Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 11:21 AM EDT

Deposition ID : D_1000251197

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

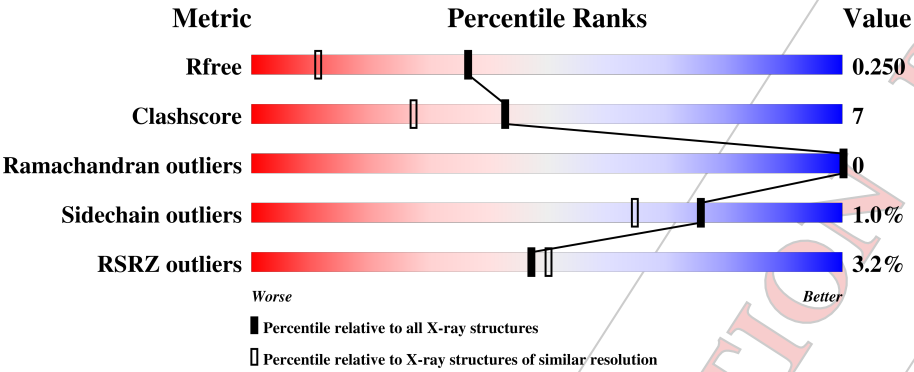
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	3% 78% 13% • 7%
1	B	257	2% 76% 10% 14%
1	C	257	3% 81% 12% 7%
1	D	257	4% 72% 8% • 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LIG	E	11	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7693 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	1	0
			1869	1195	320	337	17			
1	B	221	Total	C	N	O	S	0	0	0
			1733	1112	297	310	14			
1	C	240	Total	C	N	O	S	0	1	0
			1890	1208	321	344	17			
1	D	210	Total	C	N	O	S	0	0	0
			1662	1070	284	294	14			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	E	1	Total	C	Cl	F	N	O	S	0	0
			37	26	1	3	1	5	1		
2	E	1	Total	C	N	O	S			0	0
			25	18	1	5	1				
2	E	1	Total	C	Cl	N	O	S		0	0
			33	25	1	1	5	1			
2	E	1	Total	C	Cl	N	O	S		0	0
			33	25	1	1	5	1			

- Molecule 3 is water.

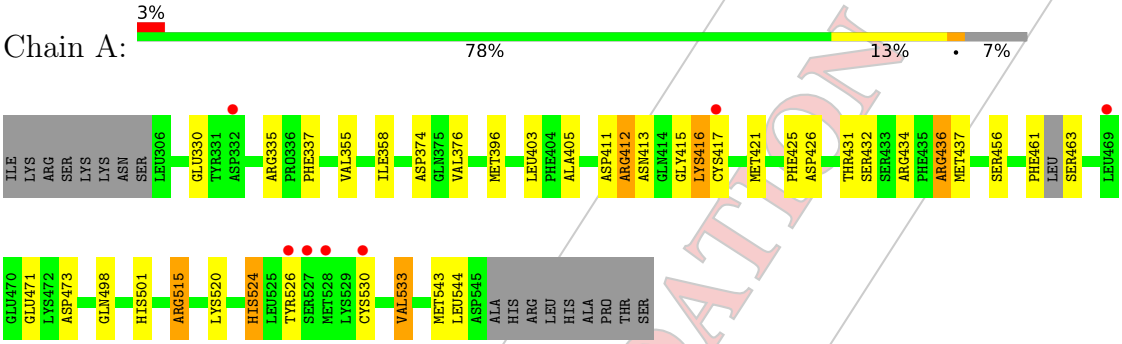
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	411	Total	O	0	0
			411	411		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

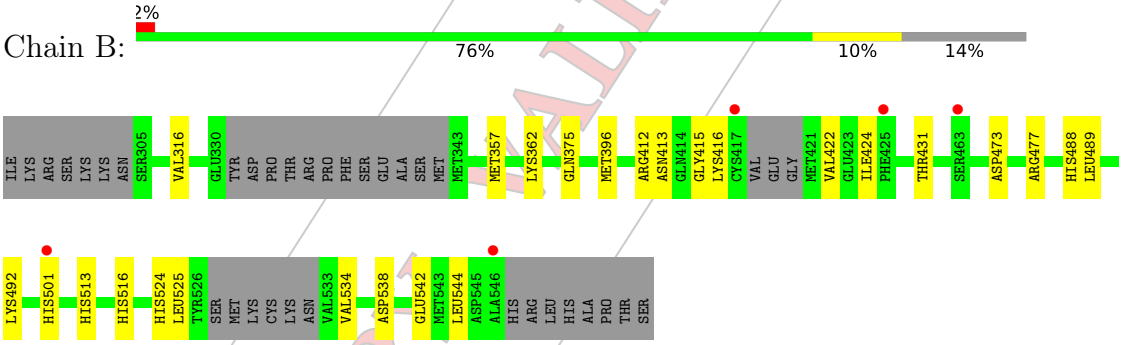
• Molecule 1: Estrogen Receptor

Chain A:



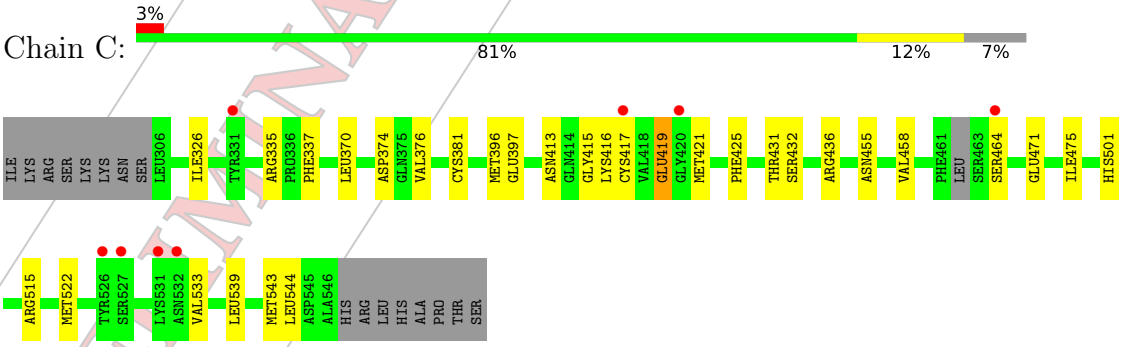
• Molecule 1: Estrogen Receptor

Chain B:



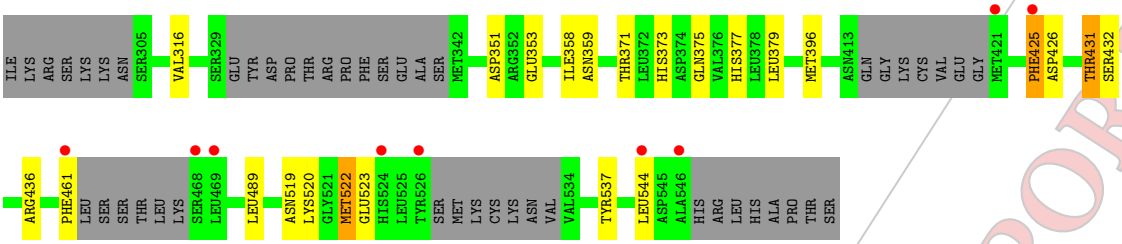
• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.49Å 58.77Å 93.21Å 86.61° 75.17° 62.96°	Depositor
Resolution (Å)	89.90 – 1.68 89.90 – 1.68	Depositor EDS
% Data completeness (in resolution range)	59.8 (89.90-1.68) 59.8 (89.90-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.199 , 0.244 0.211 , 0.250	Depositor DCC
R_{free} test set	3267 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.085 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7693	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.04	5/1896 (0.3%)	0.93	8/2568 (0.3%)
1	B	1.04	2/1750 (0.1%)	0.89	2/2363 (0.1%)
1	C	0.95	2/1917 (0.1%)	0.93	3/2594 (0.1%)
1	D	1.16	3/1679 (0.2%)	0.94	3/2267 (0.1%)
All	All	1.05	12/7242 (0.2%)	0.92	16/9792 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	431	THR	C-N	-22.69	0.81	1.34
1	B	431	THR	C-N	-19.98	0.88	1.34
1	D	522	MET	C-N	-19.33	0.89	1.34
1	A	412	ARG	C-N	-15.16	0.99	1.34
1	C	419	GLU	C-N	-13.85	1.08	1.33
1	A	411	ASP	C-N	-12.26	1.05	1.34
1	A	415	GLY	C-N	-11.12	1.08	1.34
1	A	431	THR	C-N	-9.47	1.12	1.34
1	B	357	MET	C-N	-8.44	1.14	1.34
1	D	425	PHE	C-N	6.57	1.49	1.34
1	C	431	THR	C-N	-6.30	1.19	1.34
1	A	432	SER	C-N	-5.61	1.21	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	411	ASP	O-C-N	8.58	136.43	122.70
1	A	432	SER	O-C-N	-7.79	110.24	122.70
1	B	396	MET	CG-SD-CE	-7.69	87.90	100.20
1	D	522	MET	O-C-N	-6.33	112.56	122.70
1	A	432	SER	CA-C-N	5.82	130.01	117.20
1	A	436	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	525	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	411	ASP	CA-C-N	-5.41	105.30	117.20
1	C	522	MET	CG-SD-CE	-5.34	91.66	100.20
1	C	432	SER	O-C-N	-5.29	114.23	122.70
1	A	416	LYS	CA-C-N	-5.25	105.66	117.20
1	D	426	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	515	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	359	ASN	CB-CA-C	5.12	120.64	110.40
1	A	515	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	416	LYS	O-C-N	5.06	130.80	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	419	GLU	Mainchain
1	C	501[A]	HIS	Mainchain
1	C	501[B]	HIS	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1869	0	1854	40	0
1	B	1733	0	1761	17	0
1	C	1890	0	1892	20	0
1	D	1662	0	1680	22	0
2	E	128	0	4	16	0
3	S	411	0	0	6	0
All	All	7693	0	7191	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:THR:CA	1:D:432:SER:N	2.03	1.20
1:C:421:MET:CB	2:E:11:LIG:C24	2.19	1.19
1:D:431:THR:C	1:D:432:SER:CA	2.12	1.18
1:D:431:THR:O	1:D:432:SER:N	1.81	1.11
1:D:425:PHE:HD2	2:E:4:LIG:CL01	1.72	1.09
1:D:425:PHE:CD2	2:E:4:LIG:CL01	2.49	1.03
1:A:413:ASN:HD22	1:A:416:LYS:HE2	1.37	0.89
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.56	0.88
1:A:355:VAL:HG22	1:A:543:MET:HE1	1.54	0.87
1:B:416:LYS:HG3	1:B:422:VAL:HG21	1.56	0.86
1:D:431:THR:C	1:D:432:SER:N	0.81	0.86
1:C:421:MET:CB	2:E:11:LIG:C23	2.56	0.83
1:A:355:VAL:HA	1:A:543:MET:CE	2.10	0.82
1:B:416:LYS:HG3	1:B:422:VAL:CG2	2.09	0.81
1:A:355:VAL:HG22	1:A:543:MET:CE	2.11	0.81
1:A:413:ASN:HD22	1:A:416:LYS:CE	1.93	0.80
1:D:522:MET:O	1:D:523:GLU:C	2.15	0.78
1:A:355:VAL:HA	1:A:543:MET:HE1	1.68	0.76
1:A:456:SER:HA	1:A:515:ARG:HH22	1.49	0.76
1:D:351:ASP:OD2	3:S:263:HOH:O	2.05	0.75
1:A:533:VAL:HG13	2:E:9:LIG:O01	1.86	0.75
1:A:355:VAL:CA	1:A:543:MET:HE1	2.22	0.69
1:A:413:ASN:ND2	1:A:416:LYS:HE2	2.06	0.68
1:A:355:VAL:CG2	1:A:543:MET:HE1	2.22	0.68
1:C:421:MET:CB	2:E:11:LIG:C25	2.75	0.65
1:A:355:VAL:HA	1:A:543:MET:HE2	1.78	0.63
1:A:456:SER:HA	1:A:515:ARG:NH2	2.15	0.62
1:C:415:GLY:HA2	2:E:11:LIG:CL01	2.37	0.61
1:B:416:LYS:CG	1:B:422:VAL:HG21	2.31	0.61
1:A:456:SER:CB	1:A:515:ARG:NH2	2.63	0.61
1:A:515:ARG:HH11	1:B:516:HIS:HB2	1.67	0.60
1:C:413:ASN:O	1:C:416:LYS:HG3	2.02	0.59
1:A:413:ASN:ND2	1:A:416:LYS:CE	2.65	0.59
1:C:533:VAL:CG1	2:E:11:LIG:O01	2.51	0.59
1:B:424:ILE:HG21	2:E:10:LIG:O04	2.03	0.58
1:B:362:LYS:NZ	1:B:544:LEU:O	2.29	0.58
1:C:464:SER:CB	3:S:329:HOH:O	2.51	0.57
1:C:533:VAL:HG13	2:E:11:LIG:O01	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ASP:O	1:B:542:GLU:HG3	2.05	0.56
1:D:353:GLU:OE1	2:E:4:LIG:O02	2.24	0.55
1:D:375:GLN:HB3	1:D:544:LEU:HD21	1.89	0.55
1:C:396:MET:O	1:C:436:ARG:HD3	2.08	0.53
1:D:396:MET:O	1:D:436:ARG:HD3	2.07	0.53
1:D:373:HIS:CD2	1:D:537:TYR:OH	2.62	0.52
1:D:377:HIS:CD2	1:D:461:PHE:CE1	2.97	0.52
1:A:335:ARG:HD3	1:A:337:PHE:CZ	2.47	0.50
1:C:425:PHE:CE1	2:E:11:LIG:CL01	3.02	0.50
1:A:520:LYS:O	1:A:524:HIS:ND1	2.45	0.49
1:B:524:HIS:NE2	2:E:10:LIG:C20	2.76	0.49
1:D:373:HIS:HD2	1:D:537:TYR:OH	1.95	0.49
1:C:539:LEU:HG	1:C:543:MET:CE	2.42	0.49
1:A:403:LEU:CD1	1:A:405:ALA:O	2.61	0.48
1:A:533:VAL:CG1	2:E:9:LIG:O01	2.59	0.48
1:A:396:MET:O	1:A:436:ARG:HD3	2.14	0.47
1:D:431:THR:N	1:D:432:SER:N	2.59	0.47
1:C:335:ARG:HD3	1:C:337:PHE:CZ	2.50	0.47
1:A:530:CYS:O	1:A:533:VAL:HB	2.14	0.46
1:A:421:MET:HB3	1:A:421:MET:HE3	1.83	0.46
1:A:403:LEU:HD12	1:A:405:ALA:O	2.15	0.46
1:A:456:SER:HB3	1:A:515:ARG:NH2	2.30	0.46
1:A:355:VAL:HG22	1:A:543:MET:HE3	1.95	0.45
1:A:456:SER:CB	1:A:515:ARG:HH21	2.30	0.45
1:C:376:VAL:HG22	1:C:544:LEU:HD12	1.98	0.45
1:D:358:ILE:CD1	1:D:379:LEU:HD13	2.46	0.45
1:A:498:GLN:HA	1:A:501[B]:HIS:CE1	2.51	0.45
1:C:533:VAL:HG11	2:E:11:LIG:O01	2.15	0.45
1:D:371:THR:HG21	3:S:458:HOH:O	2.16	0.45
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.99	0.45
1:D:431:THR:O	1:D:432:SER:CA	2.49	0.45
1:B:375:GLN:HB3	1:B:544:LEU:HD21	1.98	0.45
1:A:412:ARG:NE	1:A:426:ASP:OD1	2.47	0.44
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.98	0.44
1:B:524:HIS:CD2	2:E:10:LIG:C20	3.01	0.44
1:B:513:HIS:ND1	3:S:366:HOH:O	2.36	0.44
1:B:413:ASN:HA	1:B:416:LYS:HD3	2.00	0.44
1:A:355:VAL:CB	1:A:543:MET:HE1	2.48	0.44
1:D:316:VAL:HG21	1:D:489:LEU:HD21	2.00	0.43
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.36	0.43
1:B:473:ASP:OD2	1:B:477:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:YCM:HD3	3:S:149:HOH:O	2.18	0.43
1:A:358:ILE:HG23	1:A:544:LEU:HD23	2.00	0.43
1:A:434:ARG:HD2	1:A:437:MET:HE2	1.99	0.43
1:A:355:VAL:HG13	1:A:543:MET:CE	2.49	0.42
1:A:461:PHE:O	1:A:463:SER:CB	2.67	0.42
1:C:397:GLU:OE1	1:C:397:GLU:HA	2.19	0.42
1:A:330:GLU:HG3	3:S:40:HOH:O	2.19	0.42
1:B:375:GLN:CB	1:B:544:LEU:HD21	2.50	0.42
1:B:412:ARG:O	1:B:415:GLY:N	2.52	0.41
1:A:524:HIS:HD1	1:A:524:HIS:N	2.18	0.41
1:B:488:HIS:CE1	1:B:492:LYS:HD2	2.56	0.41
1:D:520:LYS:HE3	1:D:523:GLU:OE2	2.21	0.41
1:A:524:HIS:C	1:A:526:TYR:N	2.72	0.41
1:A:421:MET:HE3	1:A:425:PHE:CE1	2.56	0.41
1:C:455:ASN:O	1:C:458:VAL:HG12	2.21	0.40
1:D:358:ILE:HD13	1:D:379:LEU:HD13	2.03	0.40
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.38	0.40
1:C:370:LEU:CD1	1:C:475:ILE:HD11	2.40	0.40
1:D:519:ASN:HA	1:D:519:ASN:HD22	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/257 (91%)	229 (97%)	6 (3%)	0	100	100
1	B	212/257 (82%)	211 (100%)	1 (0%)	0	100	100
1	C	236/257 (92%)	233 (99%)	3 (1%)	0	100	100
1	D	199/257 (77%)	198 (100%)	1 (0%)	0	100	100
All	All	882/1028 (86%)	871 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/232 (87%)	197 (98%)	4 (2%)	55	36
1	B	189/232 (82%)	187 (99%)	2 (1%)	73	61
1	C	206/232 (89%)	204 (99%)	2 (1%)	76	65
1	D	180/232 (78%)	180 (100%)	0	100	100
All	All	776/928 (84%)	768 (99%)	8 (1%)	76	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	CYS
1	A	473	ASP
1	A	524	HIS
1	A	533	VAL
1	B	501	HIS
1	B	534	VAL
1	C	326	ILE
1	C	417	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	HIS
1	A	413	ASN
1	A	500	GLN
1	A	519	ASN
1	B	398	HIS
1	B	474	HIS
1	B	488	HIS
1	B	519	ASN
1	C	359	ASN

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Mol	Chain	Res	Type
1	C	498	GLN
1	C	502	GLN
1	C	519	ASN
1	D	373	HIS
1	D	519	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

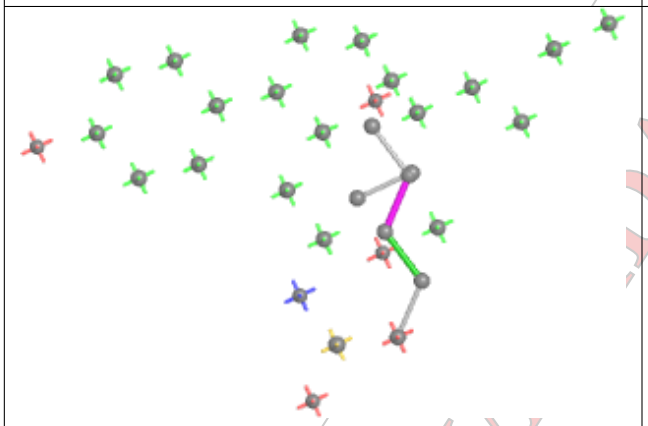
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

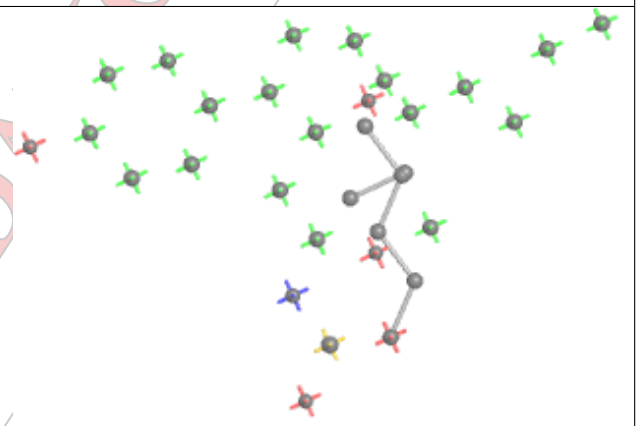
Ligand LIG E 11

Bond lengths

Bond angles

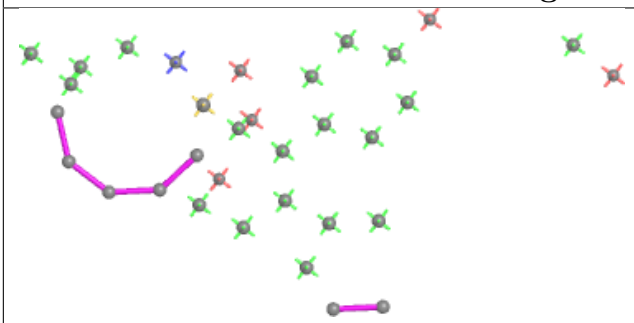


Torsions

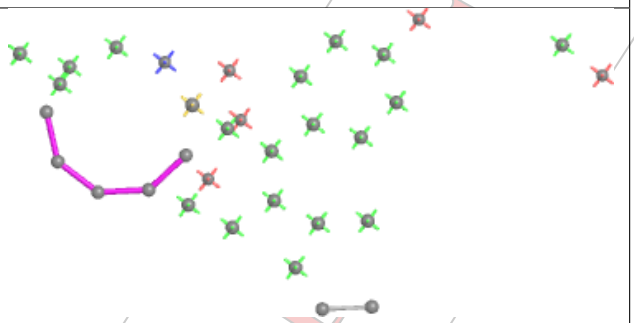


Rings

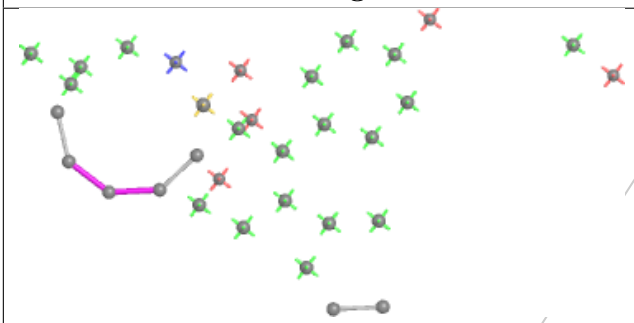
Ligand LIG E 10



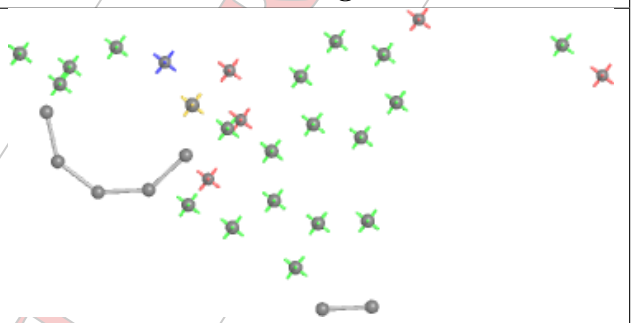
Bond lengths



Bond angles

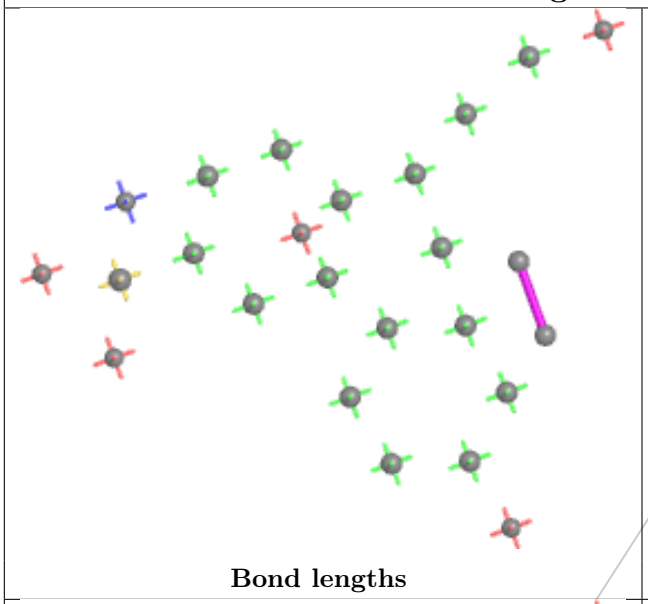


Torsions

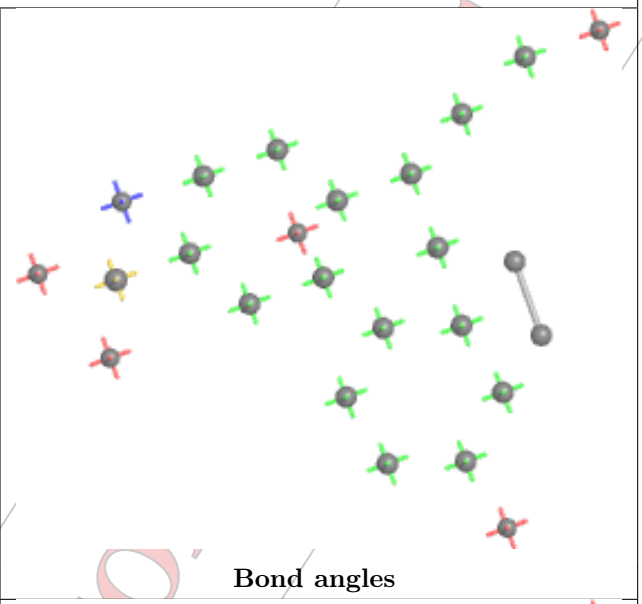


Rings

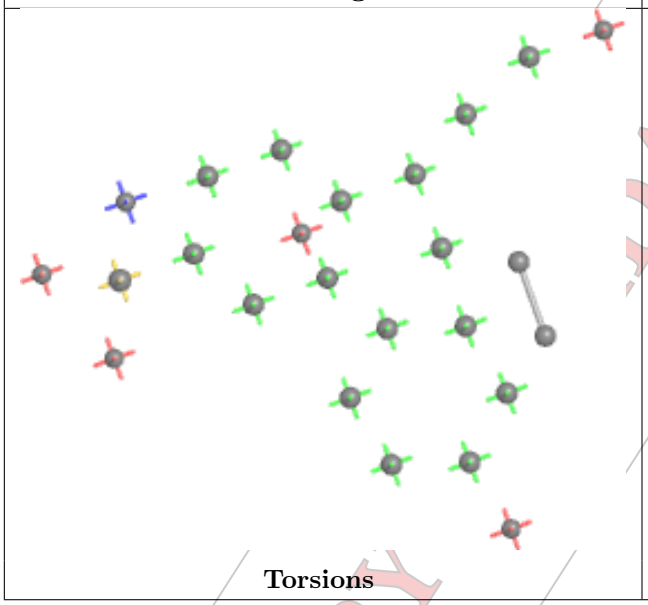
Ligand LIG E 9



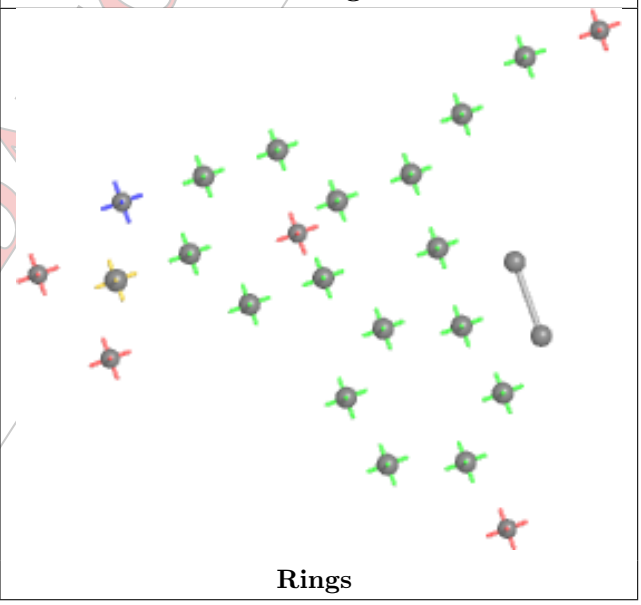
Bond lengths



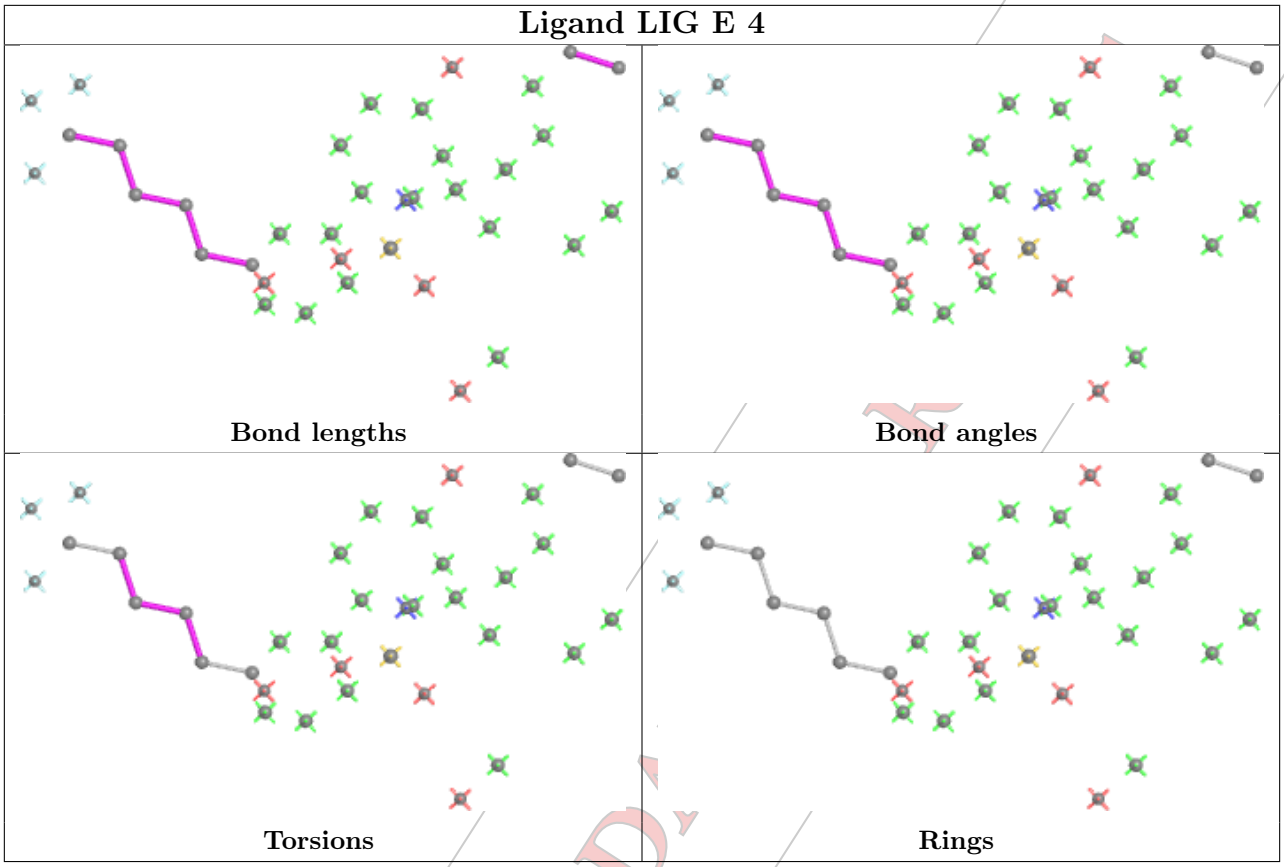
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	B	2
1	D	2
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	431:THR	C	432:SER	N	1.19
1	B	357:MET	C	358:ILE	N	1.14
1	A	431:THR	C	432:SER	N	1.12
1	A	415:GLY	C	416:LYS	N	1.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	419:GLU	C	420:GLY	N	1.08
1	A	411:ASP	C	412:ARG	N	1.05
1	A	412:ARG	C	413:ASN	N	0.99
1	D	522:MET	C	523:GLU	N	0.89
1	B	431:THR	C	432:SER	N	0.88
1	D	431:THR	C	432:SER	N	0.81

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	238/257 (92%)	0.24	7 (2%)	51	54	16, 32, 63, 79	0
1	B	220/257 (85%)	0.16	5 (2%)	60	64	15, 29, 59, 97	0
1	C	239/257 (92%)	0.18	8 (3%)	46	49	15, 29, 59, 83	0
1	D	209/257 (81%)	0.18	9 (4%)	35	37	16, 29, 60, 77	0
All	All	906/1028 (88%)	0.19	29 (3%)	47	50	15, 30, 61, 97	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	546	ALA	4.6
1	A	530	CYS	4.4
1	A	417	CYS	3.8
1	D	468	SER	3.6
1	D	469	LEU	3.6
1	A	526	TYR	3.6
1	A	469	LEU	3.5
1	B	417	CYS	3.1
1	D	425	PHE	3.0
1	C	417	CYS	3.0
1	B	425	PHE	3.0
1	D	421	MET	2.9
1	C	464	SER	2.7
1	C	527	SER	2.7
1	C	331	TYR	2.5
1	C	420	GLY	2.5
1	A	527	SER	2.5
1	C	531	LYS	2.4
1	D	544	LEU	2.4
1	C	526	TYR	2.3
1	A	528	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	546	ALA	2.2
1	D	526	TYR	2.2
1	D	524	HIS	2.2
1	A	332	ASP	2.2
1	B	501	HIS	2.1
1	B	463	SER	2.1
1	D	461	PHE	2.1
1	C	532	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

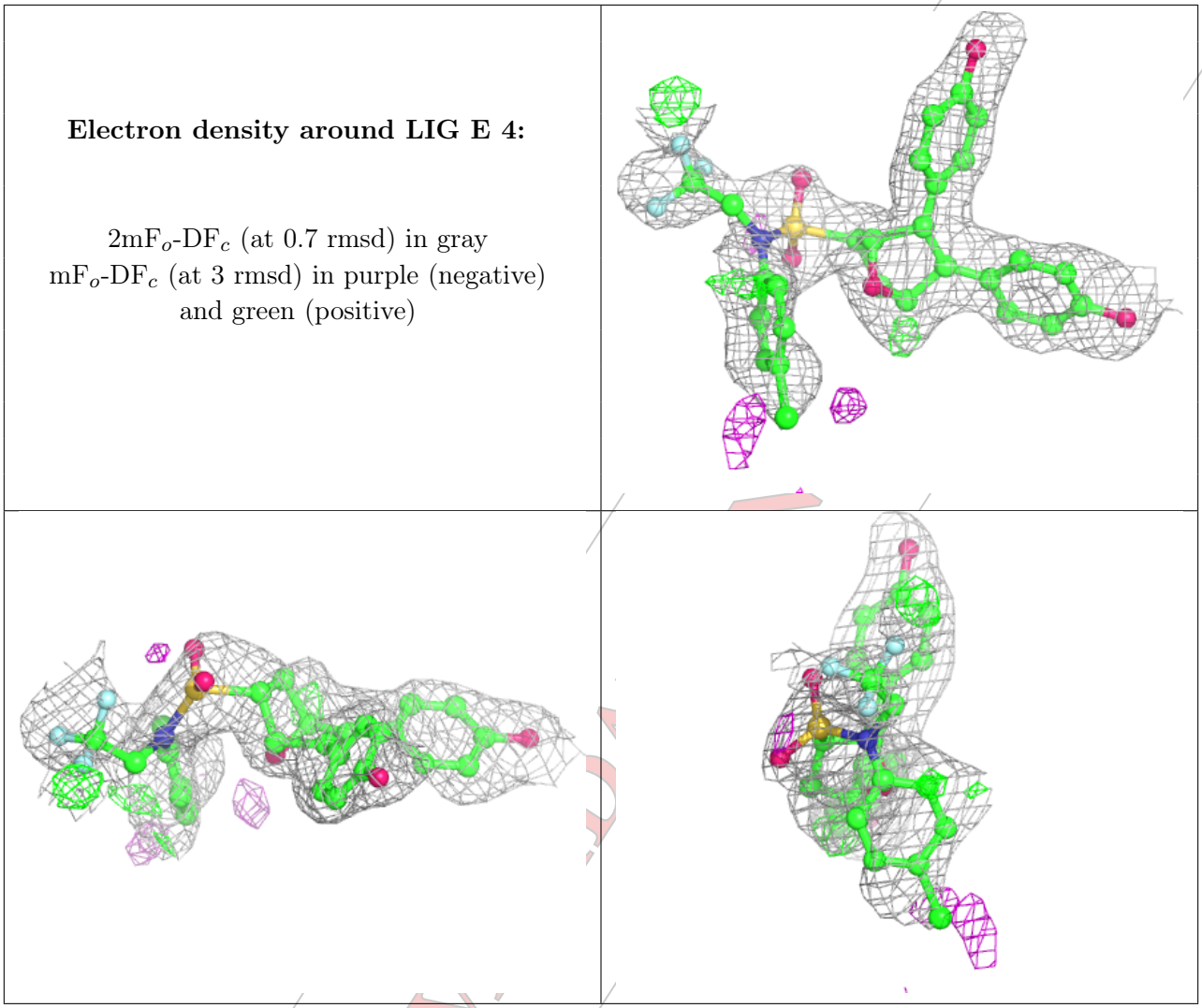
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	E	4	37/?	0.78	0.19	36,60,105,107	0
2	LIG	E	10	33/?	0.82	0.20	33,60,139,170	0
2	LIG	E	9	25/?	0.85	0.17	28,41,61,94	0
2	LIG	E	11	33/?	0.87	0.19	28,47,103,106	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

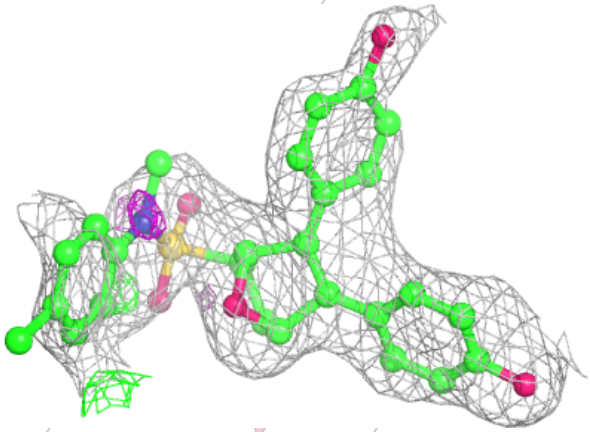
Electron density around LIG E 4:

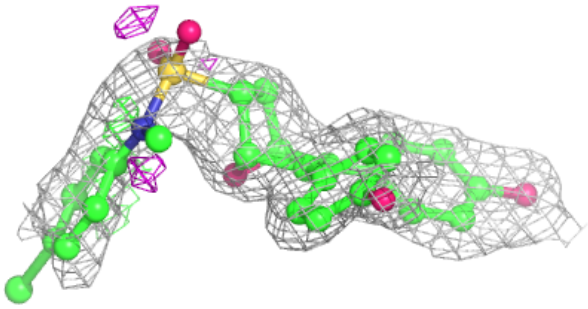
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

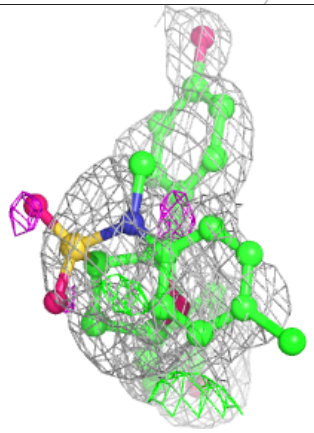


Electron density around LIG E 10:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

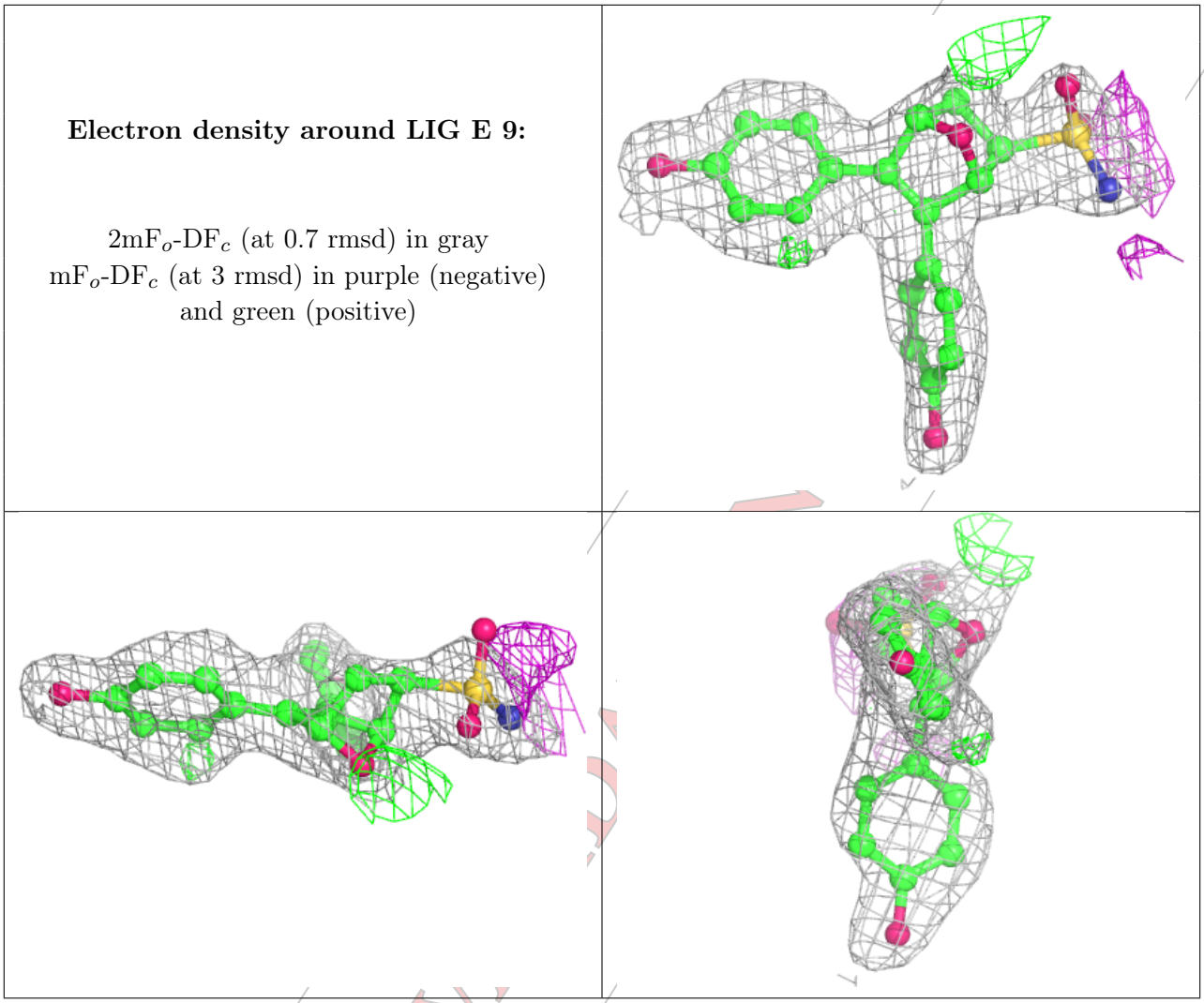






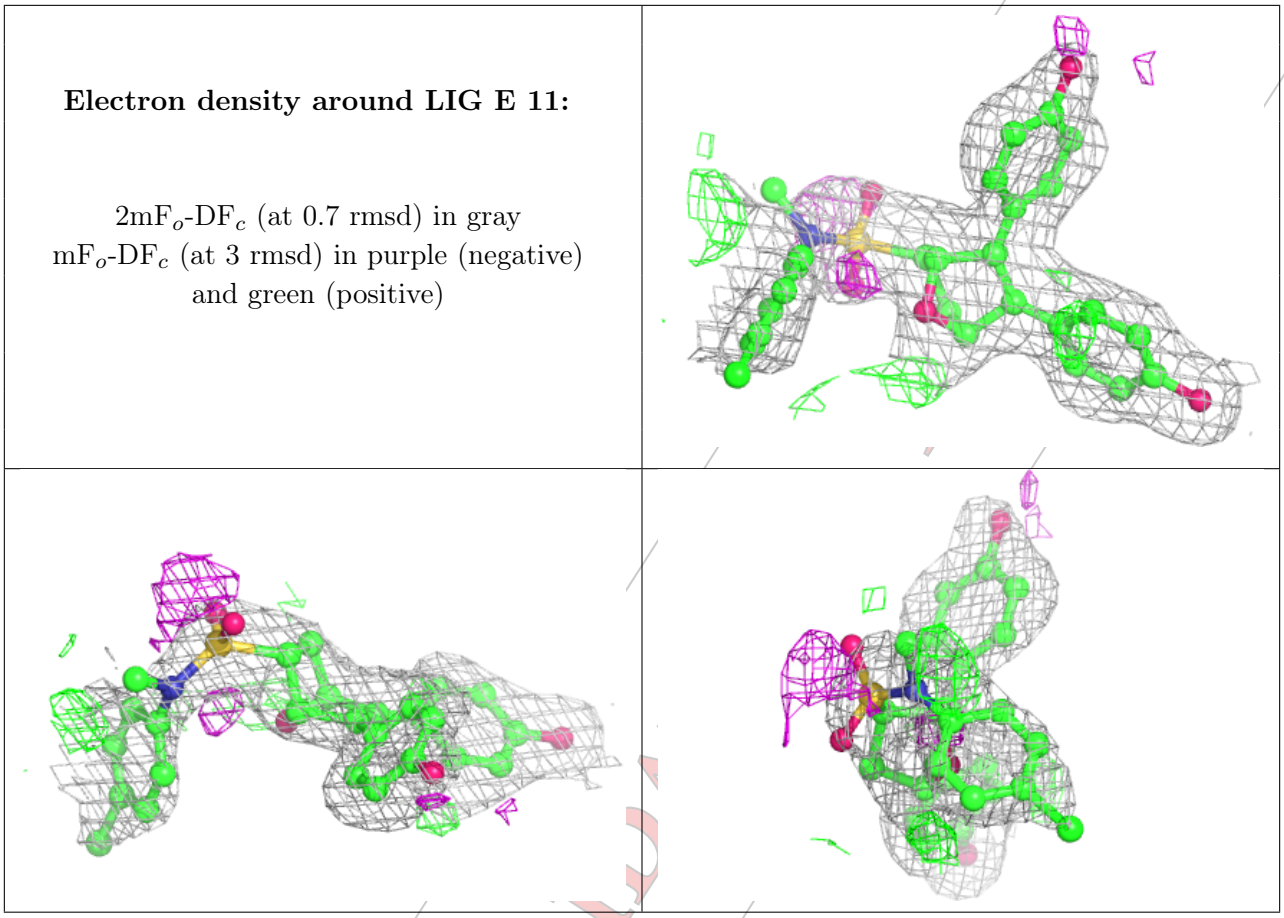
Electron density around LIG E 9:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG E 11:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 04:50 PM EDT

Deposition ID : D_1000251198

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

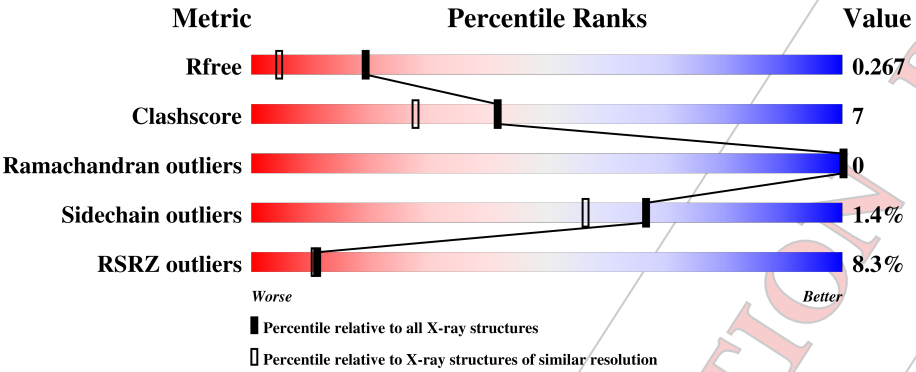
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	8% 77% 13% • 9%
1	B	257	11% 74% 12% 14%
1	C	257	6% 76% 14% 9%
1	D	257	5% 75% 9% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LIG	E	1	-	-	X	-
2	LIG	E	3	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7846 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1873	1199	316	341	17			
1	B	220	Total	C	N	O	S	0	0	0
			1767	1137	297	318	15			
1	C	234	Total	C	N	O	S	0	1	0
			1877	1198	319	341	19			
1	D	216	Total	C	N	O	S	0	0	0
			1726	1108	293	309	16			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	F	N	O	S	0	0
			45	33	3	2	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			45	33	3	2	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

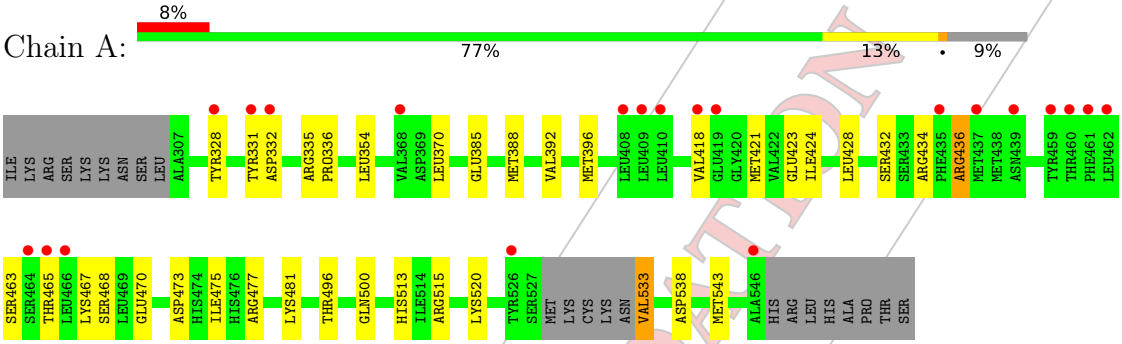
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	437	Total O 437 437	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

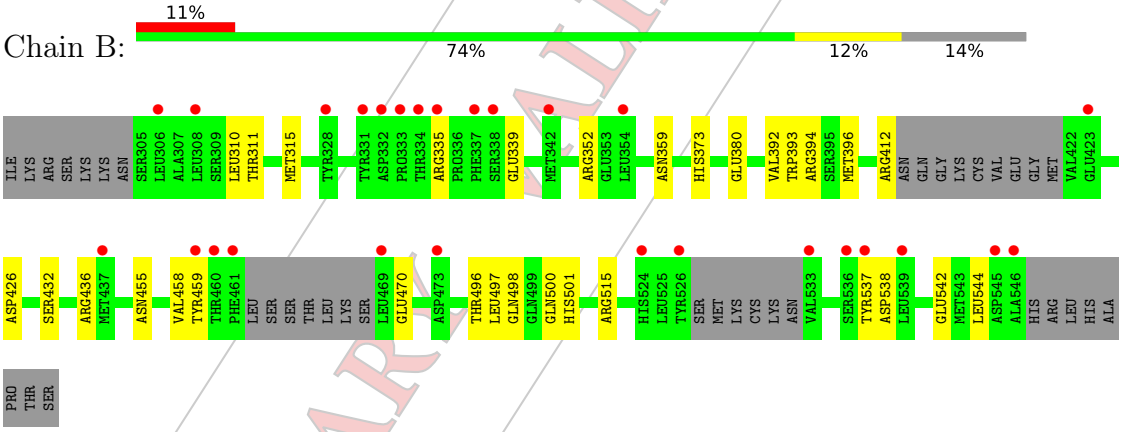
• Molecule 1: Estrogen Receptor

Chain A:



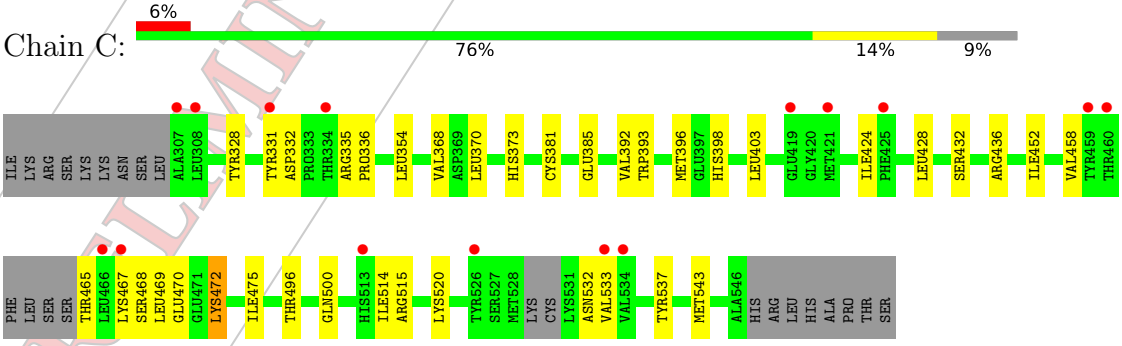
• Molecule 1: Estrogen Receptor

Chain B:



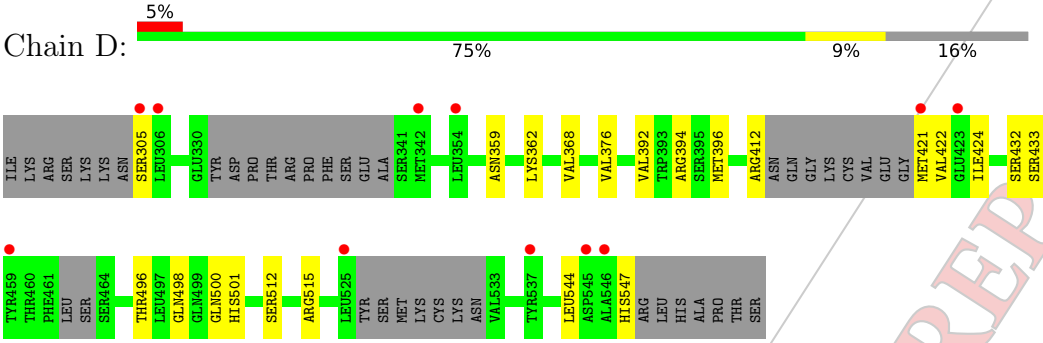
• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.78Å 58.75Å 94.44Å 86.91° 74.81° 62.77°	Depositor
Resolution (Å)	52.14 – 1.78 52.08 – 1.78	Depositor EDS
% Data completeness (in resolution range)	87.0 (52.14-1.78) 81.2 (52.08-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.265 0.243 , 0.267	Depositor DCC
R_{free} test set	3961 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.197 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7846	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.58	0/1897	0.74	4/2564 (0.2%)
1	B	0.58	0/1789	0.82	5/2418 (0.2%)
1	C	0.57	0/1889	0.73	0/2550
1	D	0.57	0/1743	0.76	4/2350 (0.2%)
All	All	0.57	0/7318	0.76	13/9882 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	394	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	515	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	D	515	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	D	515	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	515	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	394	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	515	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	515	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	352	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	538	ASP	CB-CG-OD1	-5.59	113.26	118.30
1	B	426	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	436	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	394	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1873	0	1909	40	2
1	B	1767	0	1799	25	2
1	C	1877	0	1913	33	1
1	D	1726	0	1774	12	1
2	E	164	0	4	16	0
3	F	2	0	0	0	0
4	S	437	0	0	11	0
All	All	7846	0	7399	104	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HB3	4:S:394:HOH:O	1.58	1.01
1:C:385:GLU:HG3	1:C:514:ILE:HG22	1.41	1.00
1:A:428:LEU:HD12	2:E:1:LIG:F02	1.59	0.90
1:B:311:THR:O	4:S:394:HOH:O	1.89	0.89
1:C:428:LEU:HD12	2:E:3:LIG:F02	1.68	0.83
1:C:385:GLU:HG3	1:C:514:ILE:CG2	2.09	0.83
1:A:513:HIS:CD2	1:B:459:TYR:CD2	2.69	0.81
1:B:335:ARG:HB3	1:B:339:GLU:OE1	1.86	0.76
1:A:418:VAL:HG11	1:A:421:MET:CE	2.16	0.75
1:C:458:VAL:HG22	1:C:472:LYS:HE3	1.69	0.75
1:A:424:ILE:HB	2:E:1:LIG:HC22	1.69	0.74
1:C:370:LEU:HD21	1:C:475:ILE:HD11	1.69	0.73
1:A:513:HIS:NE2	1:B:459:TYR:CD2	2.58	0.72
1:A:424:ILE:HD11	1:A:520:LYS:HB3	1.75	0.68
1:A:370:LEU:HD21	1:A:475:ILE:HD11	1.74	0.68
1:C:465:THR:HG23	1:C:468:SER:H	1.58	0.67
1:C:424:ILE:HD11	1:C:520:LYS:HB3	1.76	0.67
1:A:428:LEU:CD1	2:E:1:LIG:F02	2.32	0.67
1:B:542:GLU:OE2	4:S:401:HOH:O	2.13	0.67
1:C:424:ILE:HB	2:E:3:LIG:HC22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:GLU:HG2	1:C:452:ILE:HD13	1.76	0.66
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.77	0.65
1:A:465:THR:HG23	1:A:468:SER:H	1.61	0.65
1:C:385:GLU:CG	1:C:514:ILE:HG22	2.21	0.64
1:A:513:HIS:NE2	1:B:459:TYR:HD2	1.95	0.64
1:A:473:ASP:OD1	1:A:477:ARG:NH1	2.31	0.63
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.80	0.63
1:C:396:MET:O	1:C:436:ARG:HD3	1.99	0.62
1:D:359:ASN:OD1	1:D:547:HIS:ND1	2.33	0.61
1:A:388:MET:HE2	2:E:1:LIG:S01	2.41	0.61
1:C:428:LEU:CD1	2:E:3:LIG:F02	2.39	0.61
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.83	0.61
1:A:396:MET:O	1:A:436:ARG:HD3	2.01	0.61
1:C:467:LYS:O	1:C:470:GLU:HG2	2.01	0.60
1:A:467:LYS:O	1:A:470:GLU:HG2	2.01	0.60
1:B:396:MET:O	1:B:436:ARG:HD3	2.02	0.59
1:A:533:VAL:HG23	2:E:1:LIG:O06	2.03	0.59
1:A:388:MET:HE2	2:E:1:LIG:O05	2.04	0.58
1:A:418:VAL:HG13	1:A:421:MET:CB	2.33	0.58
1:C:370:LEU:HD21	1:C:475:ILE:CD1	2.33	0.58
1:A:418:VAL:CG1	1:A:421:MET:SD	2.92	0.58
1:C:424:ILE:HD12	2:E:3:LIG:C23	2.36	0.56
1:A:513:HIS:CD2	1:B:459:TYR:CE2	2.94	0.56
1:B:380:GLU:OE1	4:S:289:HOH:O	2.18	0.55
1:A:385:GLU:OE1	4:S:211:HOH:O	2.18	0.55
1:A:428:LEU:HD11	2:E:1:LIG:O04	2.05	0.55
1:A:424:ILE:CB	2:E:1:LIG:HC22	2.36	0.53
1:A:424:ILE:HD12	2:E:1:LIG:C23	2.38	0.53
1:C:373:HIS:HD2	1:C:537:TYR:OH	1.92	0.53
1:B:393:TRP:HE3	1:B:396:MET:HE1	1.74	0.53
1:D:368:VAL:HG22	4:S:5:HOH:O	2.08	0.53
1:B:393:TRP:CE3	1:B:396:MET:CE	2.93	0.51
1:C:424:ILE:CB	2:E:3:LIG:HC22	2.41	0.51
1:B:315:MET:N	4:S:394:HOH:O	2.42	0.51
1:C:370:LEU:CD2	1:C:475:ILE:HD11	2.39	0.50
1:C:515:ARG:HD3	1:D:512:SER:O	2.12	0.50
1:B:393:TRP:CE3	1:B:396:MET:HE1	2.47	0.49
1:A:434:ARG:NH1	4:S:242:HOH:O	2.40	0.49
1:A:331:TYR:CE2	1:A:332:ASP:HB2	2.47	0.49
1:A:467:LYS:HA	1:A:470:GLU:OE2	2.12	0.48
1:A:418:VAL:HG13	1:A:421:MET:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:SER:N	4:S:314:HOH:O	2.46	0.48
1:C:331:TYR:CE2	1:C:332:ASP:HB2	2.48	0.48
1:B:373:HIS:NE2	1:B:537:TYR:OH	2.43	0.47
1:D:392:VAL:HG13	1:D:432:SER:HA	1.97	0.47
1:A:418:VAL:HG11	1:A:421:MET:SD	2.54	0.47
1:C:381[B]:YCM:NZ2	1:C:381[B]:YCM:HA	2.30	0.47
1:C:496:THR:O	1:C:500:GLN:HG3	2.15	0.46
1:B:310:LEU:CB	4:S:394:HOH:O	2.38	0.46
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.51	0.46
1:C:424:ILE:HD11	1:C:520:LYS:CB	2.45	0.46
1:A:370:LEU:HD21	1:A:475:ILE:CD1	2.42	0.46
1:B:392:VAL:HG13	1:B:432:SER:HA	1.98	0.45
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.51	0.45
1:D:421:MET:SD	1:D:424:ILE:HG13	2.56	0.45
1:A:496:THR:O	1:A:500:GLN:HG3	2.16	0.45
1:A:513:HIS:HE1	1:B:455:ASN:O	1.99	0.45
1:B:496:THR:O	1:B:500:GLN:HG3	2.16	0.45
1:A:423:GLU:N	1:A:423:GLU:OE1	2.49	0.45
2:E:1:LIG:C12	2:E:1:LIG:C07	2.94	0.44
1:C:398:HIS:CE1	1:C:403:LEU:HD12	2.51	0.44
1:C:370:LEU:CD1	1:C:475:ILE:HD11	2.46	0.44
1:C:354:LEU:HD23	1:C:543:MET:HE1	1.99	0.44
2:E:3:LIG:C13	2:E:3:LIG:C07	2.95	0.44
1:A:513:HIS:CE1	1:B:459:TYR:HD2	2.37	0.43
1:A:513:HIS:NE2	1:B:459:TYR:CE2	2.86	0.43
1:D:496:THR:O	1:D:500:GLN:HG3	2.19	0.42
1:B:458:VAL:HG13	1:B:459:TYR:CD2	2.55	0.42
1:D:396:MET:O	1:D:436:ARG:NE	2.48	0.42
1:D:362:LYS:HG3	1:D:547:HIS:CD2	2.55	0.41
1:A:392:VAL:HG13	1:A:432:SER:HA	2.01	0.41
1:A:335:ARG:HA	1:A:336:PRO:C	2.39	0.41
1:C:335:ARG:HA	1:C:336:PRO:C	2.40	0.41
1:C:465:THR:CG2	1:C:468:SER:HB3	2.51	0.41
1:C:458:VAL:CG2	1:C:472:LYS:HE3	2.46	0.41
1:B:393:TRP:CE3	1:B:396:MET:HE3	2.56	0.41
1:C:393:TRP:CE3	1:C:396:MET:SD	3.14	0.41
1:A:354:LEU:HD23	1:A:543:MET:HE1	2.02	0.41
1:C:368:VAL:HG22	4:S:405:HOH:O	2.21	0.41
1:D:362:LYS:HE2	1:D:544:LEU:HD22	2.04	0.41
1:A:463:SER:HA	1:A:468:SER:OG	2.21	0.40
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:LEU:HA	1:B:497:LEU:HD23	1.92	0.40
1:C:392:VAL:HG13	1:C:432:SER:HA	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LYS:NZ	1:B:538:ASP:OD2[1_655]	1.76	0.44
1:A:328:TYR:OH	1:B:359:ASN:ND2[1_565]	1.85	0.35
1:C:328:TYR:OH	1:D:359:ASN:ND2[1_645]	2.04	0.16

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/257 (90%)	226 (98%)	4 (2%)	0	100	100
1	B	211/257 (82%)	210 (100%)	1 (0%)	0	100	100
1	C	227/257 (88%)	225 (99%)	2 (1%)	0	100	100
1	D	205/257 (80%)	204 (100%)	1 (0%)	0	100	100
All	All	873/1028 (85%)	865 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/232 (90%)	209 (100%)	1 (0%)	88	86
1	B	197/232 (85%)	194 (98%)	3 (2%)	65	53
1	C	209/232 (90%)	205 (98%)	4 (2%)	57	43
1	D	194/232 (84%)	191 (98%)	3 (2%)	65	53
All	All	810/928 (87%)	799 (99%)	11 (1%)	67	56

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	VAL
1	B	412	ARG
1	B	470	GLU
1	B	544	LEU
1	C	469	LEU
1	C	472	LYS
1	C	532	ASN
1	C	533	VAL
1	D	412	ARG
1	D	422	VAL
1	D	433	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	455	ASN
1	A	519	ASN
1	B	398	HIS
1	B	476	HIS
1	B	519	ASN
1	C	373	HIS
1	C	398	HIS
1	C	498	GLN
1	C	519	ASN
1	D	373	HIS
1	D	439	ASN
1	D	488	HIS
1	D	498	GLN
1	D	519	ASN
1	D	524	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

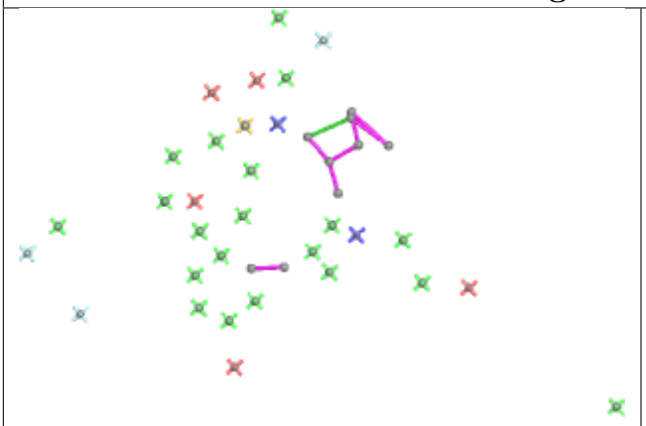
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

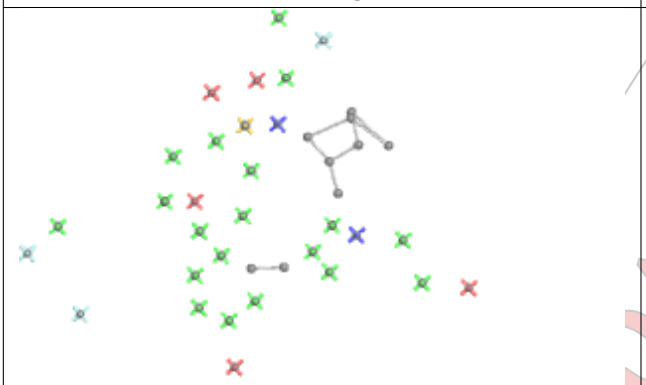
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LIG E 3

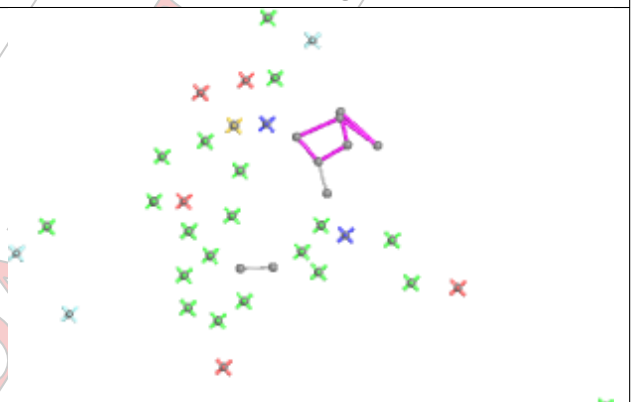


Bond lengths

Bond angles

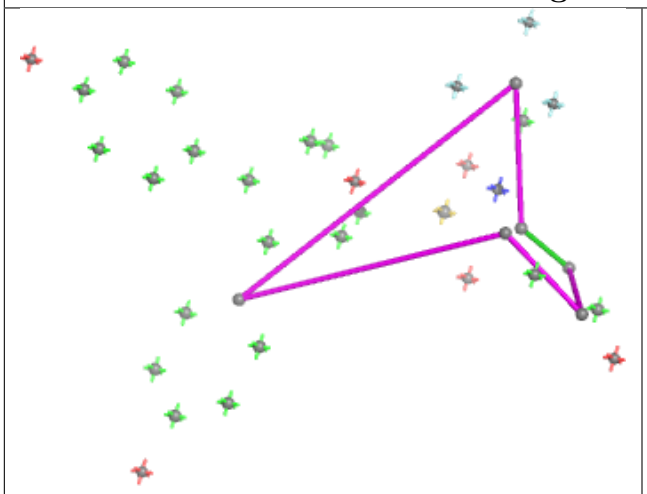


Torsions

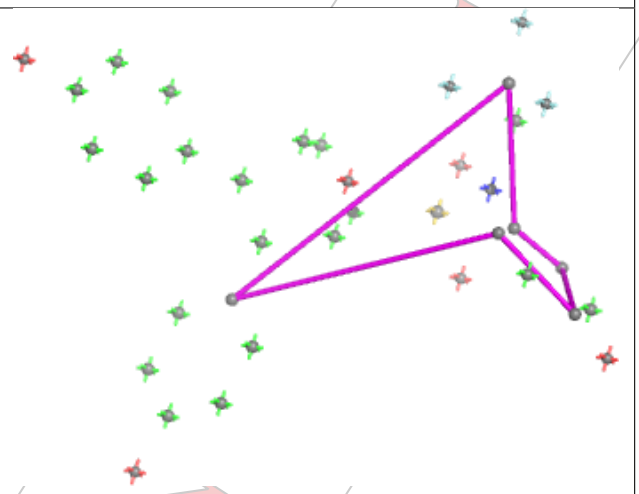


Rings

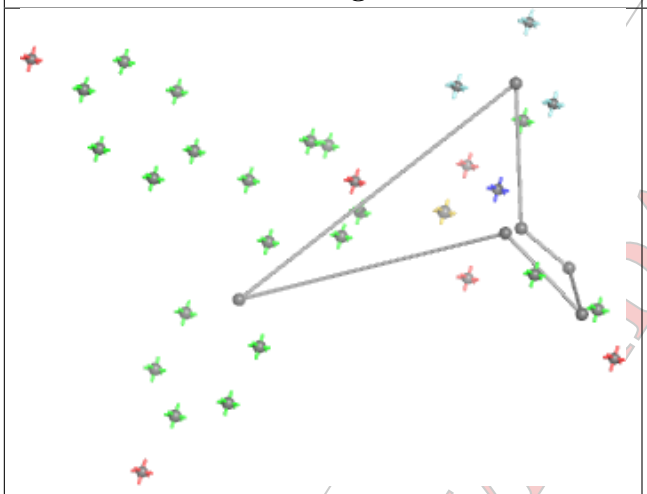
Ligand LIG E 4



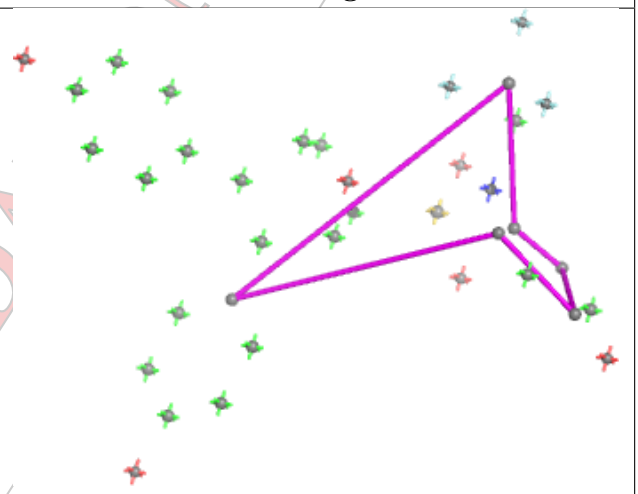
Bond lengths



Bond angles

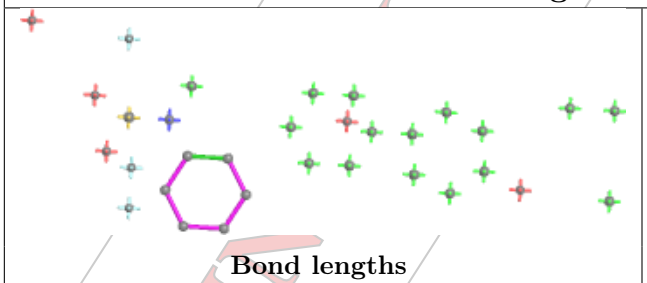


Torsions

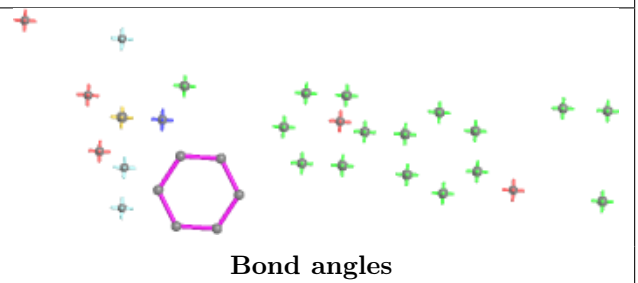


Rings

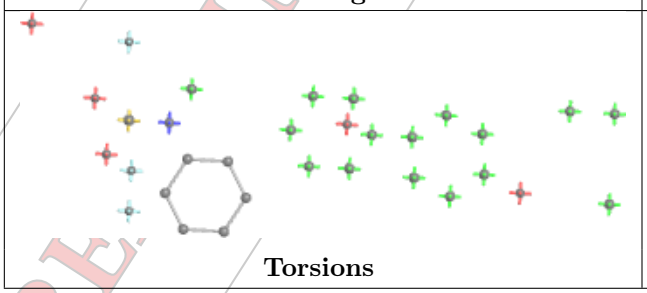
Ligand LIG E 2



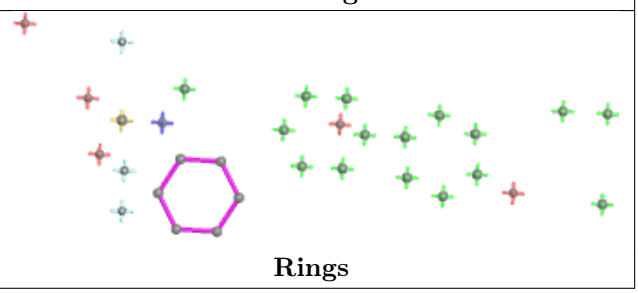
Bond lengths



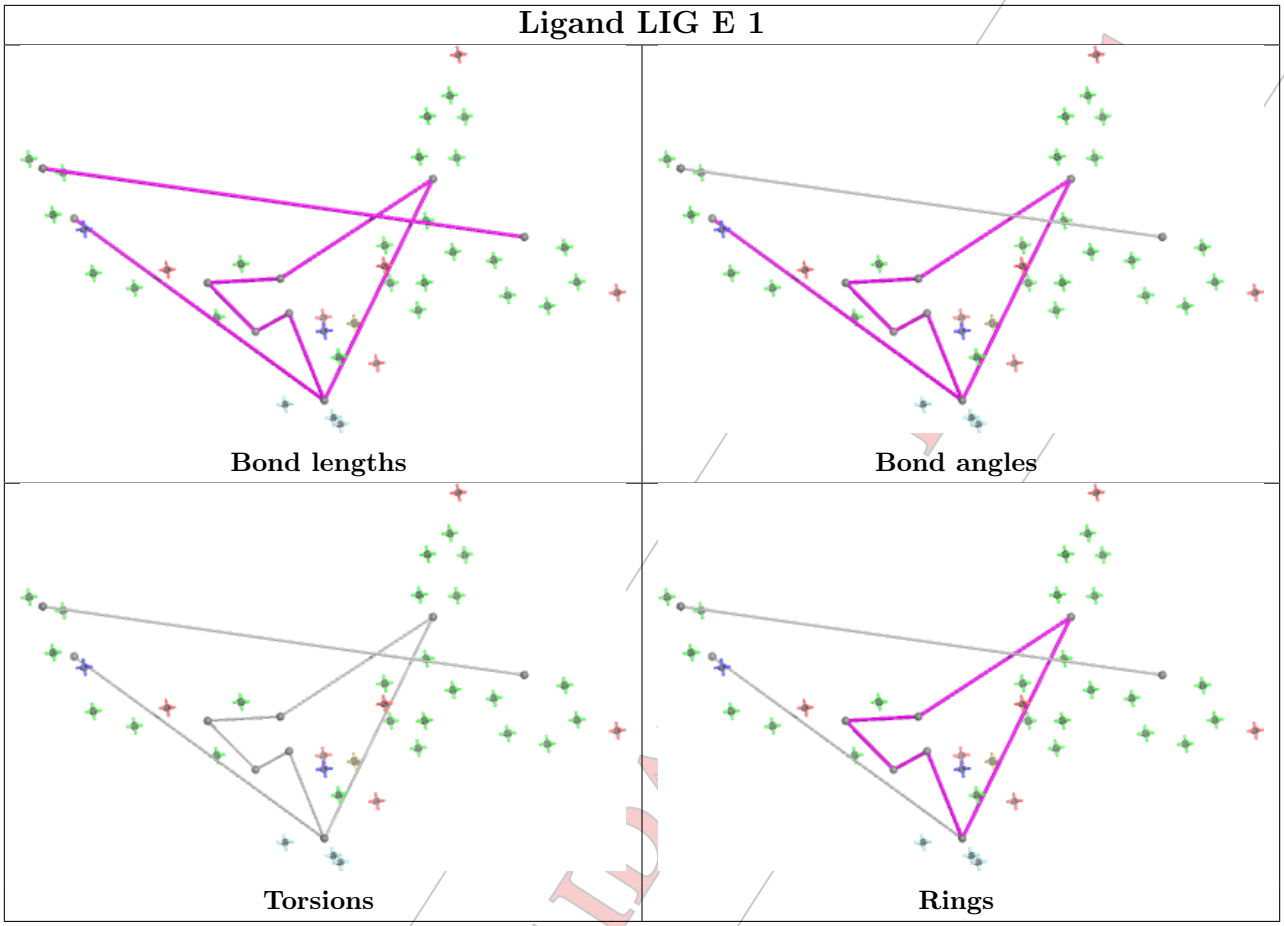
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	234/257 (91%)	0.78	21 (8%) 9 9	19, 33, 64, 83	0
1	B	219/257 (85%)	0.98	27 (12%) 4 4	19, 35, 56, 68	0
1	C	233/257 (90%)	0.72	15 (6%) 19 18	20, 35, 58, 82	0
1	D	215/257 (83%)	0.65	12 (5%) 24 23	20, 34, 53, 71	0
All	All	901/1028 (87%)	0.78	75 (8%) 11 11	19, 34, 57, 83	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	THR	6.3
1	C	466	LEU	6.2
1	B	337	PHE	6.0
1	A	462	LEU	6.0
1	B	333	PRO	6.0
1	B	331	TYR	5.8
1	B	461	PHE	5.6
1	B	459	TYR	5.3
1	A	526	TYR	5.2
1	B	524	HIS	4.8
1	A	460	THR	4.6
1	B	546	ALA	4.6
1	D	306	LEU	4.5
1	C	526	TYR	4.4
1	A	461	PHE	4.4
1	B	533	VAL	4.1
1	B	537	TYR	4.1
1	A	464	SER	3.9
1	D	342	MET	3.9
1	A	459	TYR	3.8
1	B	332	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	421	MET	3.8
1	C	331	TYR	3.5
1	A	331	TYR	3.5
1	A	418	VAL	3.4
1	B	536	SER	3.4
1	D	354	LEU	3.4
1	C	460	THR	3.2
1	C	425	PHE	3.2
1	B	342	MET	3.2
1	B	335	ARG	3.2
1	B	460	THR	3.2
1	A	332	ASP	3.1
1	C	307	ALA	3.1
1	A	408	LEU	3.1
1	B	545	ASP	3.1
1	B	338	SER	3.1
1	C	459	TYR	3.0
1	D	459	TYR	2.9
1	D	546	ALA	2.9
1	A	546	ALA	2.8
1	C	419	GLU	2.7
1	D	458	VAL	2.6
1	B	306	LEU	2.6
1	B	423	GLU	2.5
1	A	437	MET	2.5
1	C	334	THR	2.5
1	B	469	LEU	2.5
1	A	409	LEU	2.5
1	C	421	MET	2.4
1	D	545	ASP	2.4
1	A	435	PHE	2.4
1	B	437	MET	2.4
1	B	308	LEU	2.3
1	B	526	TYR	2.3
1	B	473	ASP	2.3
1	B	539	LEU	2.3
1	A	419	GLU	2.3
1	C	467	LYS	2.3
1	A	410	LEU	2.2
1	C	513	HIS	2.2
1	B	328	TYR	2.2
1	C	308	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	533	VAL	2.2
1	C	534	VAL	2.2
1	B	354	LEU	2.2
1	D	537	TYR	2.1
1	A	466	LEU	2.1
1	A	439	ASN	2.1
1	A	465	THR	2.1
1	D	423	GLU	2.1
1	D	525	LEU	2.1
1	A	328	TYR	2.1
1	D	305	SER	2.1
1	A	368	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

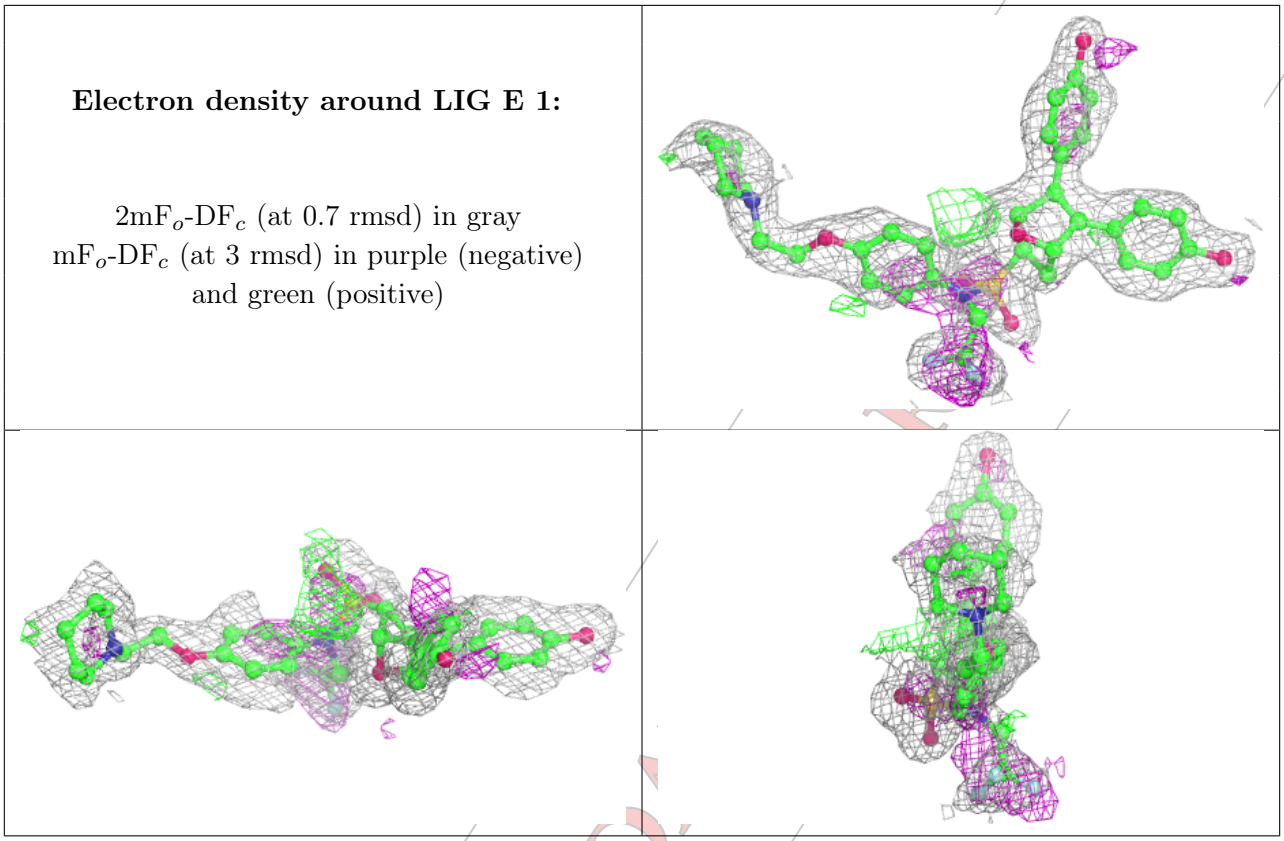
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	E	1	45/?	0.82	0.20	20,31,38,39	0
2	LIG	E	4	37/?	0.83	0.17	21,34,51,54	0
2	LIG	E	2	37/?	0.87	0.16	22,35,55,59	0
2	LIG	E	3	45/?	0.88	0.17	20,33,38,38	0
3	CL	F	1	1/?	0.96	0.05	26,26,26,26	0
3	CL	F	2	1/?	0.97	0.06	24,24,24,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

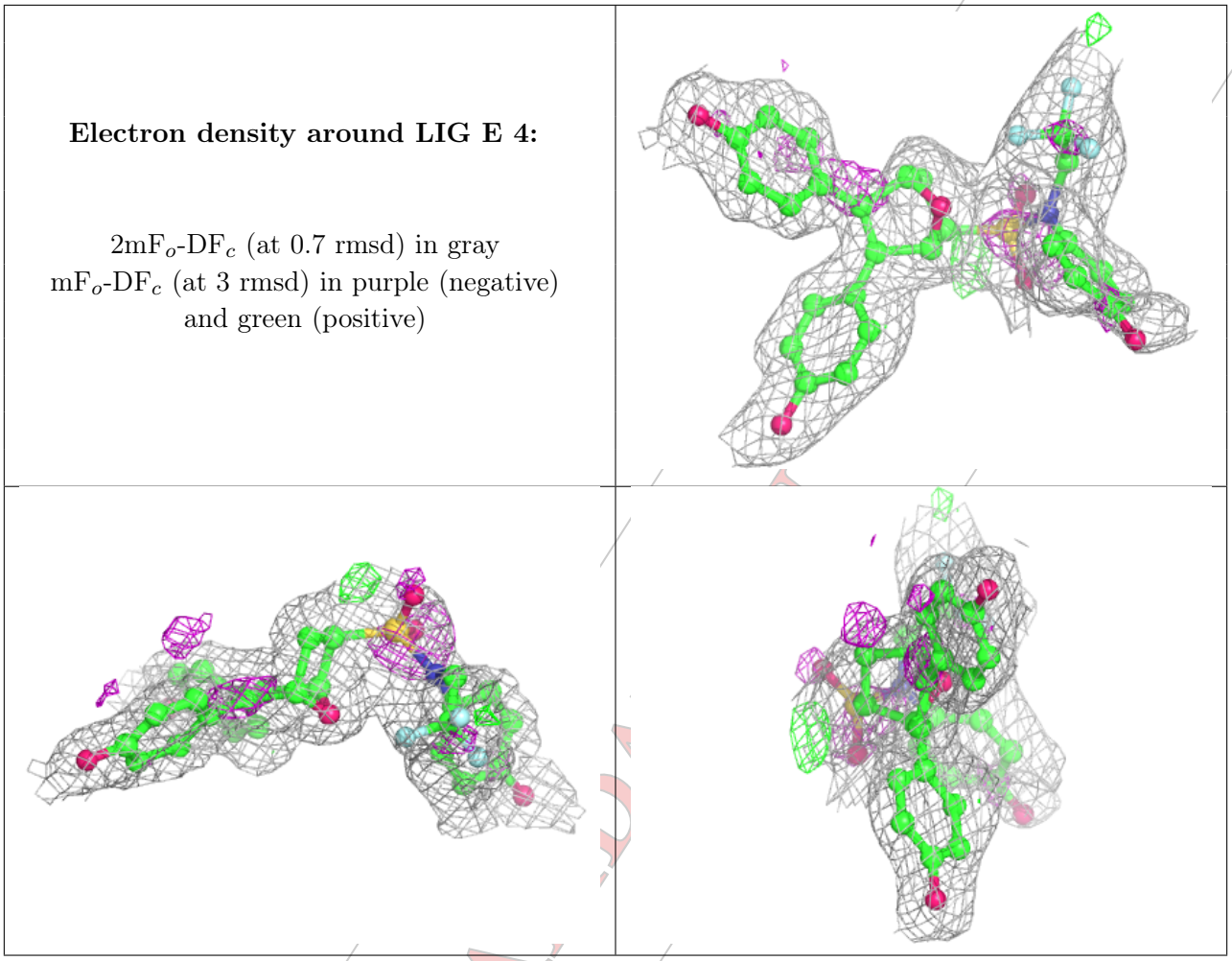
Electron density around LIG E 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



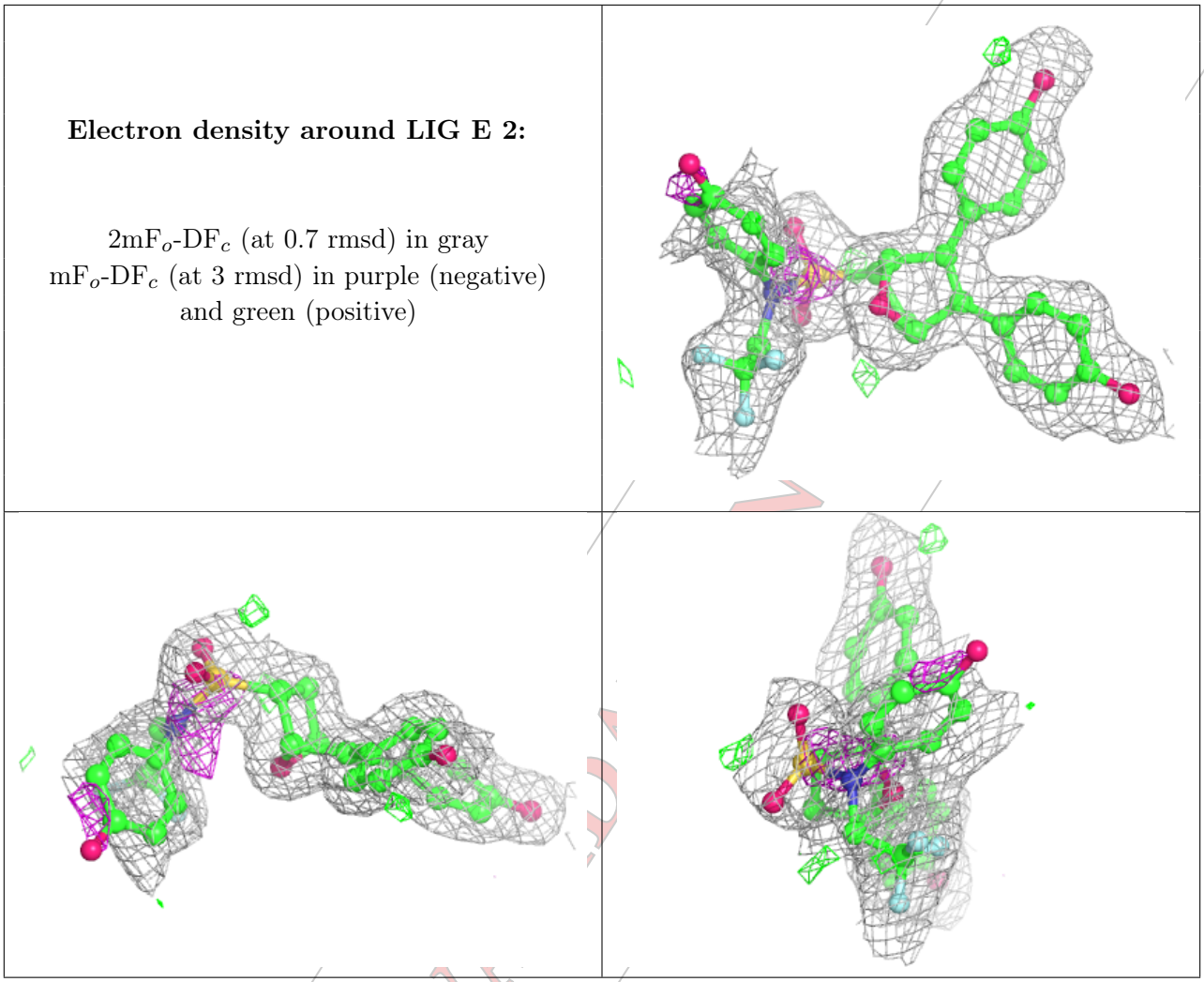
Electron density around LIG E 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



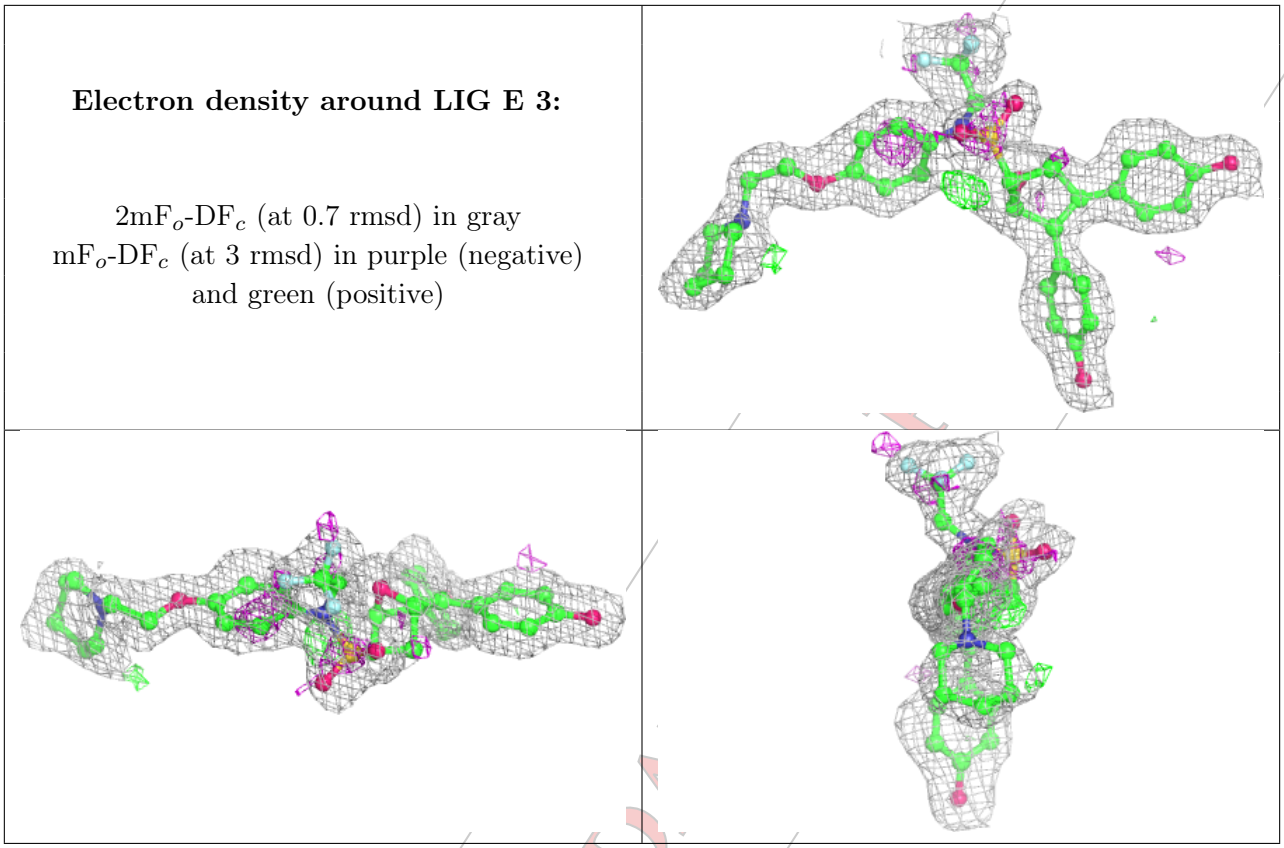
Electron density around LIG E 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG E 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 06:37 PM EDT

Deposition ID : D_1000251211

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

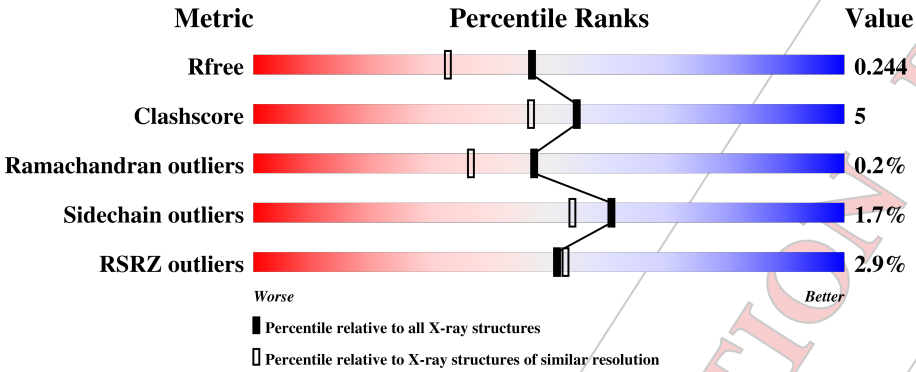
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	2% 84% 7% 9%
1	B	257	3% 79% 5% 14%
1	C	257	2% 79% 9% 12%
1	D	257	4% 73% 8% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	2	0
			1843	1176	321	329	17			
1	B	221	Total	C	N	O	S	0	2	0
			1758	1128	304	310	16			
1	C	227	Total	C	N	O	S	0	4	0
			1834	1173	321	323	17			
1	D	209	Total	C	N	O	S	0	0	0
			1639	1050	280	293	16			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

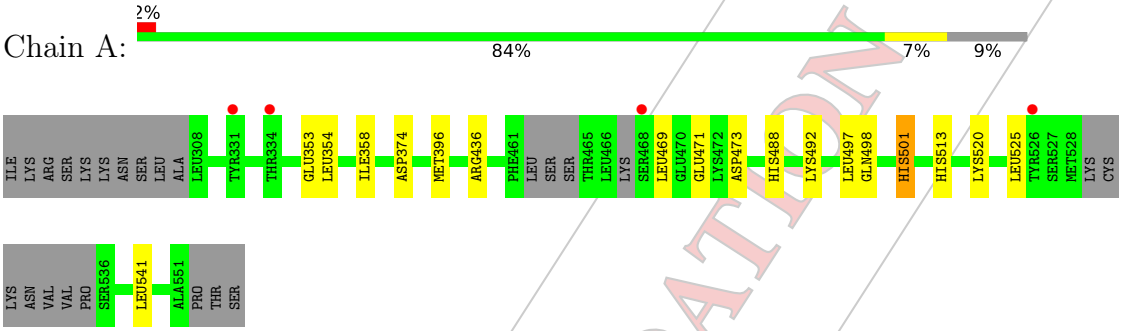
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	219	Total O 219 219	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

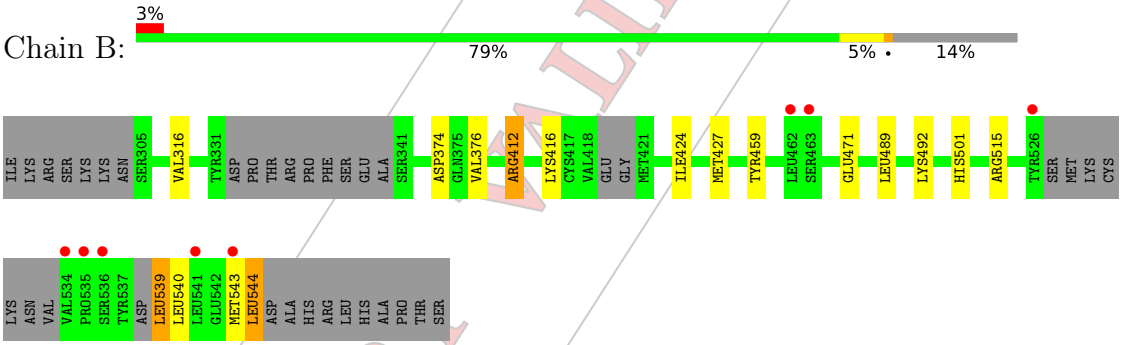
• Molecule 1: Estrogen Receptor

Chain A:



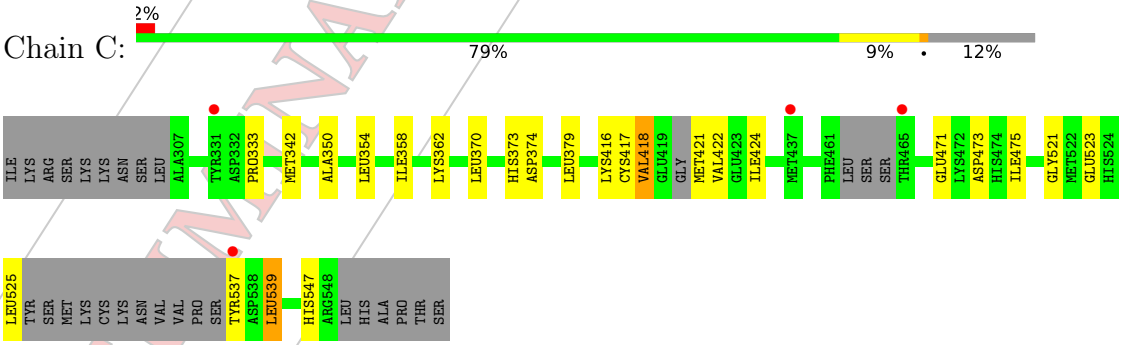
• Molecule 1: Estrogen Receptor

Chain B:



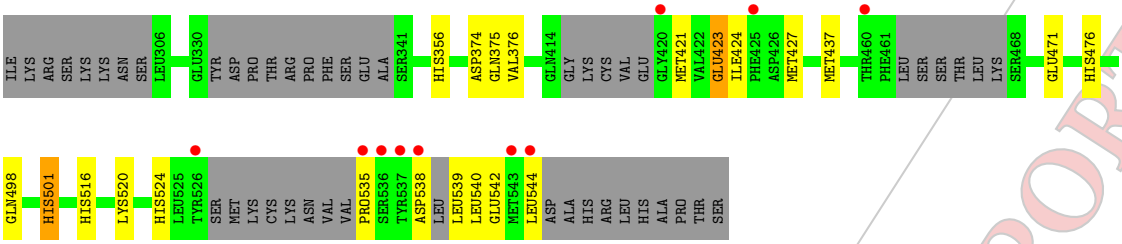
• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.42Å 59.12Å 93.52Å 86.54° 74.98° 63.19°	Depositor
Resolution (Å)	90.13 – 1.87 90.13 – 1.87	Depositor EDS
% Data completeness (in resolution range)	76.0 (90.13-1.87) 76.0 (90.13-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.207 , 0.236 0.218 , 0.244	Depositor DCC
R_{free} test set	3095 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.109 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7470	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.71	0/1854	0.75	0/2502
1	B	0.72	0/1770	0.77	0/2385
1	C	0.71	0/1846	0.76	0/2490
1	D	0.75	0/1652	0.76	0/2227
All	All	0.72	0/7122	0.76	0/9604

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1843	0	1833	19	0
1	B	1758	0	1780	17	0
1	C	1834	0	1831	29	0
1	D	1639	0	1657	18	0
2	E	175	0	8	3	0
3	F	2	0	0	0	0
4	S	219	0	0	5	0
All	All	7470	0	7109	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:LEU:HD12	1:C:539:LEU:H	1.23	1.04
1:D:374:ASP:OD2	1:D:471:GLU:OE1	1.78	1.01
1:A:501[A]:HIS:NE2	1:B:501:HIS:HE1	1.65	0.94
1:C:539:LEU:CD1	1:C:539:LEU:H	1.93	0.82
1:A:501[A]:HIS:CD2	1:B:501:HIS:CE1	2.69	0.80
1:A:488:HIS:ND1	4:S:139:HOH:O	2.15	0.80
1:A:501[A]:HIS:CD2	1:B:501:HIS:HE1	2.03	0.76
1:C:333:PRO:HD2	4:S:227:HOH:O	1.91	0.71
1:A:497:LEU:O	1:A:501[A]:HIS:CD2	2.43	0.70
1:D:421:MET:SD	2:E:4:LIG:O05	2.49	0.70
1:A:354:LEU:O	1:A:358:ILE:HD13	1.91	0.70
1:B:412:ARG:HH11	1:B:412:ARG:HG3	1.60	0.67
1:B:412:ARG:NH1	1:B:412:ARG:HG3	2.08	0.67
1:A:396:MET:O	1:A:436:ARG:HD3	1.95	0.66
1:A:501[A]:HIS:NE2	1:B:501:HIS:CE1	2.56	0.65
1:C:539:LEU:HD12	1:C:539:LEU:N	2.05	0.64
1:B:412:ARG:CG	1:B:412:ARG:HH11	2.12	0.63
1:B:376:VAL:CG2	1:B:544:LEU:HD23	2.30	0.61
1:C:418:VAL:O	1:C:421:MET:HB3	2.02	0.58
1:A:541:LEU:HD21	1:C:373:HIS:CG	2.40	0.57
1:D:376:VAL:HG13	1:D:540:LEU:HB2	1.87	0.57
1:D:356:HIS:HD2	4:S:198:HOH:O	1.88	0.56
1:D:421:MET:SD	2:E:4:LIG:C19	2.96	0.54
1:C:416:LYS:HG2	1:C:422:VAL:HG21	1.90	0.53
1:B:376:VAL:HG22	1:B:544:LEU:HD23	1.92	0.52
1:A:525:LEU:HD13	1:A:525:LEU:C	2.30	0.52
1:C:525:LEU:C	1:C:525:LEU:HD13	2.29	0.52
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.92	0.51
1:A:520:LYS:NZ	4:S:134:HOH:O	2.43	0.50
1:B:376:VAL:HG23	1:B:544:LEU:HD23	1.93	0.50
1:D:423:GLU:CD	1:D:524:HIS:HE1	2.14	0.50
1:C:537:TYR:CD1	1:C:537:TYR:C	2.85	0.50
1:D:375:GLN:HB3	1:D:544:LEU:HD11	1.94	0.50
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.30	0.50
1:A:541:LEU:CD2	1:C:373:HIS:ND1	2.76	0.49
1:C:374:ASP:OD2	1:C:471:GLU:OE2	2.31	0.49
1:A:541:LEU:HD23	1:C:373:HIS:CE1	2.49	0.48
1:B:374:ASP:OD2	1:B:471:GLU:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:LYS:C	1:C:418:VAL:H	2.17	0.47
1:C:350:ALA:O	1:C:354:LEU:HD23	2.16	0.46
1:C:539:LEU:CD1	1:C:539:LEU:N	2.71	0.46
1:D:538:ASP:O	1:D:542:GLU:CB	2.63	0.46
1:B:515[B]:ARG:HD3	1:B:515[B]:ARG:HA	1.74	0.45
1:A:501[A]:HIS:CD2	1:A:501[A]:HIS:N	2.85	0.45
1:C:358:ILE:CD1	1:C:379:LEU:HD13	2.46	0.45
1:D:427:MET:CE	1:D:516:HIS:CD2	3.00	0.45
1:B:424:ILE:HD13	1:B:427:MET:CE	2.48	0.44
1:D:356:HIS:HE1	4:S:10:HOH:O	1.99	0.44
1:C:537:TYR:CD1	1:C:537:TYR:O	2.70	0.44
1:C:537:TYR:O	1:C:537:TYR:CG	2.71	0.44
1:D:423:GLU:OE2	1:D:520:LYS:HE3	2.17	0.44
1:B:376:VAL:HG13	1:B:540:LEU:HB2	1.99	0.43
1:D:427:MET:HE3	1:D:516:HIS:CD2	2.53	0.43
1:C:416:LYS:C	1:C:418:VAL:N	2.70	0.43
1:B:539:LEU:CD1	1:B:543:MET:SD	3.07	0.43
1:D:535:PRO:HB3	1:D:539:LEU:HD23	2.01	0.43
1:D:427:MET:CE	1:D:516:HIS:HD2	2.32	0.43
1:D:423:GLU:HG3	1:D:424:ILE:N	2.34	0.43
1:B:316:VAL:HG21	1:B:489:LEU:HD21	2.01	0.42
1:C:416:LYS:HA	1:C:422:VAL:CG2	2.50	0.42
1:C:362:LYS:HG3	1:C:547:HIS:CE1	2.55	0.41
1:D:539:LEU:HD12	1:D:539:LEU:O	2.20	0.41
1:C:424:ILE:HD13	1:C:521:GLY:HA2	2.02	0.41
1:C:342:MET:HE1	1:C:417:YCM:HB3	2.02	0.41
1:A:513:HIS:HB2	1:B:459:TYR:CD2	2.55	0.41
1:C:350:ALA:O	1:C:354:LEU:CD2	2.69	0.41
1:C:475:ILE:HD13	1:C:475:ILE:HA	1.92	0.41
1:C:523:GLU:OE1	1:C:523:GLU:HA	2.20	0.41
1:D:476:HIS:CD2	1:D:476:HIS:C	2.94	0.41
1:A:353:GLU:OE1	2:E:1:LIG:O03	2.39	0.40
1:A:541:LEU:HD21	1:C:373:HIS:ND1	2.36	0.40
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.56	0.40
1:A:498:GLN:HA	1:A:501[B]:HIS:CE1	2.57	0.40
1:C:418:VAL:O	1:C:421:MET:CB	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/257 (88%)	223 (99%)	2 (1%)	0	100	100
1	B	211/257 (82%)	209 (99%)	1 (0%)	1 (0%)	29	17
1	C	221/257 (86%)	218 (99%)	2 (1%)	1 (0%)	29	17
1	D	196/257 (76%)	195 (100%)	1 (0%)	0	100	100
All	All	853/1028 (83%)	845 (99%)	6 (1%)	2 (0%)	47	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	416	LYS
1	C	418	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/232 (84%)	191 (97%)	5 (3%)	46	36
1	B	191/232 (82%)	187 (98%)	4 (2%)	53	45
1	C	195/232 (84%)	193 (99%)	2 (1%)	76	73
1	D	178/232 (77%)	175 (98%)	3 (2%)	60	54
All	All	760/928 (82%)	746 (98%)	14 (2%)	60	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	LEU
1	A	473	ASP
1	A	492	LYS
1	A	501[A]	HIS
1	A	501[B]	HIS
1	B	412	ARG
1	B	492	LYS
1	B	539	LEU
1	B	544	LEU
1	C	473	ASP
1	C	539	LEU
1	D	423	GLU
1	D	437	MET
1	D	501	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	398	HIS
1	B	439	ASN
1	B	488	HIS
1	B	501	HIS
1	C	398	HIS
1	C	519	ASN
1	C	547	HIS
1	D	356	HIS
1	D	398	HIS
1	D	476	HIS
1	D	513	HIS
1	D	516	HIS
1	D	519	ASN
1	D	524	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

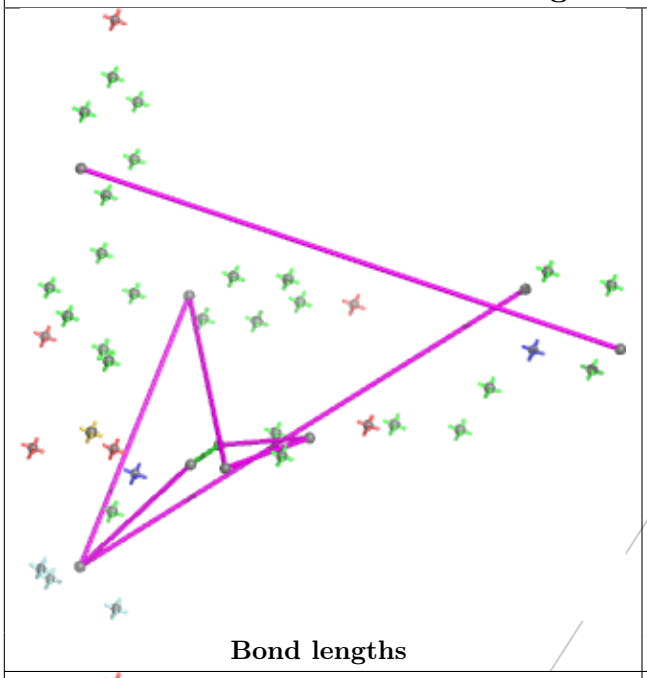
There are no torsion outliers.

There are no ring outliers.

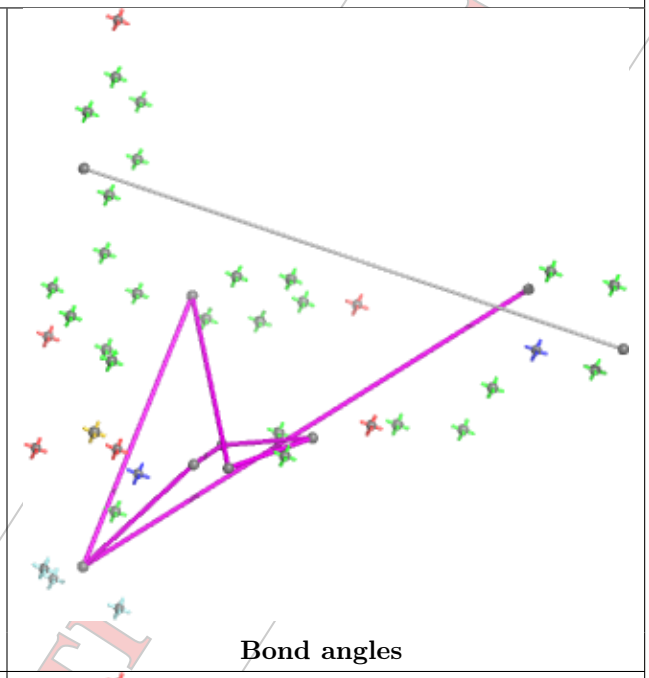
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

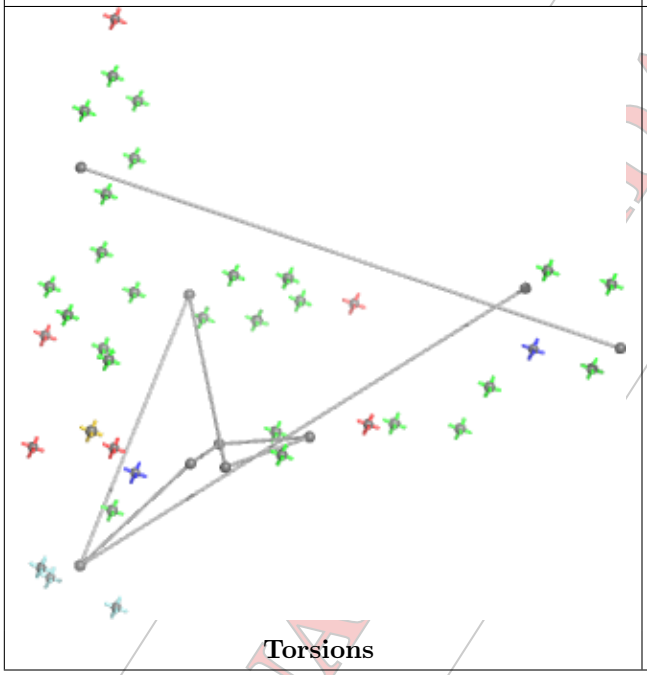
Ligand LIG E 3



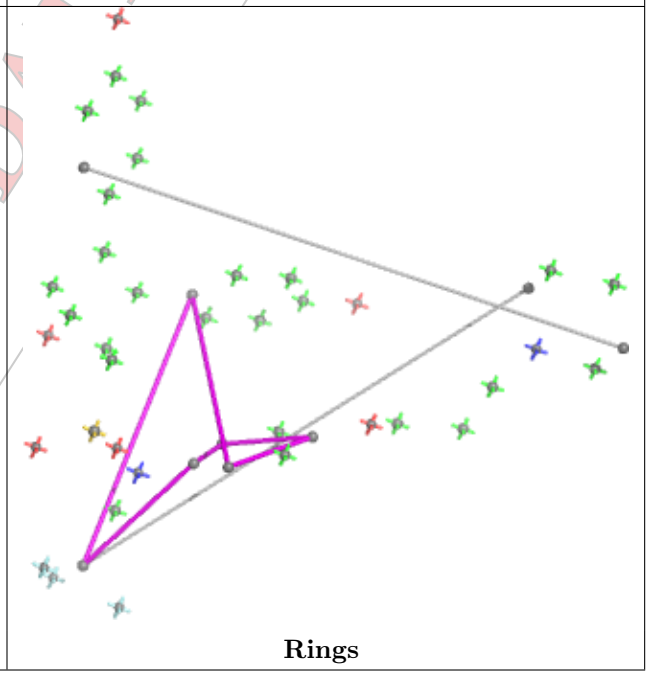
Bond lengths



Bond angles

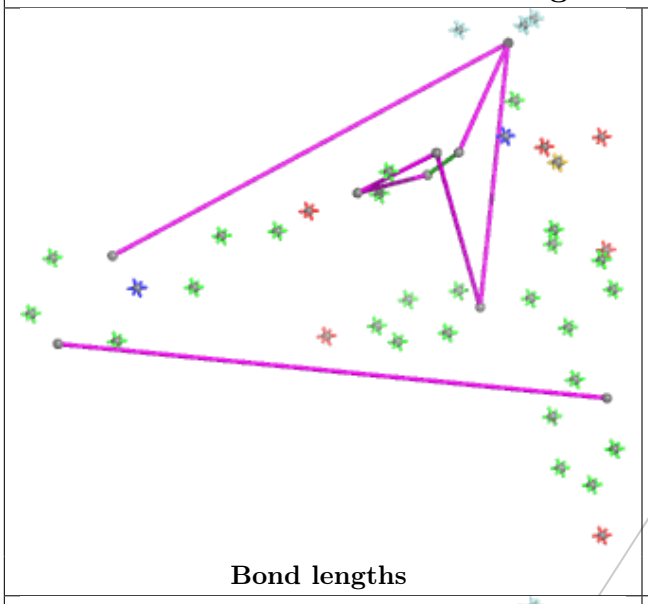


Torsions

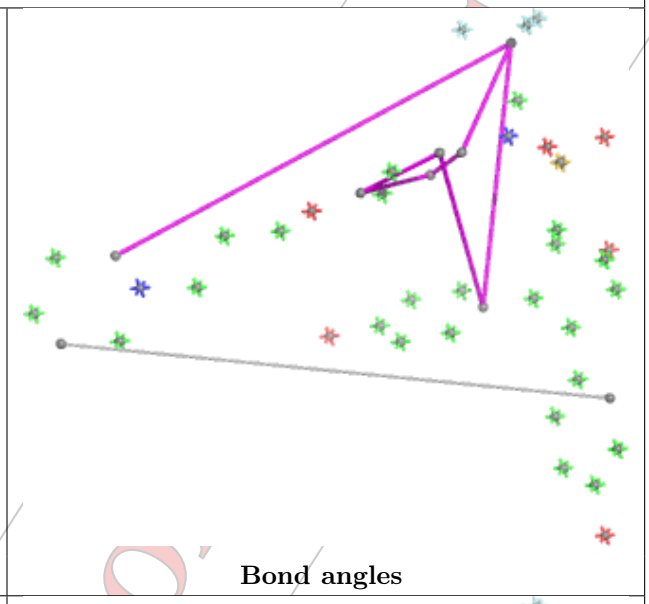


Rings

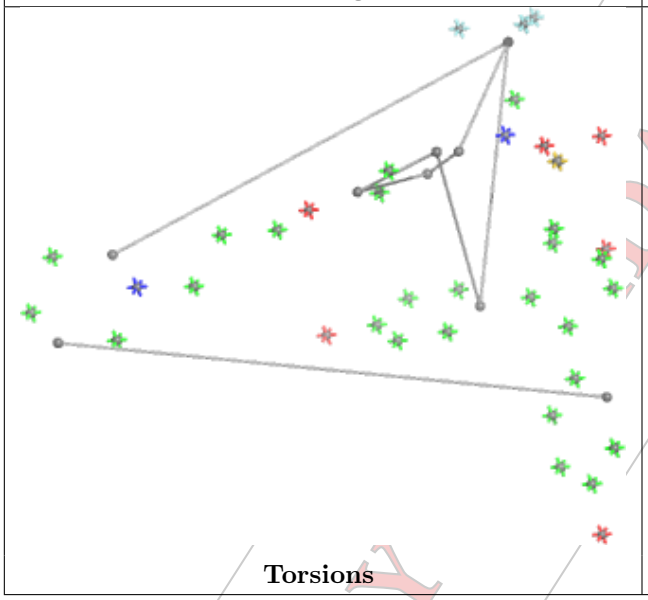
Ligand LIG E 4



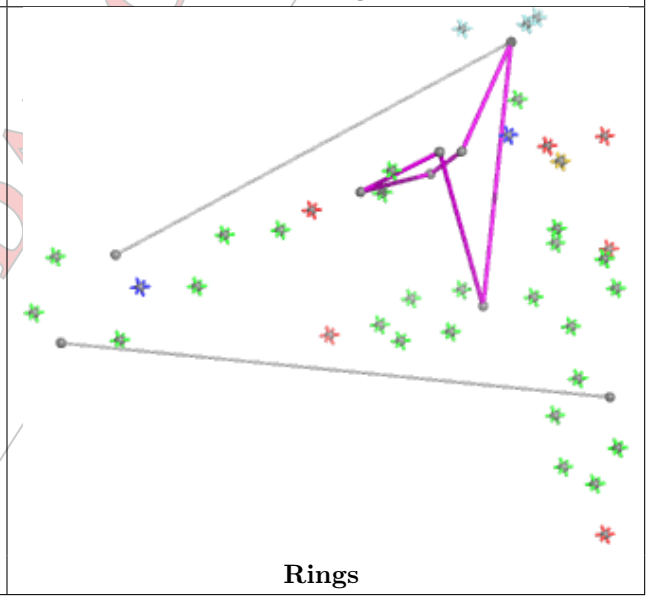
Bond lengths



Bond angles

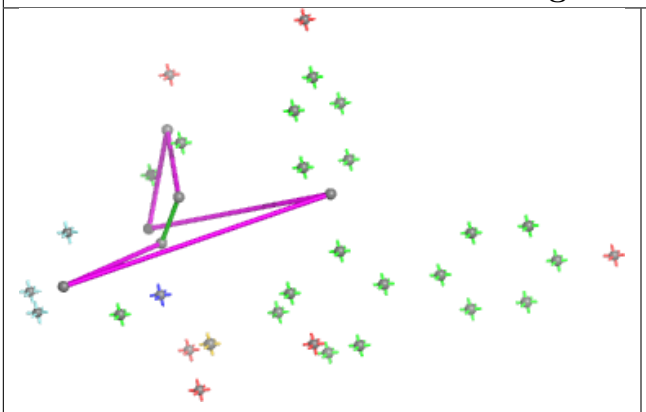


Torsions



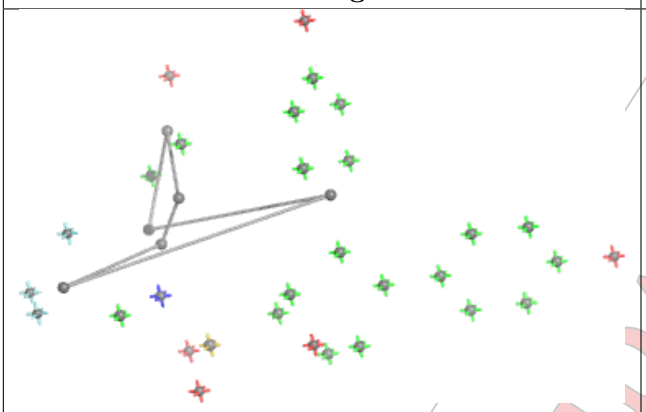
Rings

Ligand LIG E 2

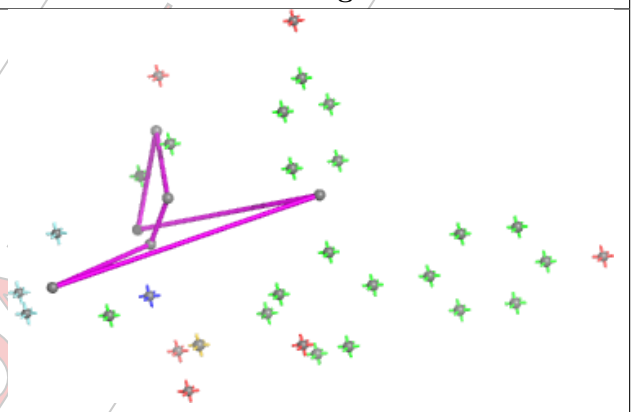


Bond lengths

Bond angles

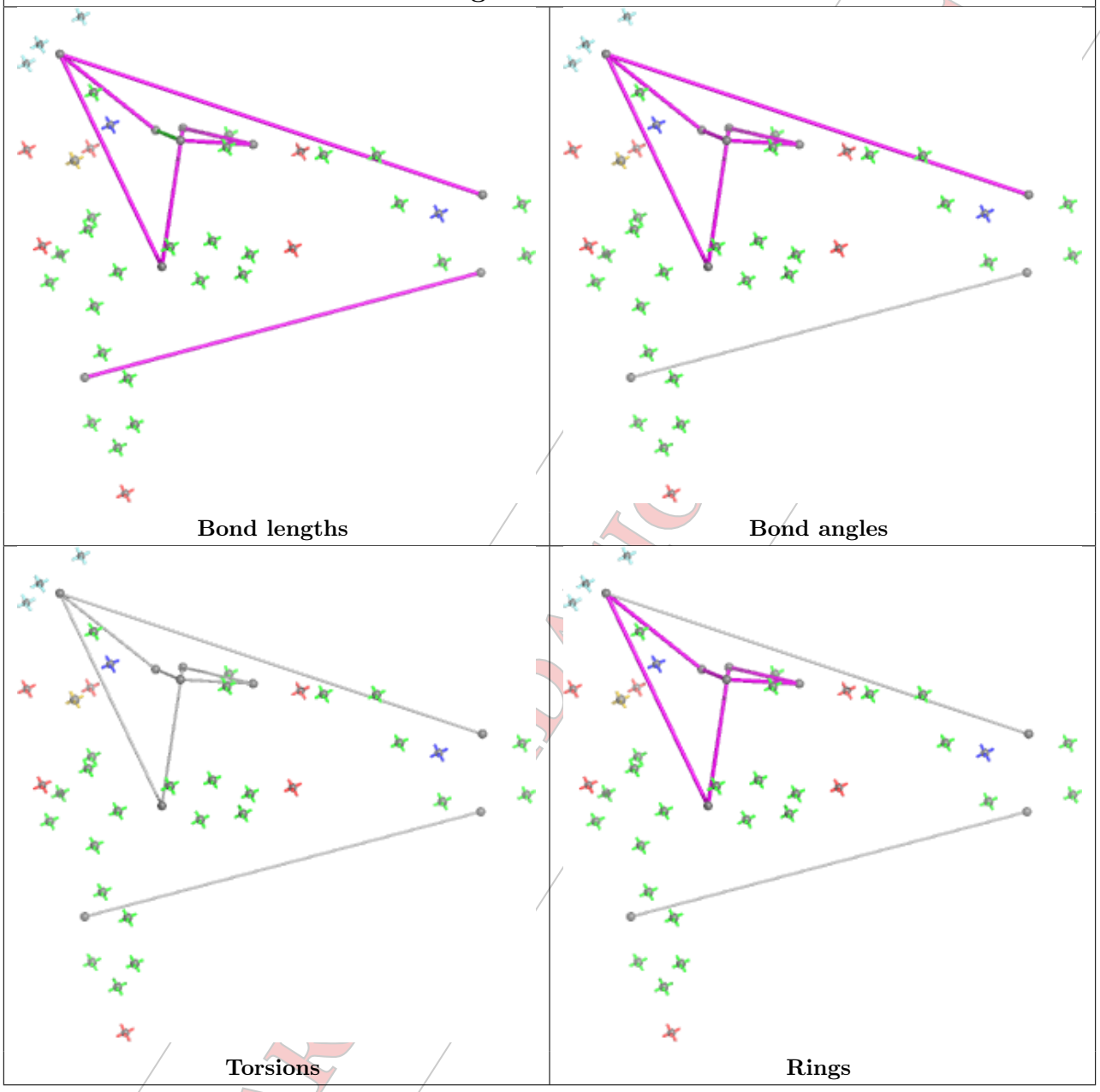


Torsions



Rings

Ligand LIG E 1



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	540:LEU	C	542:GLU	N	3.32

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	231/257 (89%)	0.13	4 (1%)	70	72	24, 44, 75, 110	0
1	B	219/257 (85%)	0.08	8 (3%)	41	43	23, 40, 78, 97	0
1	C	225/257 (87%)	0.04	4 (1%)	68	70	23, 39, 70, 97	0
1	D	208/257 (80%)	0.10	10 (4%)	30	32	24, 39, 75, 94	0
All	All	883/1028 (85%)	0.09	26 (2%)	51	53	23, 41, 75, 110	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	544	LEU	6.2
1	B	536	SER	3.7
1	B	535	PRO	3.4
1	D	536	SER	3.0
1	D	460	THR	3.0
1	D	535	PRO	2.9
1	C	331	TYR	2.8
1	B	534	VAL	2.7
1	A	526	TYR	2.6
1	C	465	THR	2.5
1	C	537	TYR	2.5
1	D	537	TYR	2.5
1	D	420	GLY	2.5
1	A	331	TYR	2.4
1	A	468	SER	2.4
1	A	334	THR	2.4
1	B	541	LEU	2.3
1	D	425	PHE	2.2
1	B	463	SER	2.2
1	B	526	TYR	2.2
1	B	462	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	538	ASP	2.2
1	B	543	MET	2.1
1	C	437	MET	2.0
1	D	526	TYR	2.0
1	D	543	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

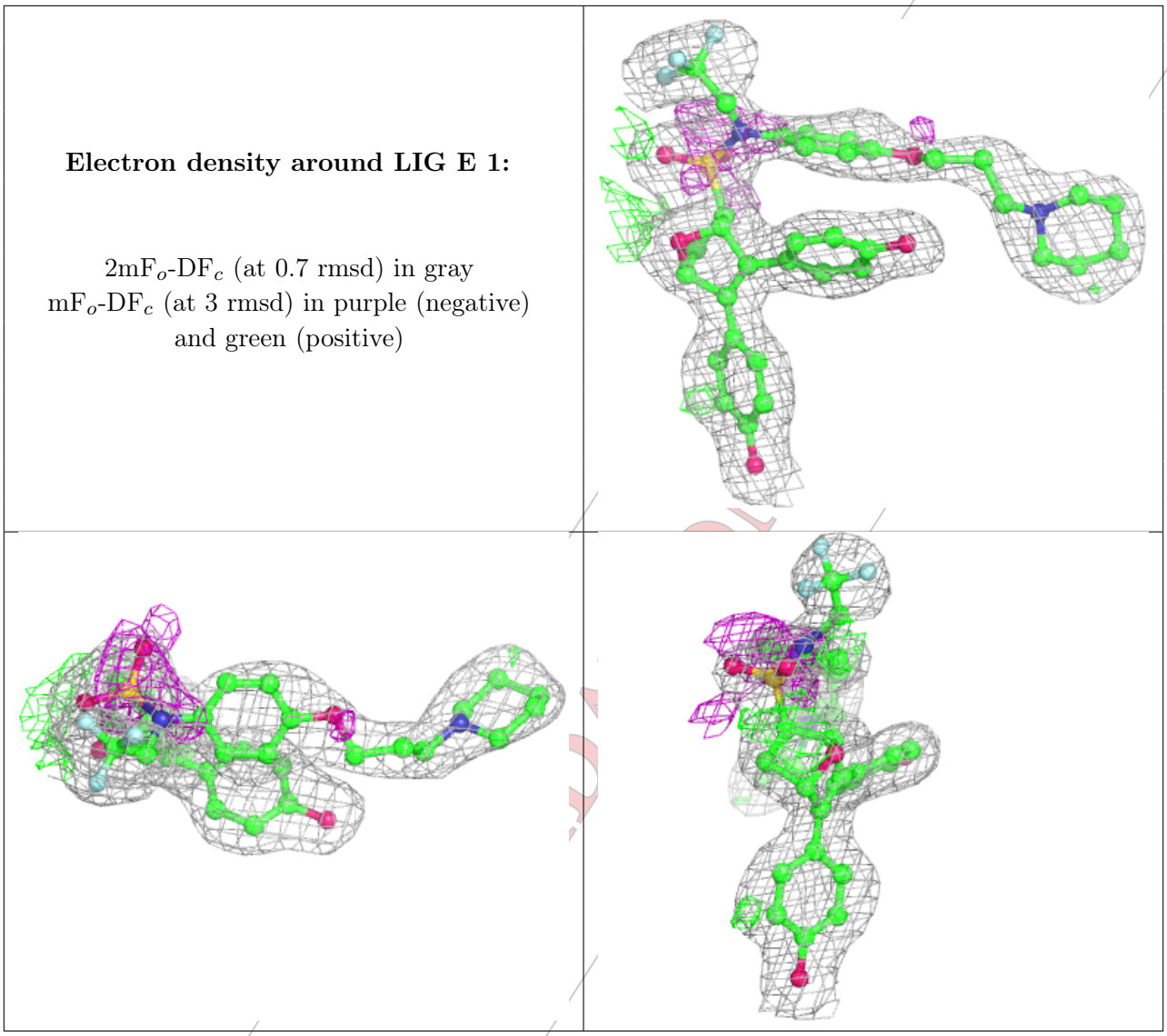
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	E	1	46/?	0.91	0.13	23,46,84,92	0
2	LIG	E	2	37/?	0.92	0.13	30,39,77,85	0
2	LIG	E	3	46/?	0.93	0.15	24,49,81,88	0
2	LIG	E	4	46/?	0.94	0.15	27,50,91,101	0
3	CL	F	2	1/?	0.98	0.09	34,34,34,34	0
3	CL	F	1	1/?	0.99	0.10	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

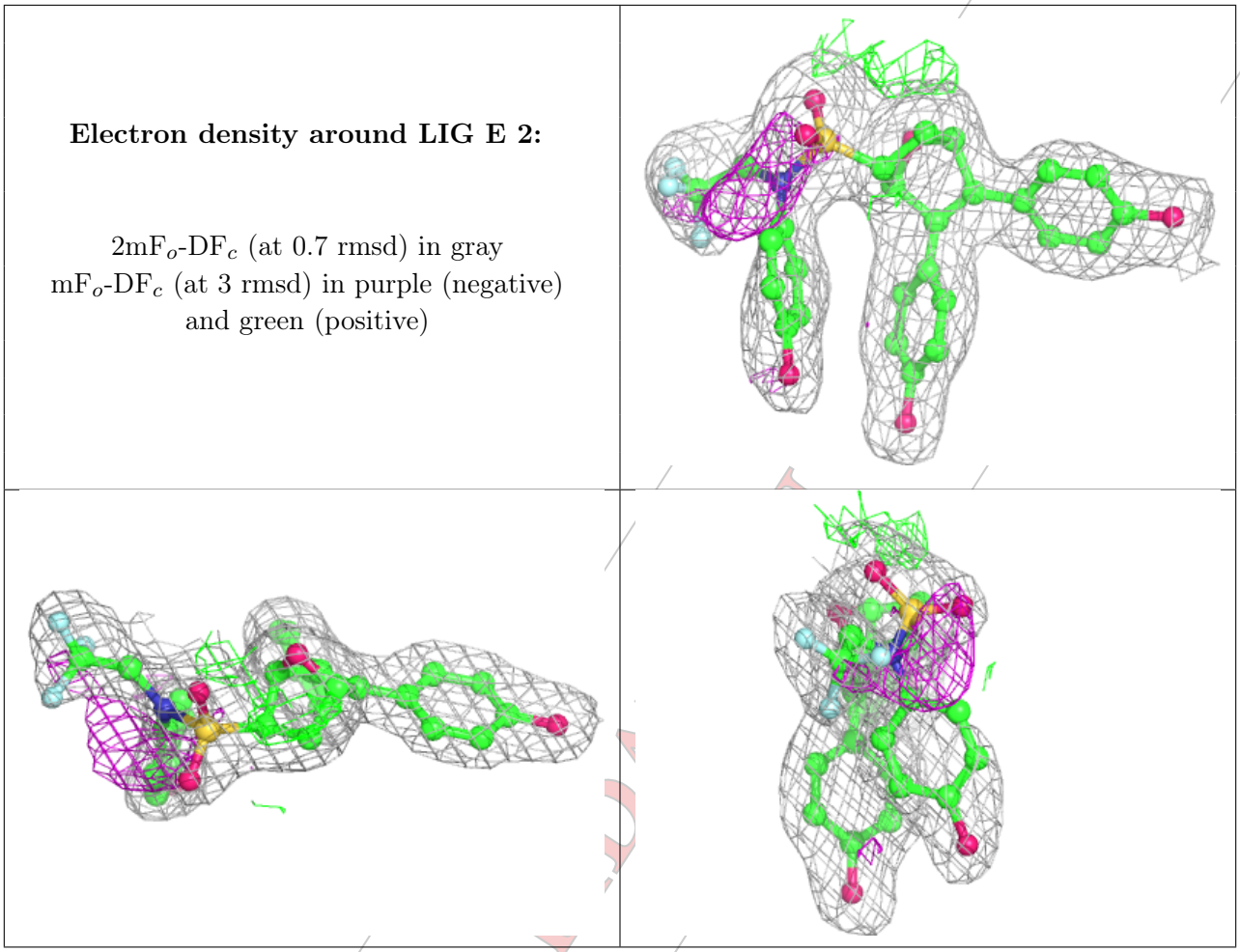
Electron density around LIG E 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



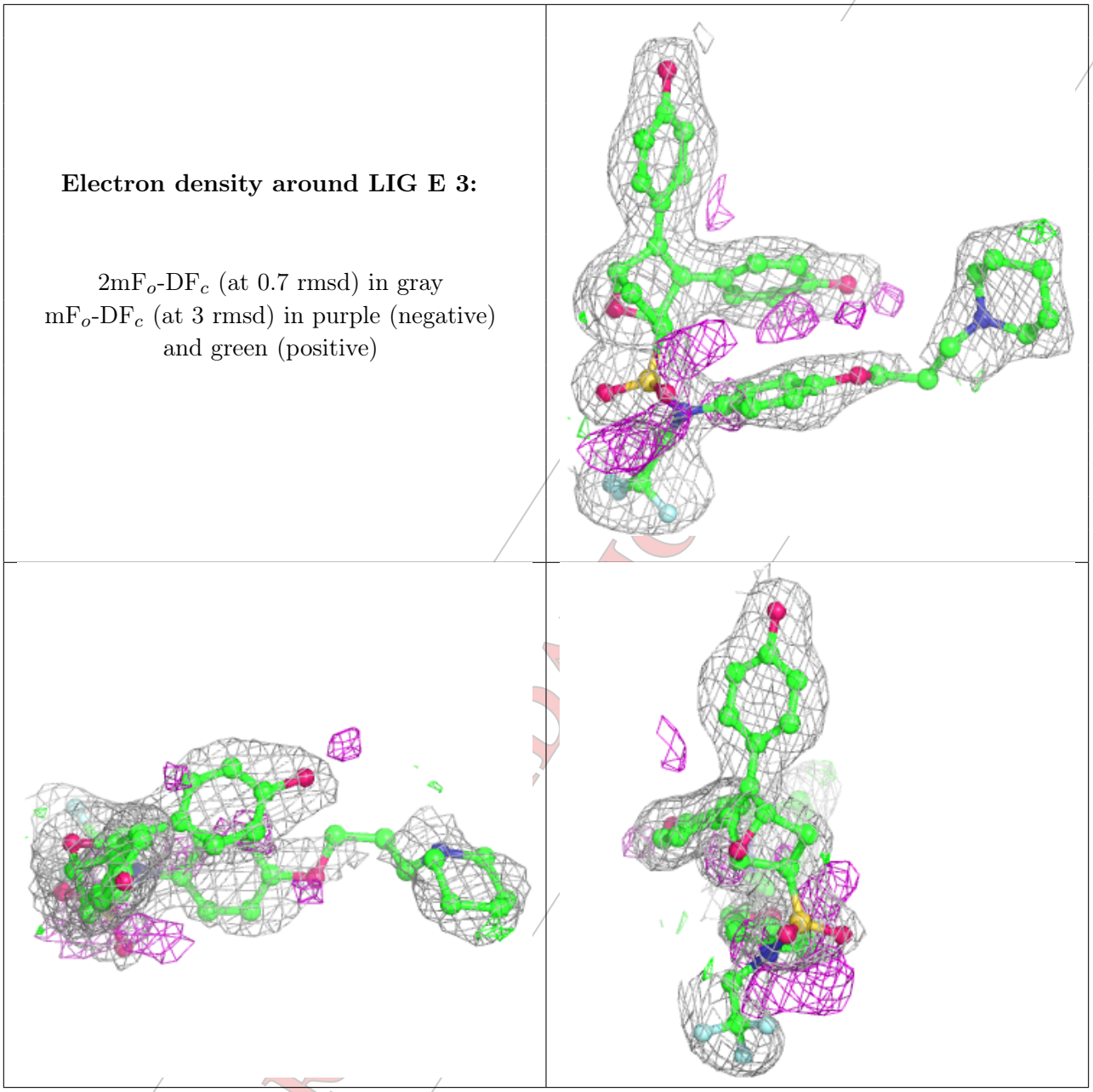
Electron density around LIG E 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



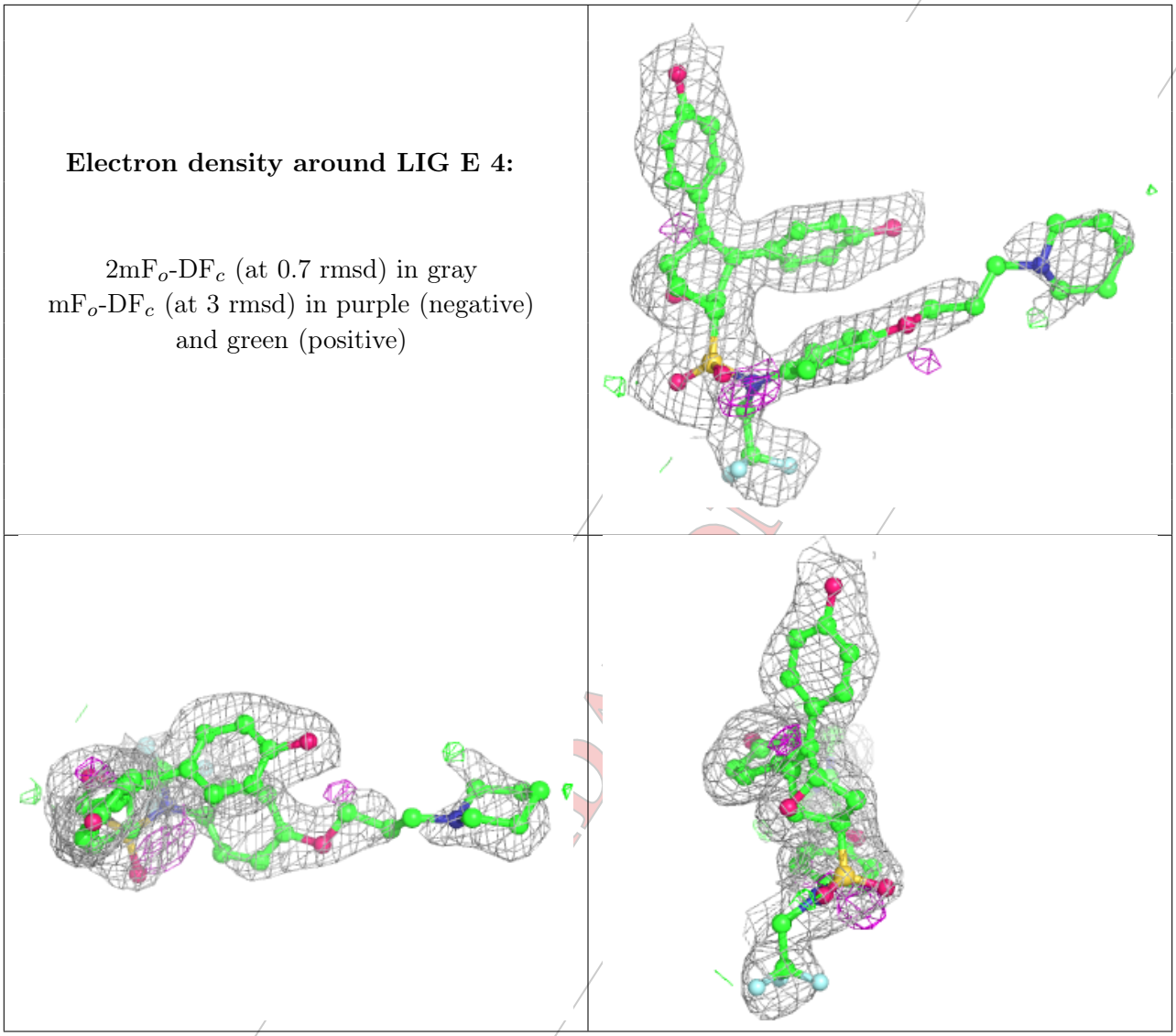
Electron density around LIG E 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG E 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 07:25 PM EDT

Deposition ID : D_1000251213

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

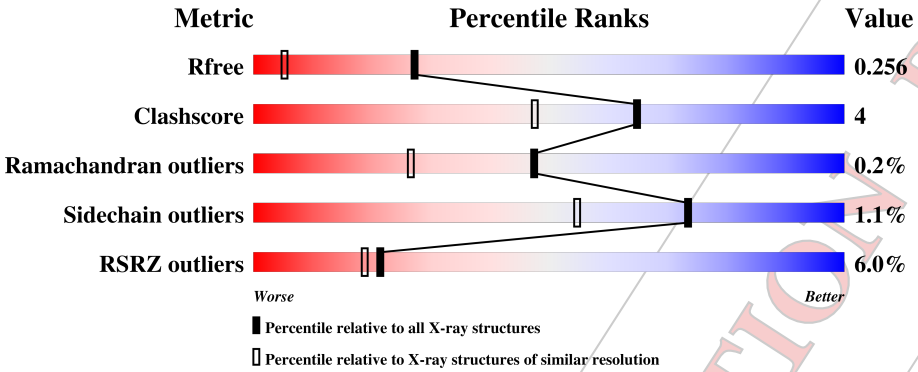
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	5%, 80%, 8% · 11%
1	B	257	7%, 81%, 7% 12%
1	C	257	4%, 81%, 7% 11%
1	D	257	5%, 75%, 9% · 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8188 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	1	0
			1836	1178	310	332	16			
1	B	227	Total	C	N	O	S	0	2	0
			1831	1172	309	334	16			
1	C	229	Total	C	N	O	S	0	1	0
			1843	1181	310	336	16			
1	D	217	Total	C	N	O	S	0	0	0
			1739	1118	291	313	17			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
2	E	1	Total	C	F	N	O	S	0	1
			88	67	3	4	12	2		
2	E	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		

- Molecule 3 is water.

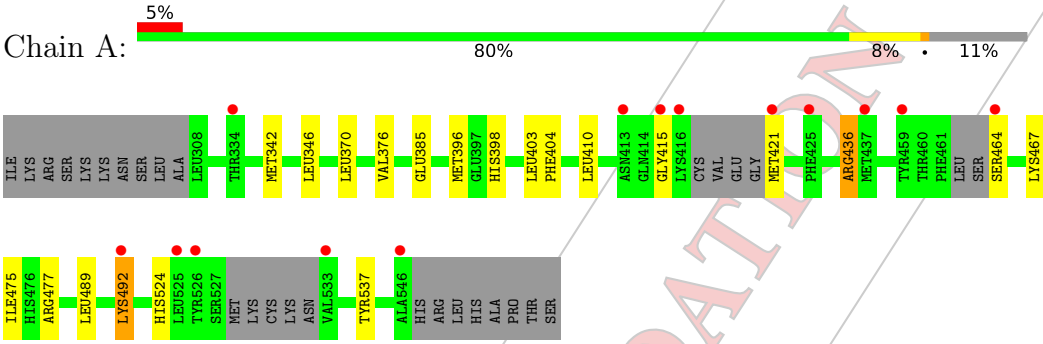
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	713	Total	O	0	0
			713	713		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

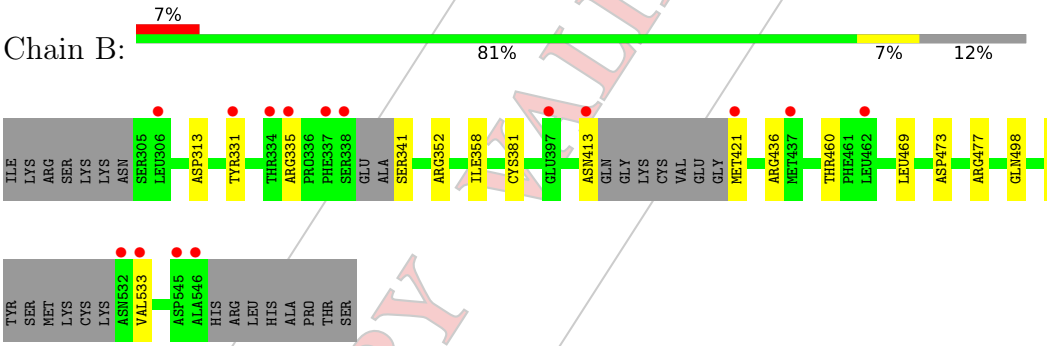
- Molecule 1: Estrogen Receptor

Chain A:



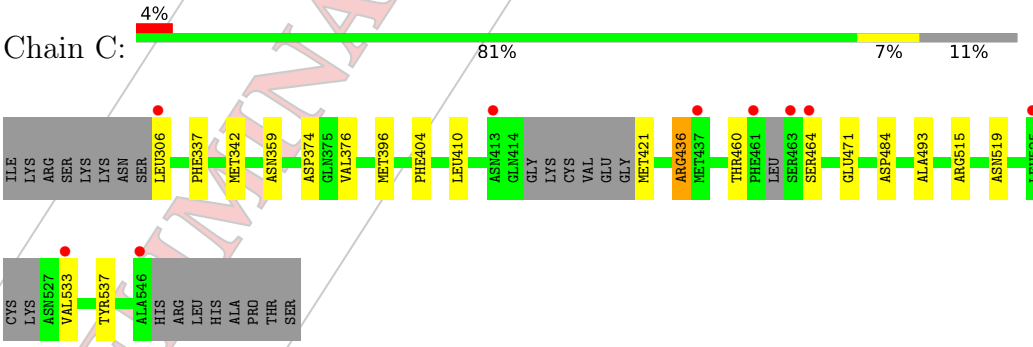
- Molecule 1: Estrogen Receptor

Chain B:



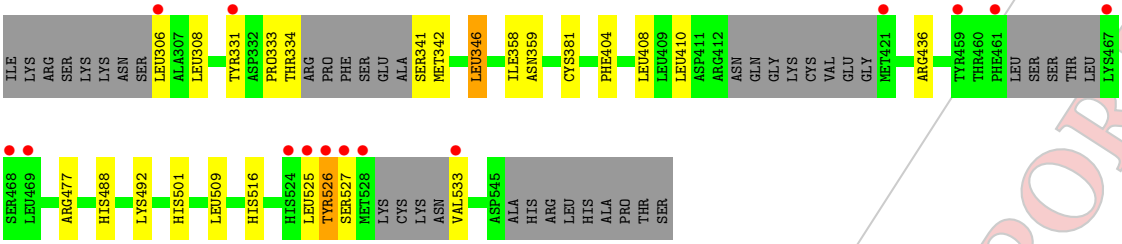
- Molecule 1: Estrogen Receptor

Chain C:



- Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.53Å 58.62Å 93.90Å 86.94° 75.26° 62.85°	Depositor
Resolution (Å)	90.57 – 1.64 90.57 – 1.64	Depositor EDS
% Data completeness (in resolution range)	69.0 (90.57-1.64) 69.0 (90.57-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.250 0.220 , 0.256	Depositor DCC
R_{free} test set	4122 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.107 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8188	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.62	0/1858	0.76	1/2508 (0.0%)
1	B	0.62	0/1852	0.81	3/2502 (0.1%)
1	C	0.64	0/1865	0.77	2/2518 (0.1%)
1	D	0.64	0/1769	0.81	3/2386 (0.1%)
All	All	0.63	0/7344	0.79	9/9914 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	1	0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	436	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	A	436	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	436	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	D	436	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	515	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	313	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	334	THR	N-CA-CB	5.59	120.91	110.30
1	B	352	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	359	ASN	CB-CA-C	5.15	120.70	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	334	THR	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1836	0	1873	18	1
1	B	1831	0	1863	15	1
1	C	1843	0	1873	14	1
1	D	1739	0	1777	16	1
2	E	226	0	1	3	0
3	S	713	0	0	15	0
All	All	8188	0	7387	61	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.33	1.06
1:D:381:CYS:SG	3:S:380:HOH:O	2.20	0.97
2:E:2[B]:LIG:C12	2:E:2[B]:LIG:O04	2.19	0.85
1:B:525:LEU:HD11	1:B:533:VAL:HG11	1.63	0.80
1:B:381:YCM:NZ2	3:S:410:HOH:O	2.17	0.77
1:D:342:MET:O	1:D:346:LEU:HD23	1.87	0.75
1:C:533:VAL:N	3:S:553:HOH:O	2.20	0.73
1:A:473:ASP:OD2	1:A:477:ARG:CZ	2.38	0.72
1:A:421:MET:HG3	1:A:524:HIS:NE2	2.04	0.72
1:A:467:LYS:NZ	3:S:642:HOH:O	2.26	0.67
1:B:524:HIS:ND1	2:E:2[B]:LIG:C06	2.58	0.67
1:A:489:LEU:O	1:A:492:LYS:HG3	1.94	0.66
1:B:477:ARG:NH2	3:S:429:HOH:O	2.26	0.65
1:A:385:GLU:OE1	3:S:147:HOH:O	2.14	0.64
1:B:341:SER:N	3:S:381:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:ASP:OD1	1:D:501:HIS:HE1	1.80	0.63
1:B:525:LEU:HD21	1:B:533:VAL:HG11	1.84	0.60
1:D:346:LEU:CD2	1:D:408:LEU:HD21	2.33	0.58
1:A:472:LYS:NZ	3:S:614:HOH:O	2.33	0.58
1:D:346:LEU:HD11	1:D:404:PHE:CD2	2.39	0.58
1:B:524:HIS:CE1	2:E:2[B]:LIG:C06	2.89	0.56
1:D:341:SER:N	3:S:629:HOH:O	2.38	0.56
1:D:346:LEU:HD22	1:D:408:LEU:HD21	1.89	0.55
1:A:489:LEU:O	1:A:492:LYS:HE3	2.07	0.54
1:C:460:THR:HG21	3:S:139:HOH:O	2.07	0.54
1:D:308:LEU:HD11	1:D:477:ARG:HE	1.73	0.54
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.23	0.53
1:C:396:MET:O	1:C:436:ARG:HD3	2.09	0.53
1:C:306:LEU:N	3:S:766:HOH:O	2.42	0.52
1:A:396:MET:O	1:A:436:ARG:HD3	2.11	0.51
1:D:404:PHE:CE1	1:D:410:LEU:HD12	2.46	0.51
1:B:525:LEU:HB3	3:S:412:HOH:O	2.11	0.51
1:D:525:LEU:O	1:D:526:TYR:HB2	2.12	0.49
1:A:473:ASP:OD2	1:A:477:ARG:NH2	2.47	0.48
1:A:421:MET:CG	1:A:524:HIS:NE2	2.77	0.47
1:A:342:MET:CE	1:A:346:LEU:HG	2.44	0.47
1:B:413:ASN:C	1:B:413:ASN:OD1	2.52	0.47
1:C:359:ASN:OD1	3:S:570:HOH:O	2.20	0.46
1:C:337:PHE:CD2	1:C:342:MET:CE	2.99	0.45
1:B:335:ARG:HB3	1:B:335:ARG:CZ	2.47	0.45
1:C:337:PHE:CD2	1:C:342:MET:HE2	2.52	0.45
1:A:342:MET:CE	1:A:346:LEU:HD21	2.47	0.44
1:C:306:LEU:CA	3:S:766:HOH:O	2.66	0.44
1:A:404:PHE:CE2	1:A:410:LEU:HD12	2.53	0.44
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.53	0.44
1:D:346:LEU:CD1	1:D:404:PHE:CD2	3.01	0.43
1:C:519:ASN:HD21	1:D:516:HIS:HA	1.83	0.43
1:A:342:MET:HE3	1:A:346:LEU:HG	2.00	0.43
1:B:473[A]:ASP:OD2	1:B:477:ARG:NH2	2.52	0.42
1:B:469:LEU:HD13	1:C:493:ALA:O	2.20	0.42
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.55	0.42
1:D:527:SER:OG	1:D:533:ALA:HB3	2.20	0.42
1:C:376:VAL:HG11	1:C:537:TYR:CD2	2.55	0.42
1:D:488:HIS:NE2	1:D:492:LYS:HD2	2.35	0.41
1:A:398:HIS:CE1	1:A:403:LEU:HD12	2.55	0.41
1:D:509:LEU:HD23	1:D:509:LEU:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:LEU:HD21	1:D:408:LEU:HD21	2.02	0.41
1:A:376:VAL:HG11	1:A:537:TYR:CD2	2.57	0.40
1:B:460:THR:HG23	3:S:116:HOH:O	2.22	0.40
1:B:525:LEU:CD1	1:B:533:VAL:HG11	2.43	0.40
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.40	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:SER:OG	1:D:333:PRO:O[1_566]	1.99	0.21
1:B:335:ARG:O	1:C:464:SER:OG[1_466]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/257 (86%)	218 (99%)	1 (0%)	1 (0%)	29	11
1	B	220/257 (86%)	216 (98%)	4 (2%)	0	100	100
1	C	221/257 (86%)	220 (100%)	1 (0%)	0	100	100
1	D	207/257 (80%)	203 (98%)	3 (1%)	1 (0%)	29	11
All	All	868/1028 (84%)	857 (99%)	9 (1%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	526	TYR
1	A	415	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/232 (89%)	205 (100%)	1 (0%)	88	80
1	B	207/232 (89%)	204 (99%)	3 (1%)	67	45
1	C	206/232 (89%)	205 (100%)	1 (0%)	88	80
1	D	196/232 (84%)	192 (98%)	4 (2%)	55	29
All	All	815/928 (88%)	806 (99%)	9 (1%)	73	55

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	LYS
1	B	331	TYR
1	B	358	ILE
1	B	421	MET
1	C	421	MET
1	D	306	LEU
1	D	331	TYR
1	D	346	LEU
1	D	358	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	519	ASN
1	B	398	HIS
1	B	498	GLN
1	B	519	ASN
1	C	519	ASN
1	D	501	HIS
1	D	513	HIS
1	D	519	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

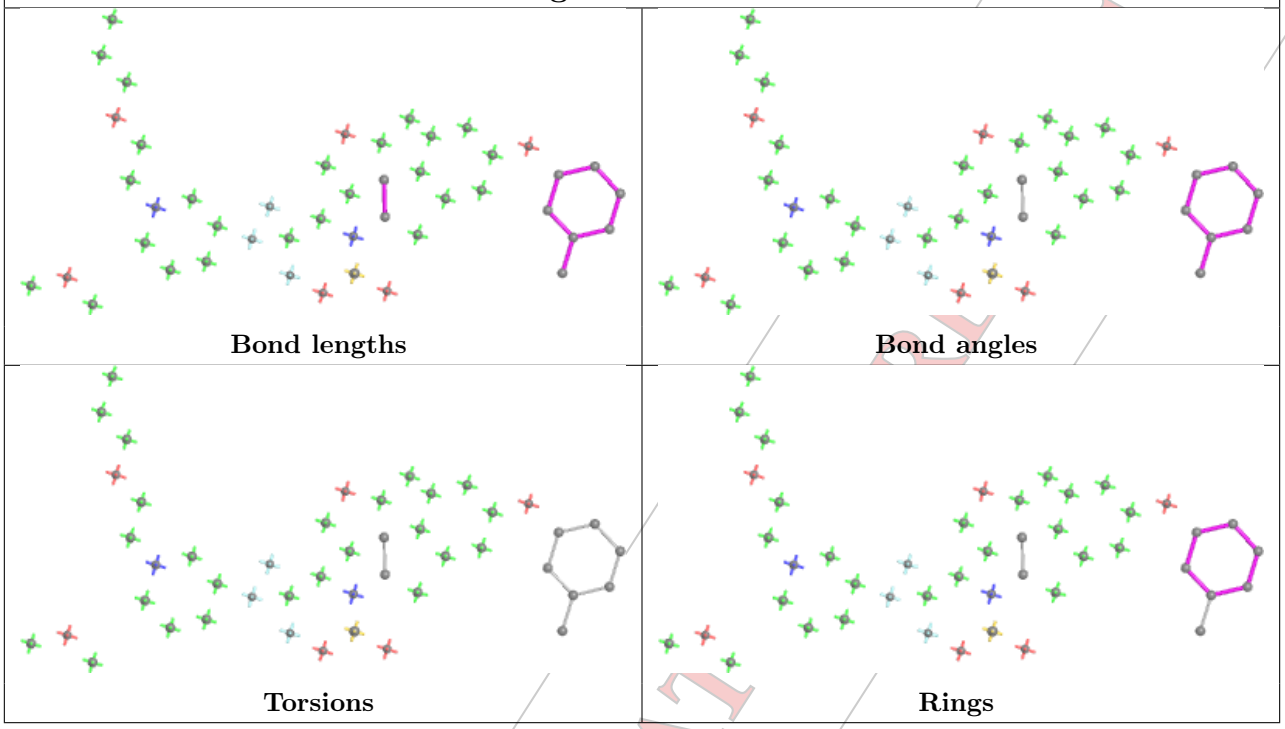
There are no torsion outliers.

There are no ring outliers.

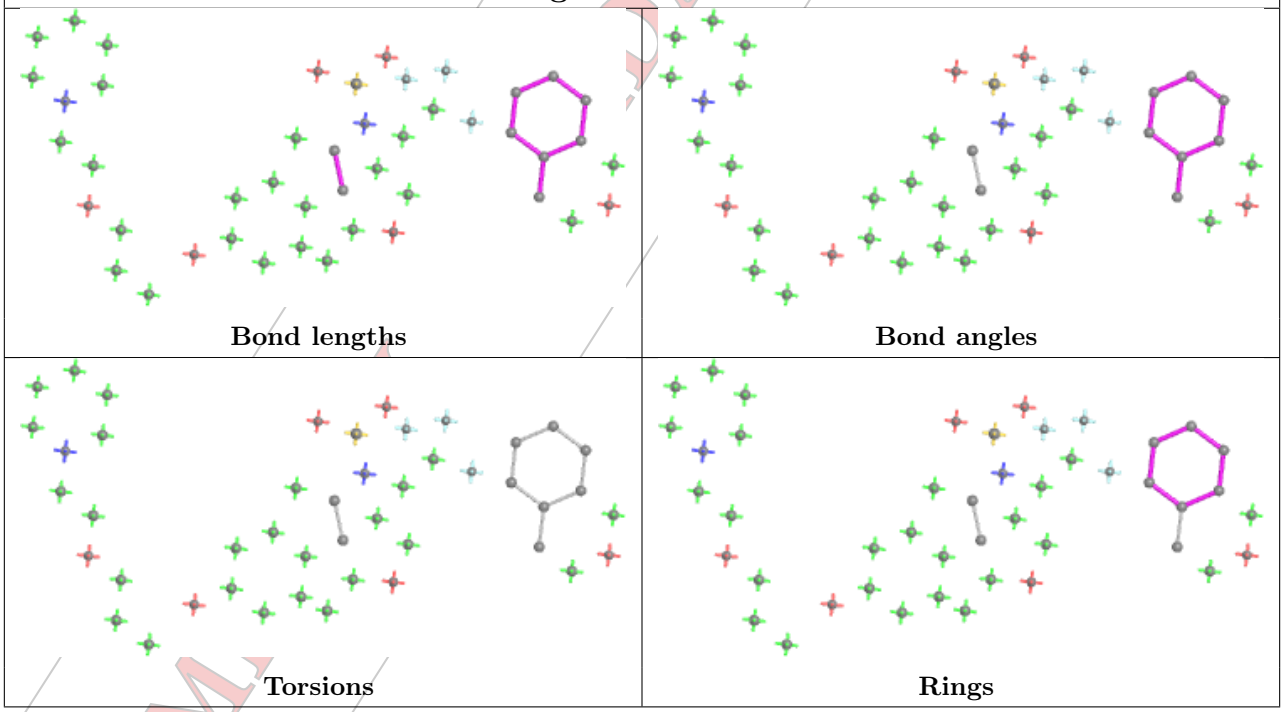
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

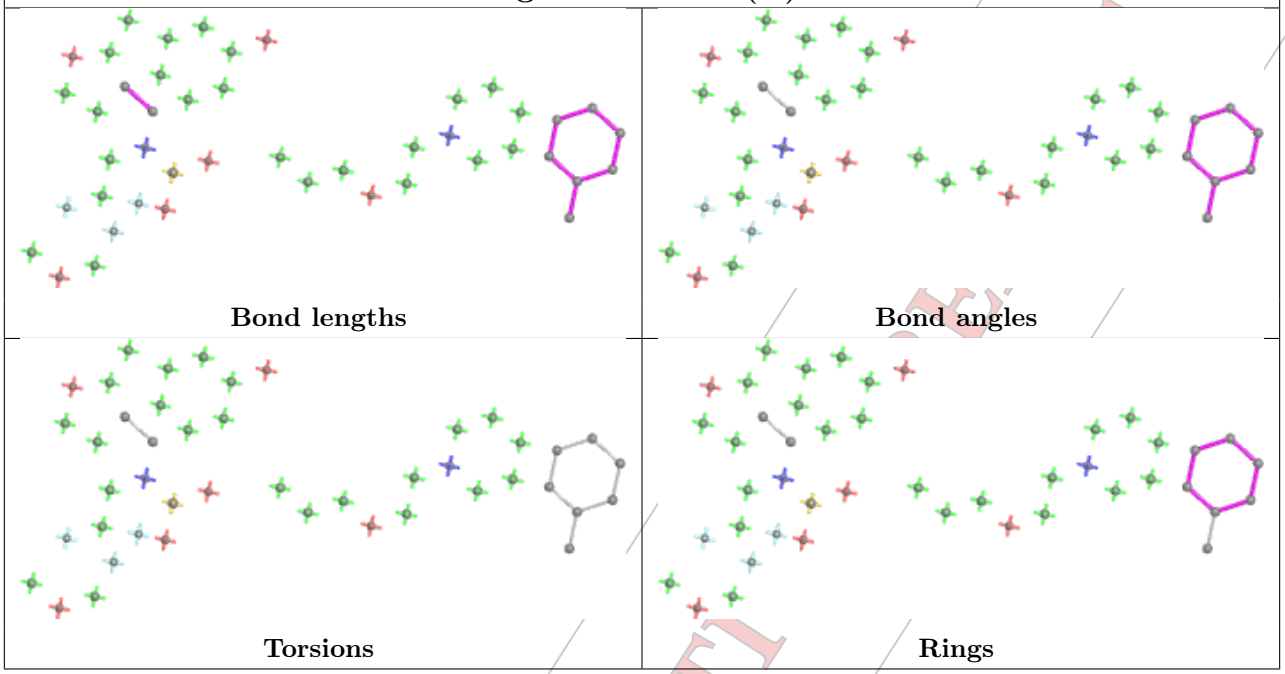
Ligand LIG E 3



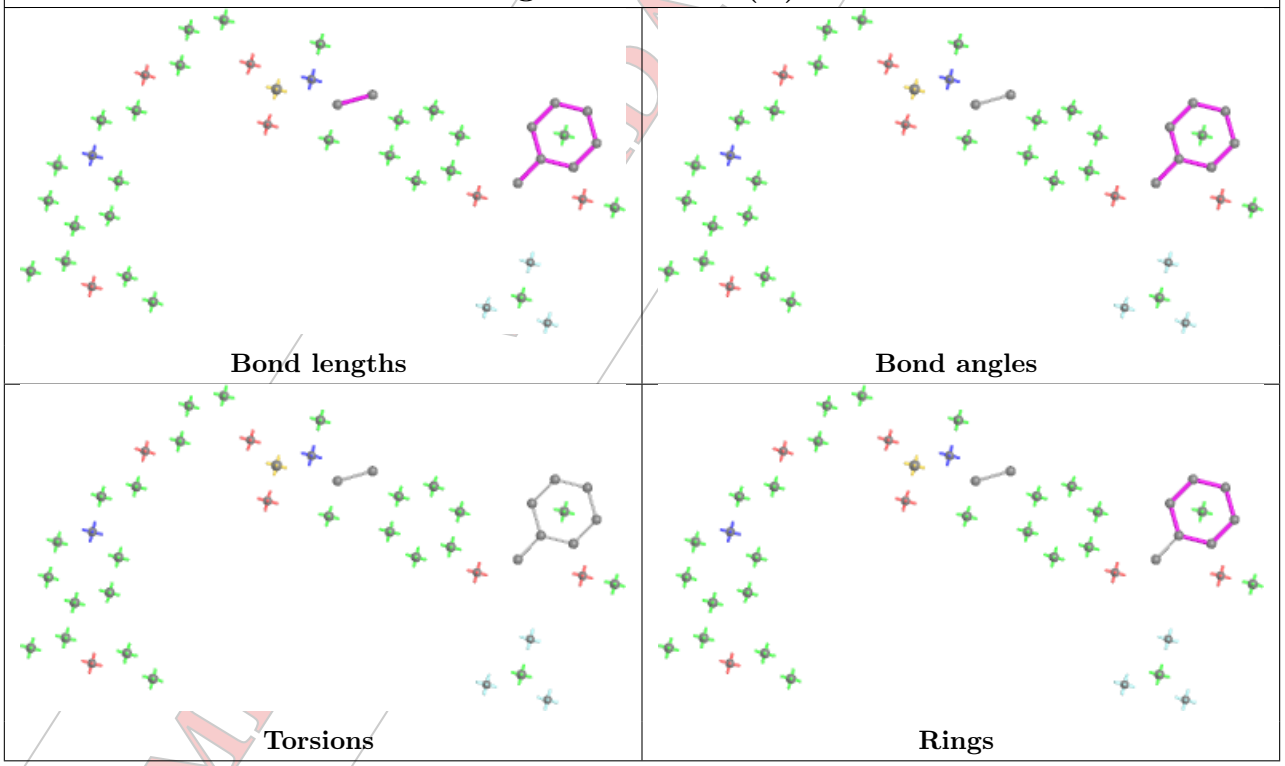
Ligand LIG E 4



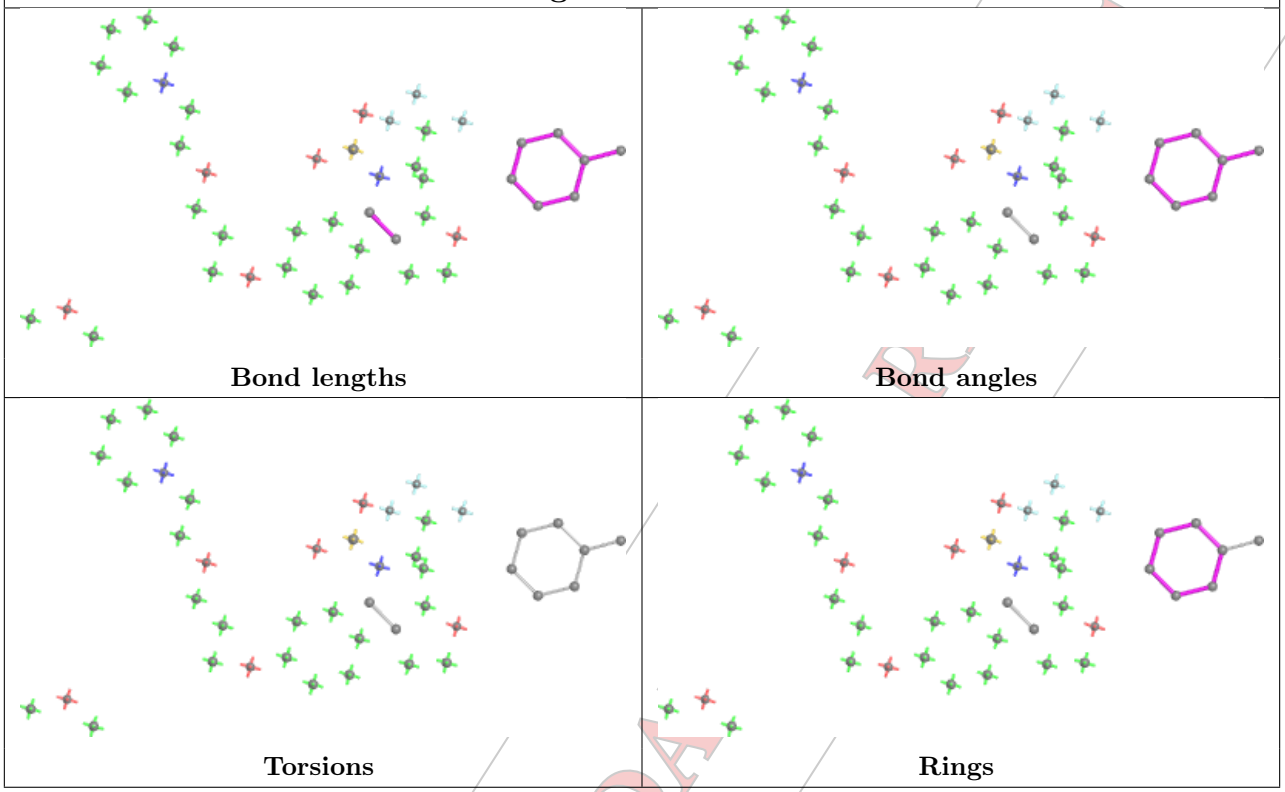
Ligand LIG E 2 (A)



Ligand LIG E 2 (B)



Ligand LIG E 1



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	527:ALA	C	533:VAL	N	10.52

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	227/257 (88%)	0.25	14 (6%)	20	17	14, 26, 50, 76	0
1	B	226/257 (87%)	0.27	17 (7%)	14	12	12, 24, 61, 74	0
1	C	228/257 (88%)	0.15	9 (3%)	39	37	12, 24, 48, 66	0
1	D	217/257 (84%)	0.25	14 (6%)	18	16	13, 24, 57, 85	0
All	All	898/1028 (87%)	0.23	54 (6%)	21	19	12, 25, 55, 85	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	VAL	7.2
1	B	546	ALA	5.6
1	B	306	LEU	5.5
1	A	546	ALA	5.5
1	B	532	ASN	5.4
1	C	533	VAL	5.0
1	D	533	ALA	4.7
1	B	337	PHE	4.6
1	D	421	MET	4.5
1	C	546	ALA	4.4
1	A	415	GLY	4.3
1	B	462	LEU	4.2
1	C	306	LEU	4.1
1	B	533	VAL	3.8
1	D	527	SER	3.8
1	B	413	ASN	3.8
1	D	468	SER	3.6
1	A	413	ASN	3.6
1	B	525	LEU	3.6
1	A	421	MET	3.5
1	D	526	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	461	PHE	3.4
1	D	524	HIS	3.3
1	C	413	ASN	3.3
1	D	525	LEU	3.3
1	D	459	TYR	3.2
1	D	469	LEU	3.1
1	D	306	LEU	3.1
1	B	524	HIS	3.1
1	B	331	TYR	3.0
1	D	467	LYS	3.0
1	A	492	LYS	2.8
1	A	464	SER	2.8
1	D	528	MET	2.8
1	B	421	MET	2.7
1	D	331	TYR	2.7
1	C	463	SER	2.7
1	B	335	ARG	2.6
1	C	464	SER	2.6
1	A	459	TYR	2.5
1	C	525	LEU	2.5
1	B	397	GLU	2.4
1	A	416	LYS	2.4
1	B	338	SER	2.3
1	A	525	LEU	2.3
1	A	437	MET	2.2
1	A	334	THR	2.2
1	B	545	ASP	2.2
1	D	461	PHE	2.2
1	A	425	PHE	2.0
1	B	437	MET	2.0
1	C	437	MET	2.0
1	A	526	TYR	2.0
1	B	334	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

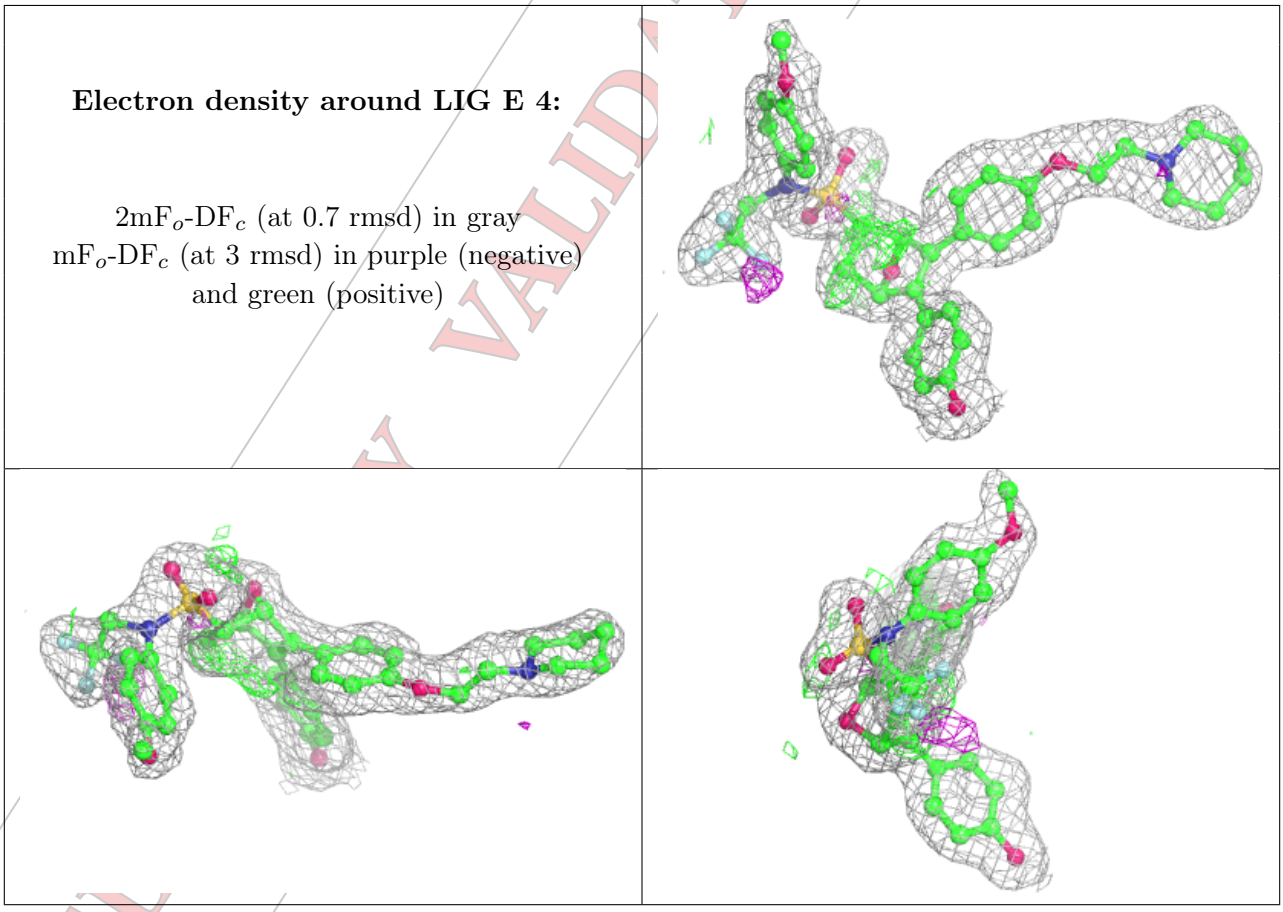
There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

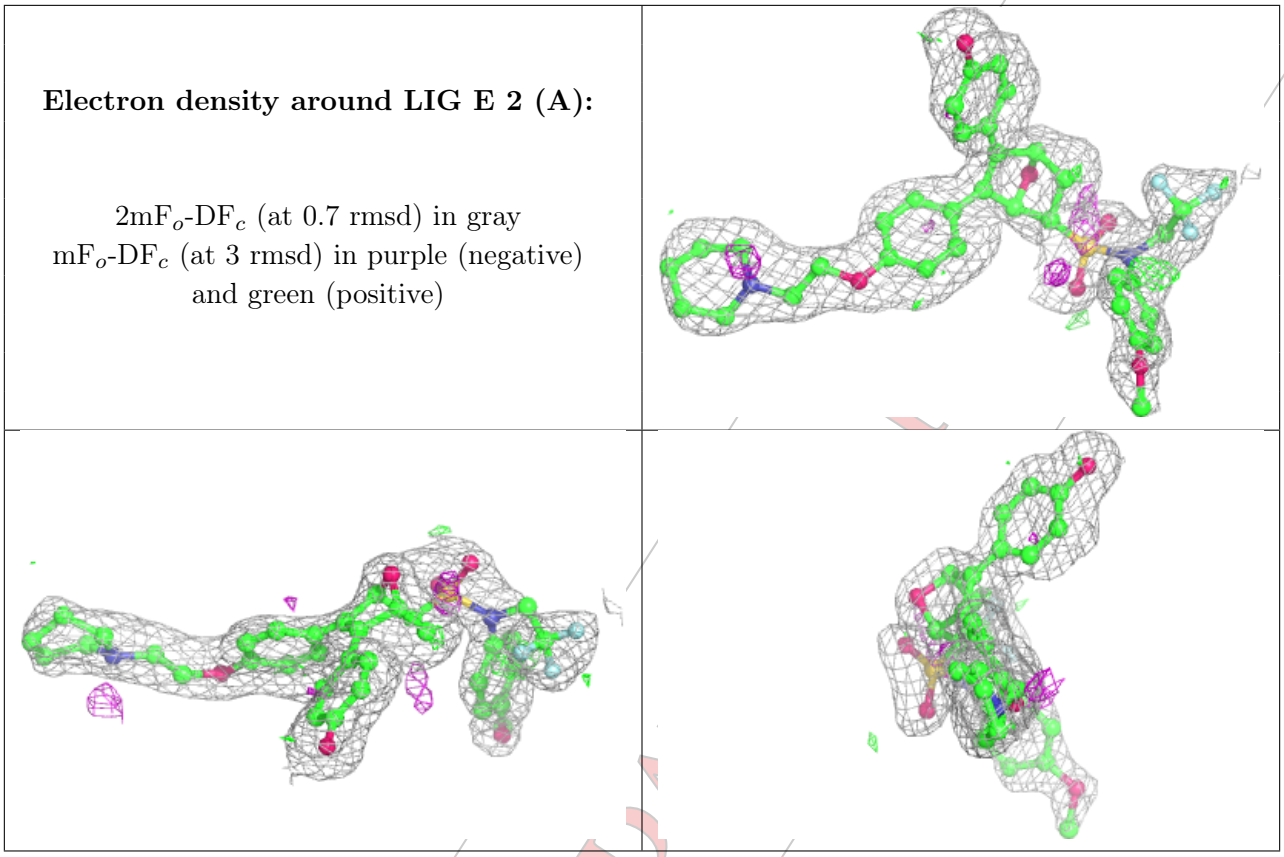
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	E	4	46/?	0.88	0.13	23,33,45,47	0
2	LIG	E	2[A]	46/?	0.88	0.16	18,25,30,30	46
2	LIG	E	2[B]	42/?	0.88	0.16	24,32,36,37	42
2	LIG	E	3	46/?	0.90	0.12	19,31,42,45	0
2	LIG	E	1	46/?	0.90	0.12	21,31,39,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



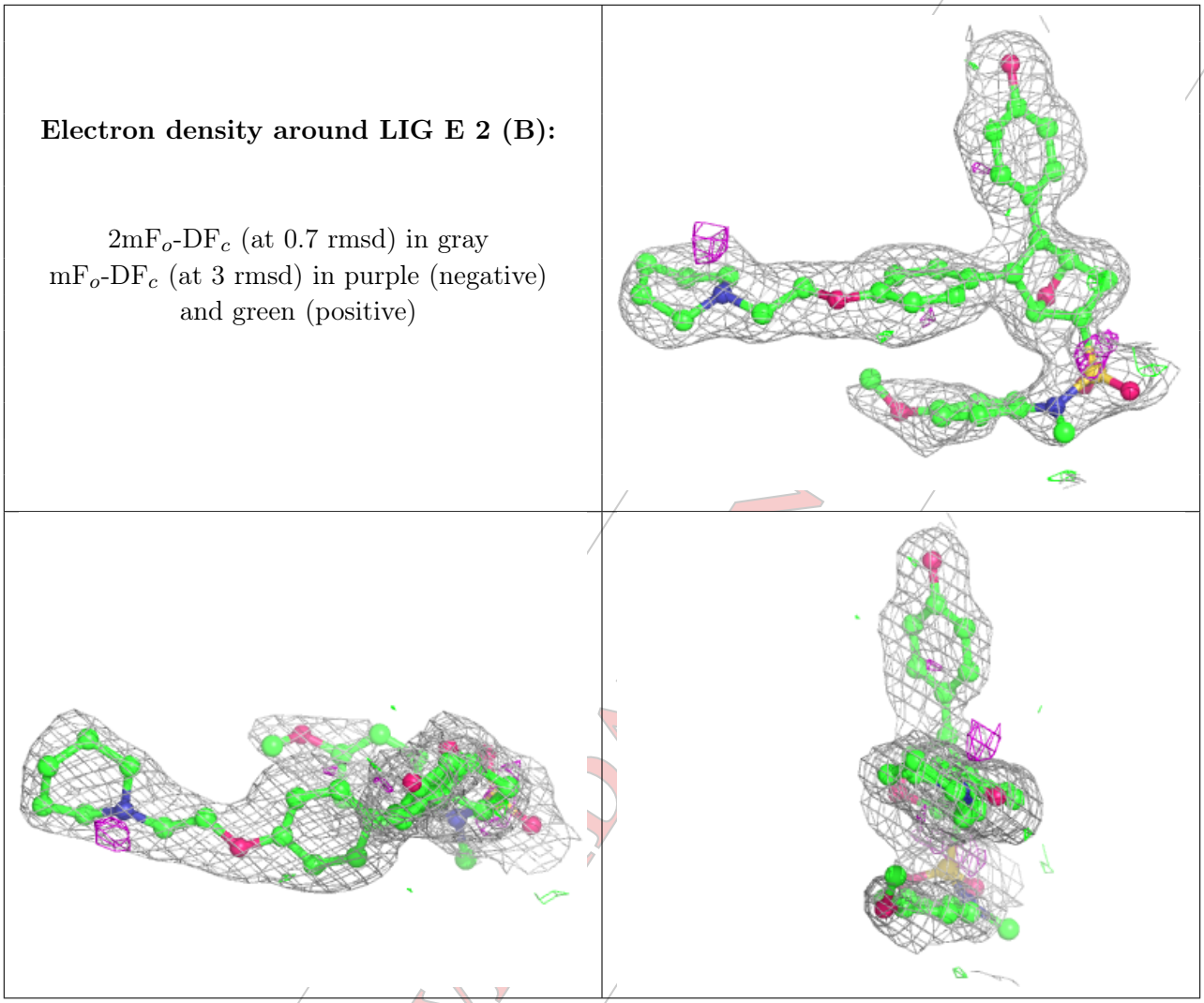
Electron density around LIG E 2 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



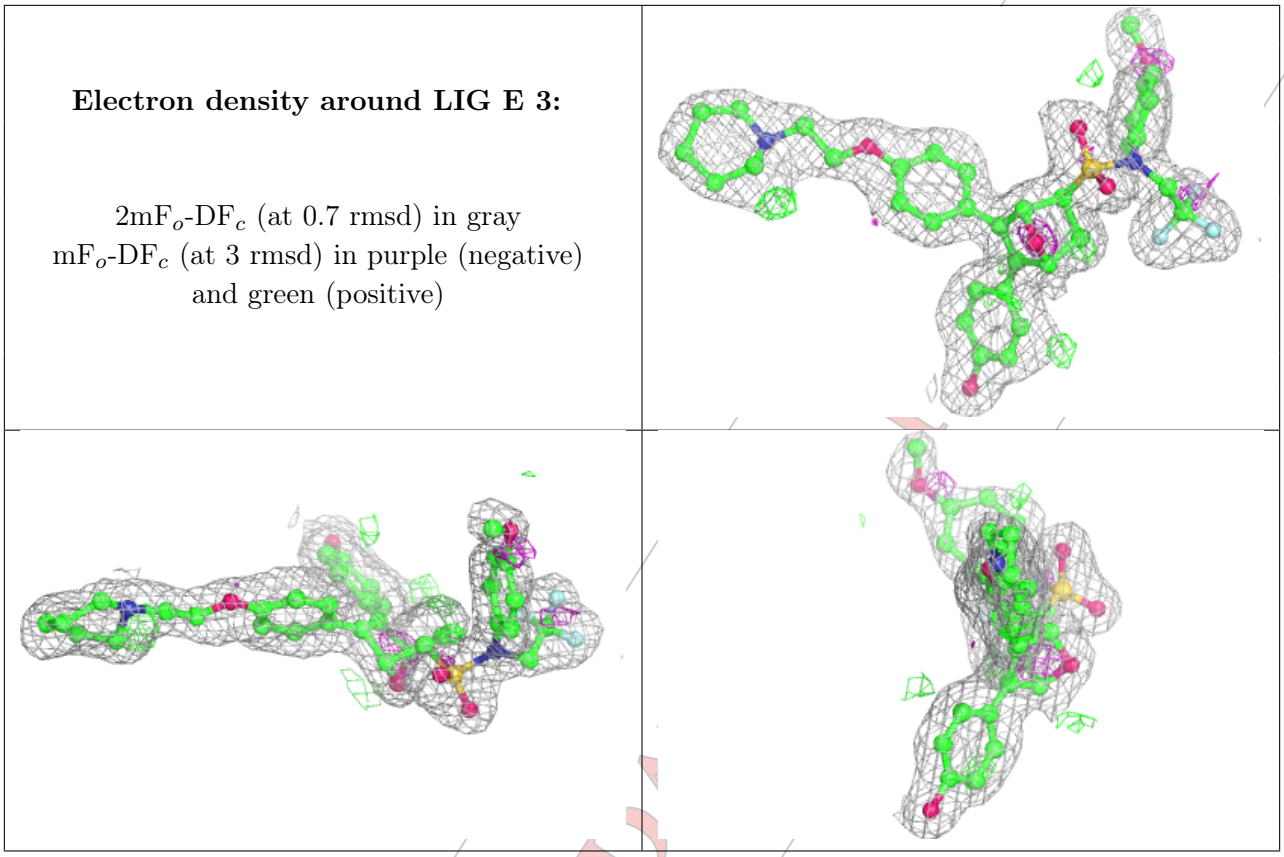
Electron density around LIG E 2 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



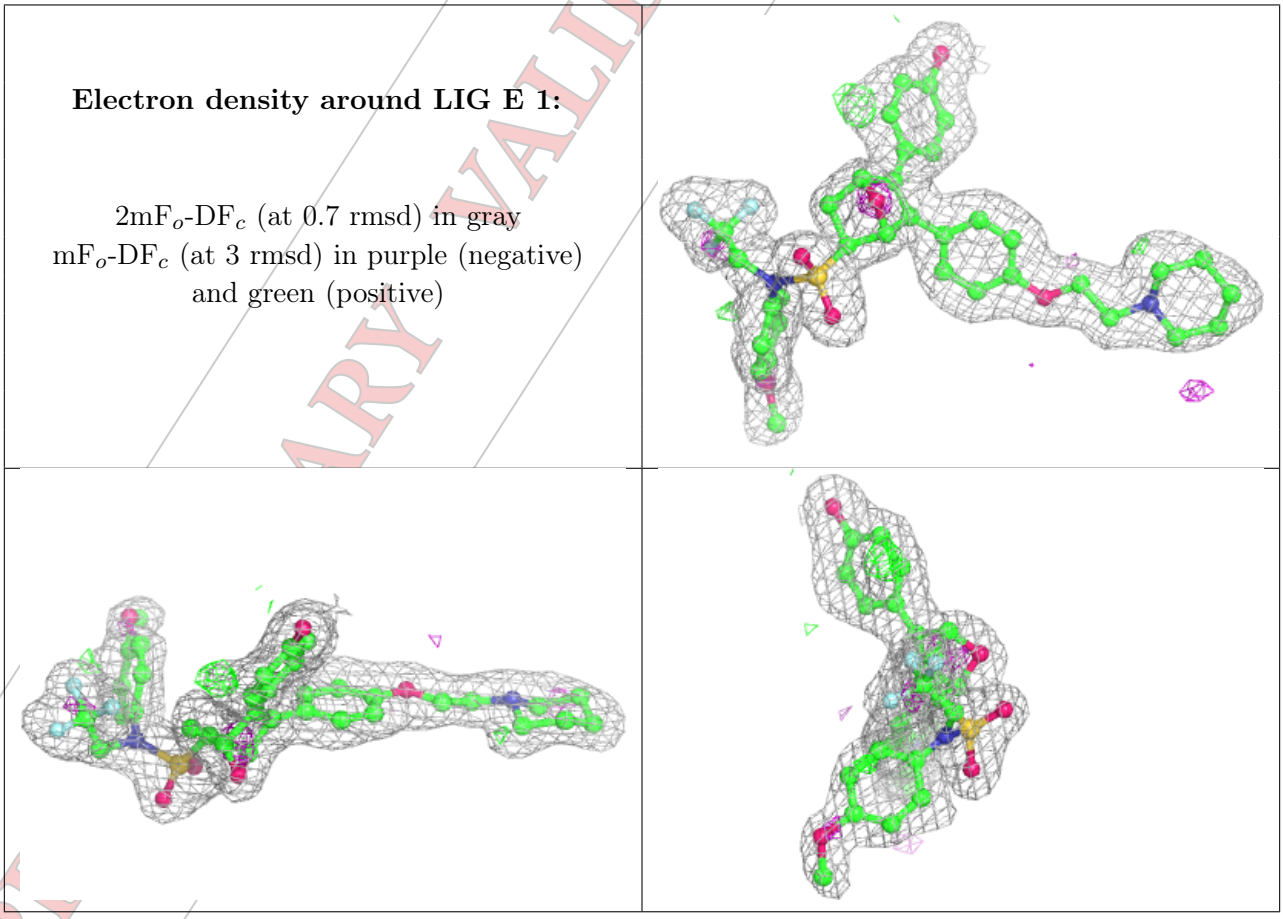
Electron density around LIG E 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG E 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 09:16 PM EDT

Deposition ID : D_1000251214

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

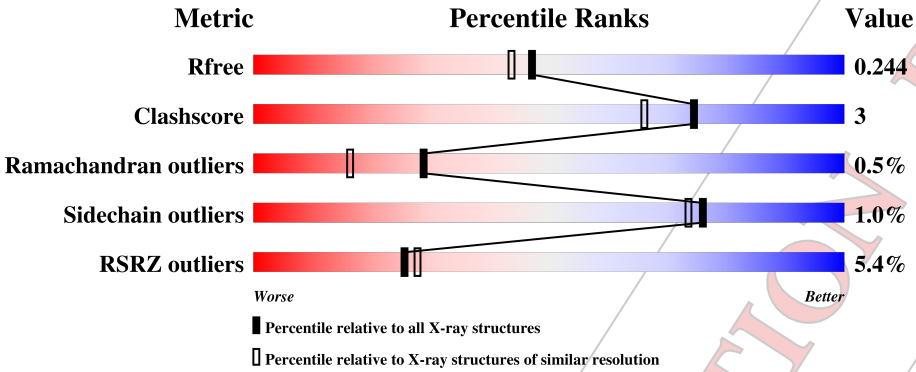
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	5%, 86%, 5%, 9%
1	B	257	4%, 84%, 5%, 11%
1	C	257	5%, 82%, 7%, 11%
1	D	257	5%, 76%, 8%, 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7785 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1870	1198	315	340	17			
1	B	229	Total	C	N	O	S	0	1	0
			1836	1177	311	331	17			
1	C	229	Total	C	N	O	S	0	1	0
			1838	1178	311	334	15			
1	D	218	Total	C	N	O	S	0	1	0
			1755	1127	297	315	16			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	1
			94	70	6	4	12	2		
2	B	1	Total	C	F	N	O	S	0	0
			47	35	3	2	6	1		
2	C	1	Total	C	N	O	S		0	0
			44	35	2	6	1			
2	D	1	Total	C	F	N	O	S	0	0
			47	35	3	2	6	1		

- Molecule 3 is water.

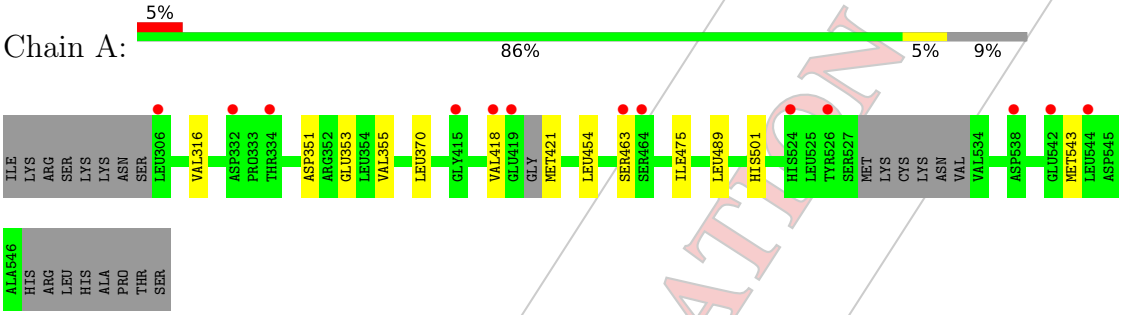
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	254	Total	O	0	0
			254	254		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

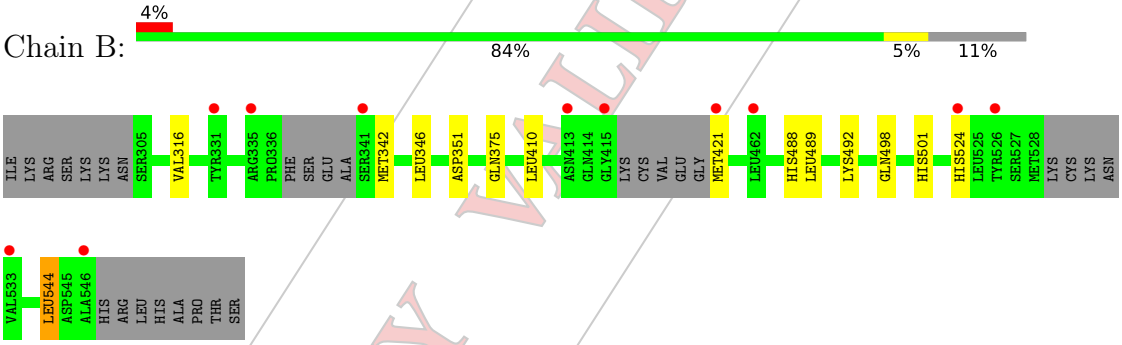
• Molecule 1: Estrogen Receptor

Chain A:



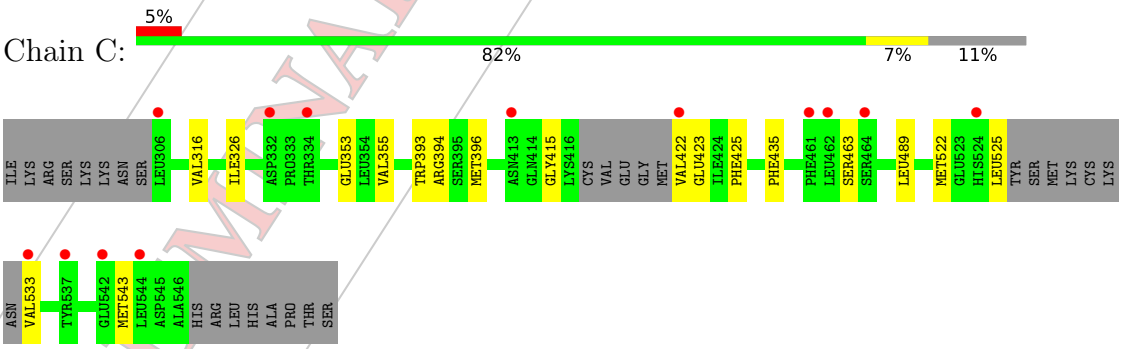
• Molecule 1: Estrogen Receptor

Chain B:



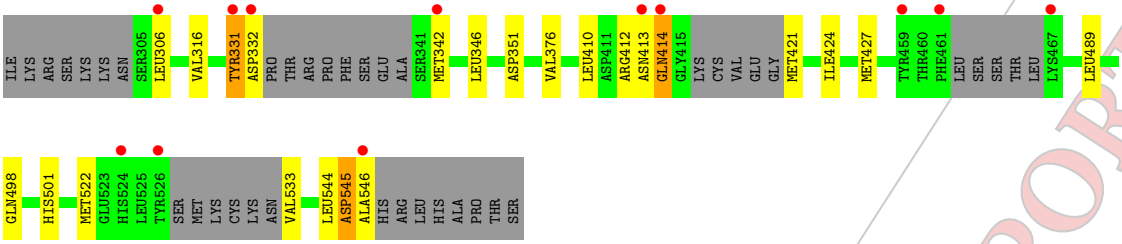
• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.55Å 58.91Å 93.46Å 87.24° 75.18° 62.93°	Depositor
Resolution (Å)	90.06 – 1.97 90.06 – 1.83	Depositor EDS
% Data completeness (in resolution range)	76.7 (90.06-1.97) 63.4 (90.06-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.202 , 0.235 0.211 , 0.244	Depositor DCC
R_{free} test set	2677 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.108 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7785	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/1893	0.53	0/2557
1	B	0.31	0/1861	0.55	0/2513
1	C	0.30	0/1860	0.53	0/2513
1	D	0.30	0/1777	0.53	0/2396
All	All	0.30	0/7391	0.53	0/9979

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1870	0	1907	10	0
1	B	1836	0	1878	9	0
1	C	1838	0	1878	13	0
1	D	1755	0	1790	14	0
2	A	94	0	6	5	0
2	B	47	0	3	1	0
2	C	44	0	2	2	0
2	D	47	0	3	2	0
3	S	254	0	0	0	0
All	All	7785	0	7467	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.38	1.02
1:A:501:HIS:CE1	1:B:501[B]:HIS:CE1	2.65	0.84
1:C:393:TRP:CE3	1:C:396:MET:HE3	2.24	0.72
1:C:326:ILE:HD12	1:C:394:ARG:HD3	1.74	0.69
1:A:355:VAL:HA	1:A:543:MET:CE	2.21	0.69
1:C:355:VAL:HG22	1:C:543:MET:CE	2.30	0.62
1:C:422:VAL:HG12	1:C:425:PHE:H	1.65	0.61
2:A:601[A]:LIG:C30	2:A:601[A]:LIG:F01	2.39	0.60
2:A:601[A]:LIG:C15	2:A:601[A]:LIG:F02	2.40	0.60
1:C:393:TRP:CE3	1:C:396:MET:CE	2.87	0.58
1:B:488:HIS:NE2	1:B:492:LYS:HD2	2.20	0.57
1:B:498:GLN:HA	1:B:501[A]:HIS:CE1	2.40	0.56
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.41	0.56
1:A:418:VAL:HG13	1:A:421:MET:N	2.23	0.53
1:A:355:VAL:HA	1:A:543:MET:HE3	1.91	0.52
1:C:525:LEU:HD11	1:C:533:VAL:N	2.24	0.52
1:A:454:LEU:HD22	1:A:475:ILE:HD12	1.92	0.51
1:D:413:ASN:O	1:D:414:GLN:HB2	2.11	0.50
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.92	0.50
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.28	0.49
1:D:331:TYR:O	1:D:332:ASP:C	2.51	0.49
2:A:601[A]:LIG:O06	2:A:601[A]:LIG:F01	2.21	0.49
1:B:342:MET:HE3	1:B:346:LEU:HD11	1.94	0.49
1:D:424:ILE:HD13	1:D:427:MET:CE	2.43	0.48
1:C:415:GLY:O	1:C:422:VAL:HG23	2.13	0.47
1:C:525:LEU:HD12	2:C:601:LIG:O03	2.15	0.47
1:C:355:VAL:HG22	1:C:543:MET:HE2	1.97	0.47
1:D:351:ASP:OD1	2:D:601:LIG:N01	2.48	0.47
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.97	0.47
1:A:353:GLU:OE1	2:A:601[B]:LIG:O05	2.35	0.45
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.99	0.45
1:D:413:ASN:O	1:D:414:GLN:CB	2.65	0.44
1:D:545:ASP:O	1:D:546:ALA:HB3	2.19	0.43
1:A:351:ASP:OD1	2:A:601[A]:LIG:N01	2.52	0.43
1:D:533:VAL:HG12	2:D:601:LIG:C10	2.49	0.43
1:D:342:MET:HE3	1:D:346:LEU:HG	2.01	0.42
1:D:342:MET:HE3	1:D:346:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:MET:CE	1:B:410:LEU:HD11	2.50	0.42
1:A:316:VAL:HG21	1:A:489:LEU:HD21	2.02	0.42
1:C:396:MET:CE	1:C:435:PHE:HB3	2.50	0.42
1:C:393:TRP:HE3	1:C:396:MET:CE	2.33	0.42
1:C:316:VAL:HG21	1:C:489:LEU:HD21	2.02	0.41
1:D:424:ILE:HD13	1:D:427:MET:HE2	2.02	0.41
1:C:353:GLU:OE1	2:C:601:LIG:O05	2.38	0.41
1:B:375:GLN:HB3	1:B:544:LEU:HD21	2.02	0.41
1:B:421:MET:HG2	1:B:524:HIS:CD2	2.57	0.40
1:B:351:ASP:OD1	2:B:601:LIG:N01	2.55	0.40
1:D:342:MET:CE	1:D:410:LEU:HD11	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	227/257 (88%)	222 (98%)	4 (2%)	1 (0%)	34 22
1	B	221/257 (86%)	217 (98%)	4 (2%)	0	100 100
1	C	223/257 (87%)	221 (99%)	1 (0%)	1 (0%)	34 22
1	D	208/257 (81%)	204 (98%)	2 (1%)	2 (1%)	15 6
All	All	879/1028 (86%)	864 (98%)	11 (1%)	4 (0%)	29 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	SER
1	C	463	SER
1	D	545	ASP
1	D	414	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/232 (90%)	210 (100%)	0	100	100
1	B	207/232 (89%)	206 (100%)	1 (0%)	88	87
1	C	206/232 (89%)	204 (99%)	2 (1%)	76	73
1	D	196/232 (84%)	191 (97%)	5 (3%)	46	37
All	All	819/928 (88%)	811 (99%)	8 (1%)	76	73

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	544	LEU
1	C	423	GLU
1	C	522	MET
1	D	306	LEU
1	D	331	TYR
1	D	412	ARG
1	D	421	MET
1	D	522	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	A	501	HIS
1	C	519	ASN
1	C	524	HIS
1	D	439	ASN
1	D	519	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

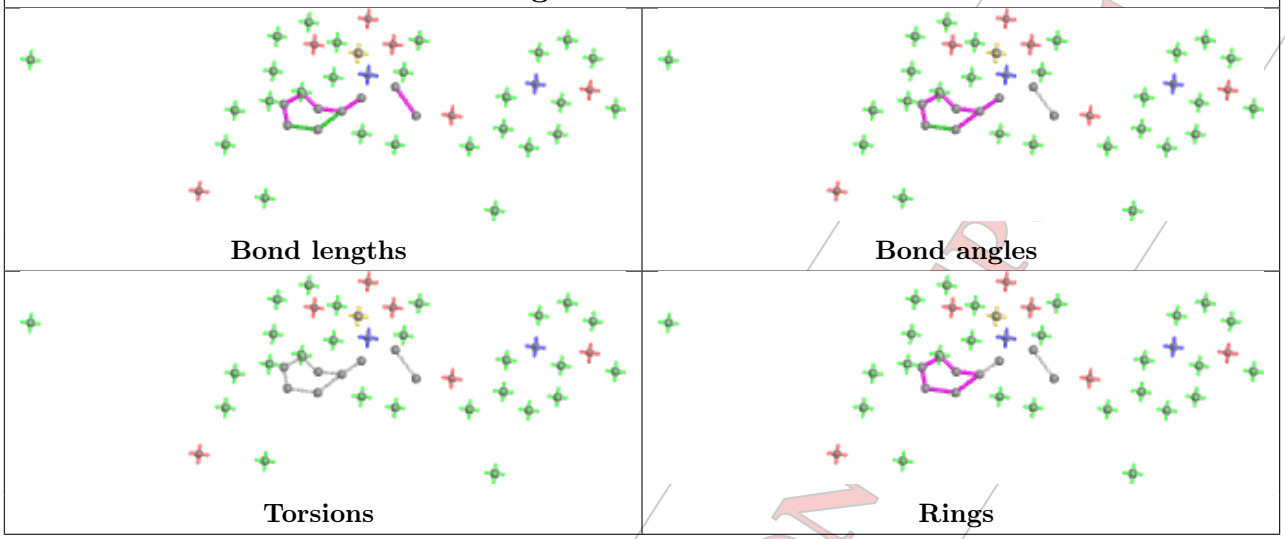
There are no torsion outliers.

There are no ring outliers.

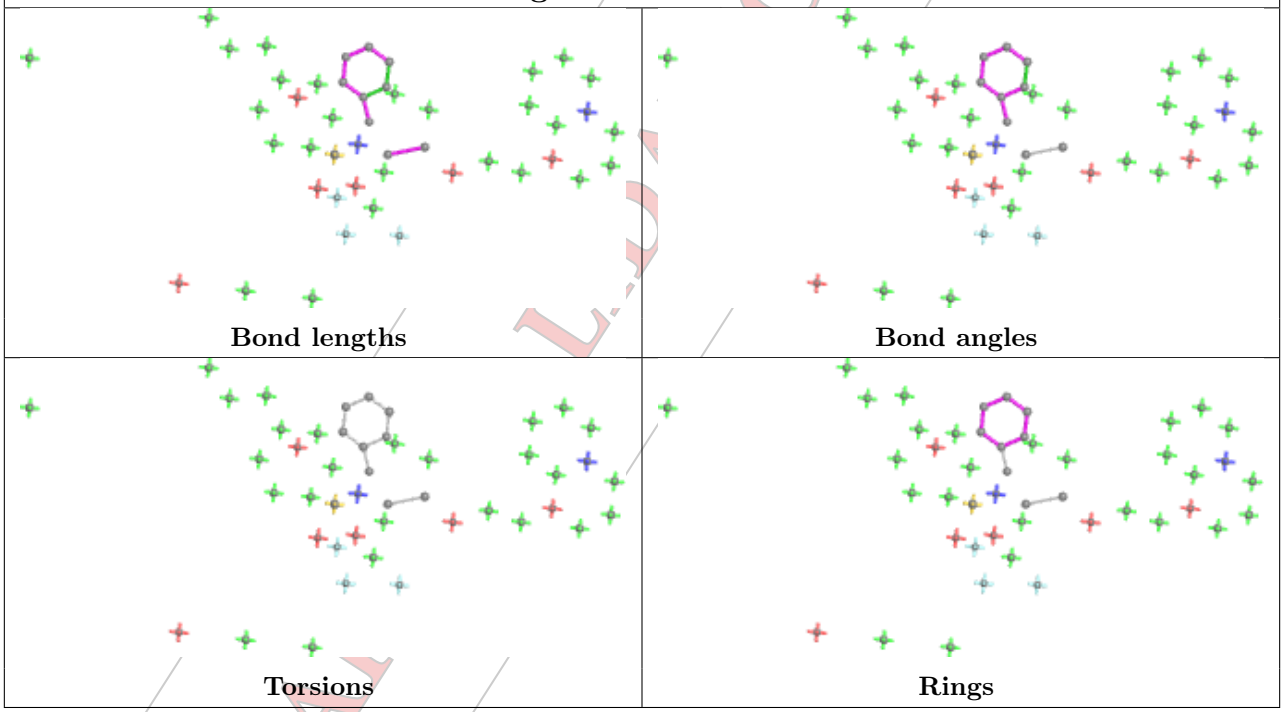
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

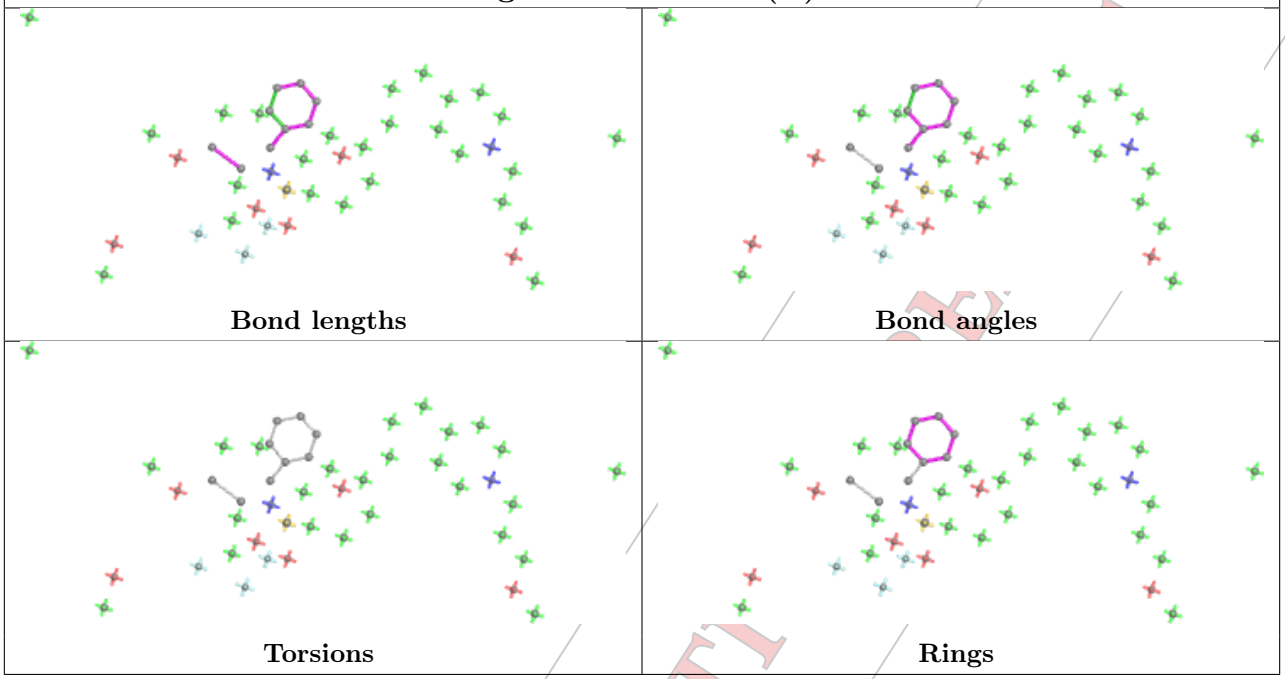
Ligand LIG C 601



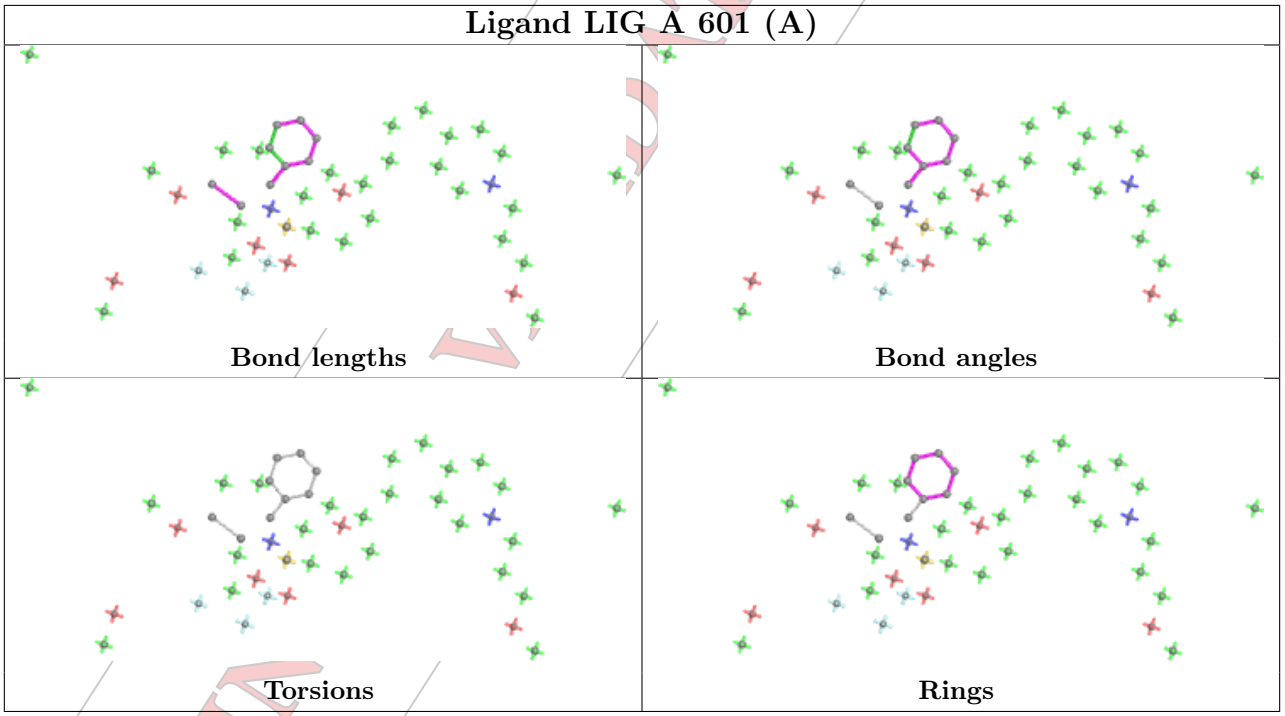
Ligand LIG D 601



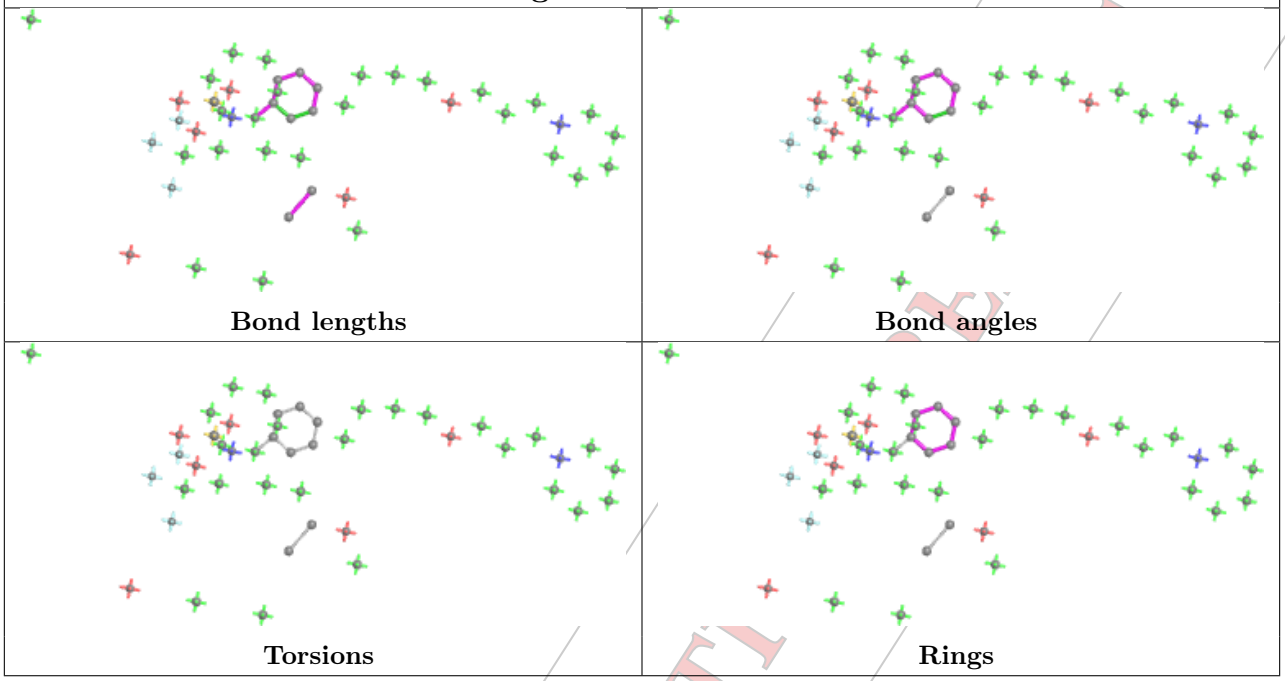
Ligand LIG A 601 (B)



Ligand LIG A 601 (A)



Ligand LIG B 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	233/257 (90%)	0.40	13 (5%)	24	26	18, 39, 82, 132	0
1	B	228/257 (88%)	0.25	11 (4%)	30	32	18, 33, 81, 106	0
1	C	228/257 (88%)	0.28	13 (5%)	23	25	17, 34, 68, 101	0
1	D	217/257 (84%)	0.26	12 (5%)	25	27	18, 33, 82, 118	0
All	All	906/1028 (88%)	0.30	49 (5%)	25	28	17, 35, 79, 132	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLU	10.5
1	A	418	VAL	8.6
1	C	462	LEU	4.3
1	B	331	TYR	4.3
1	A	463	SER	4.0
1	A	526	TYR	3.9
1	A	464	SER	3.8
1	D	332	ASP	3.7
1	A	306	LEU	3.6
1	D	413	ASN	3.5
1	B	415	GLY	3.2
1	C	537	TYR	3.1
1	D	546	ALA	3.1
1	A	334	THR	3.1
1	D	461	PHE	3.1
1	C	524	HIS	3.1
1	B	526	TYR	3.0
1	D	459	TYR	2.9
1	D	306	LEU	2.9
1	D	526	TYR	2.9
1	A	544	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	533	VAL	2.8
1	D	467	LYS	2.8
1	B	413	ASN	2.7
1	B	524	HIS	2.7
1	A	415	GLY	2.6
1	B	341	SER	2.6
1	C	413	ASN	2.6
1	B	335	ARG	2.6
1	B	462	LEU	2.5
1	D	524	HIS	2.5
1	C	464	SER	2.4
1	B	546	ALA	2.4
1	C	542	GLU	2.4
1	A	538	ASP	2.3
1	C	544	LEU	2.3
1	C	306	LEU	2.2
1	A	332	ASP	2.2
1	D	414	GLN	2.2
1	C	533	VAL	2.1
1	C	332	ASP	2.1
1	A	524	HIS	2.1
1	D	331	TYR	2.1
1	C	461	PHE	2.1
1	C	334	THR	2.1
1	D	342	MET	2.1
1	C	422	VAL	2.0
1	A	542	GLU	2.0
1	B	421	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

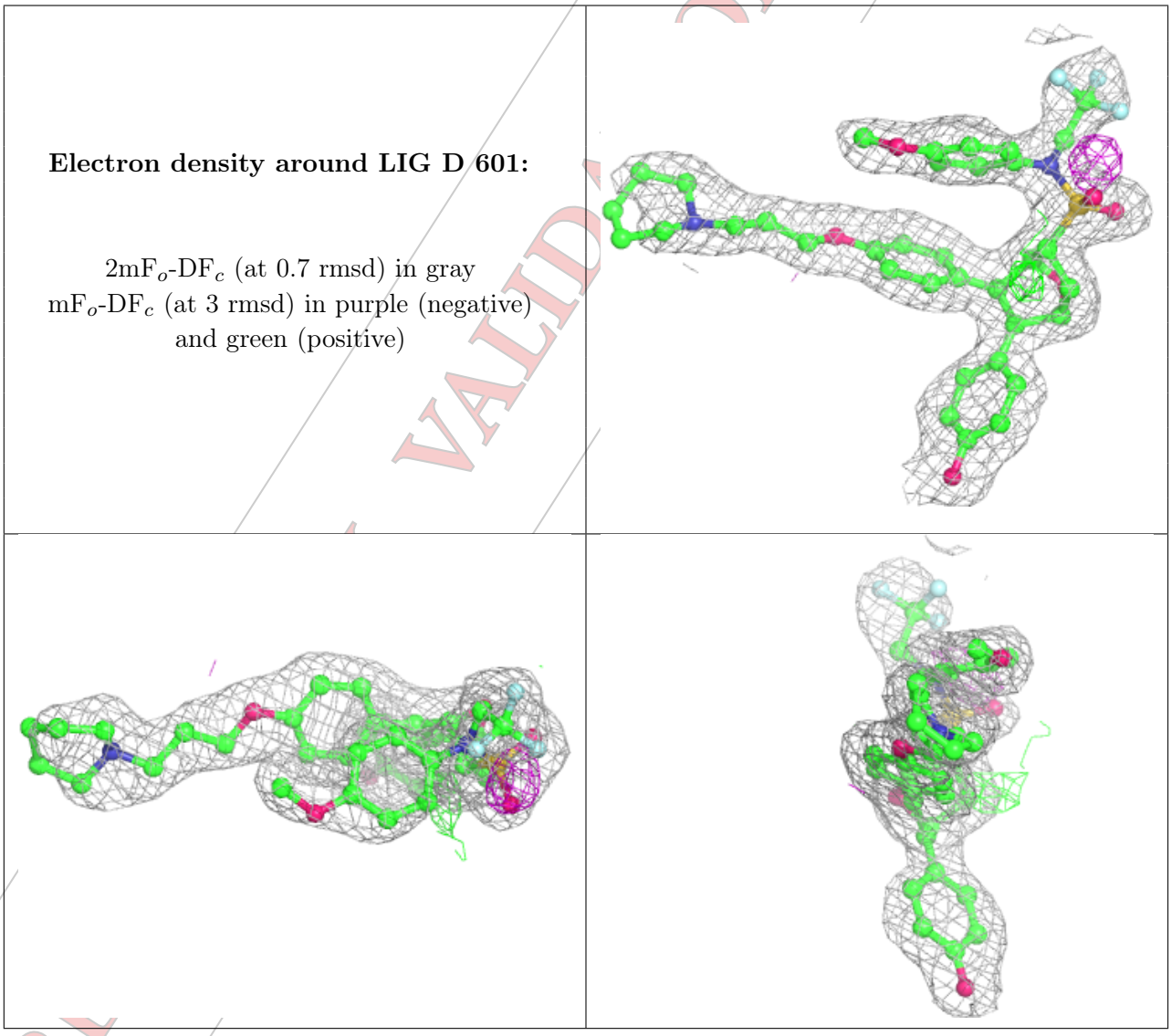
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	D	601	47/?	0.92	0.13	21,40,78,108	0
2	LIG	A	601[B]	47/?	0.92	0.17	16,28,44,62	47
2	LIG	A	601[A]	47/?	0.92	0.17	22,35,62,79	47
2	LIG	B	601	47/?	0.92	0.14	21,36,74,86	0
2	LIG	C	601	44/?	0.94	0.13	17,34,71,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

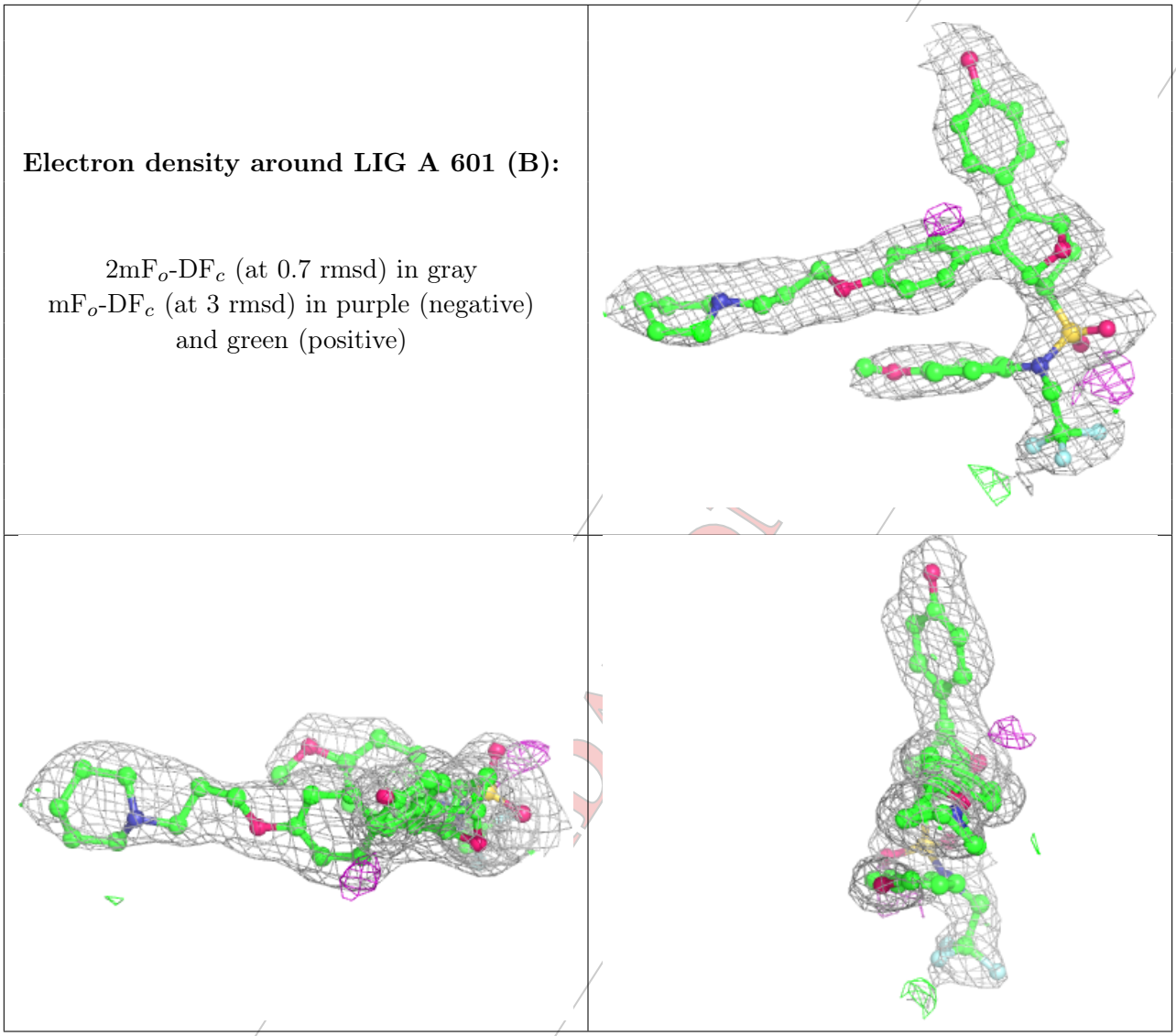
Electron density around LIG D 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



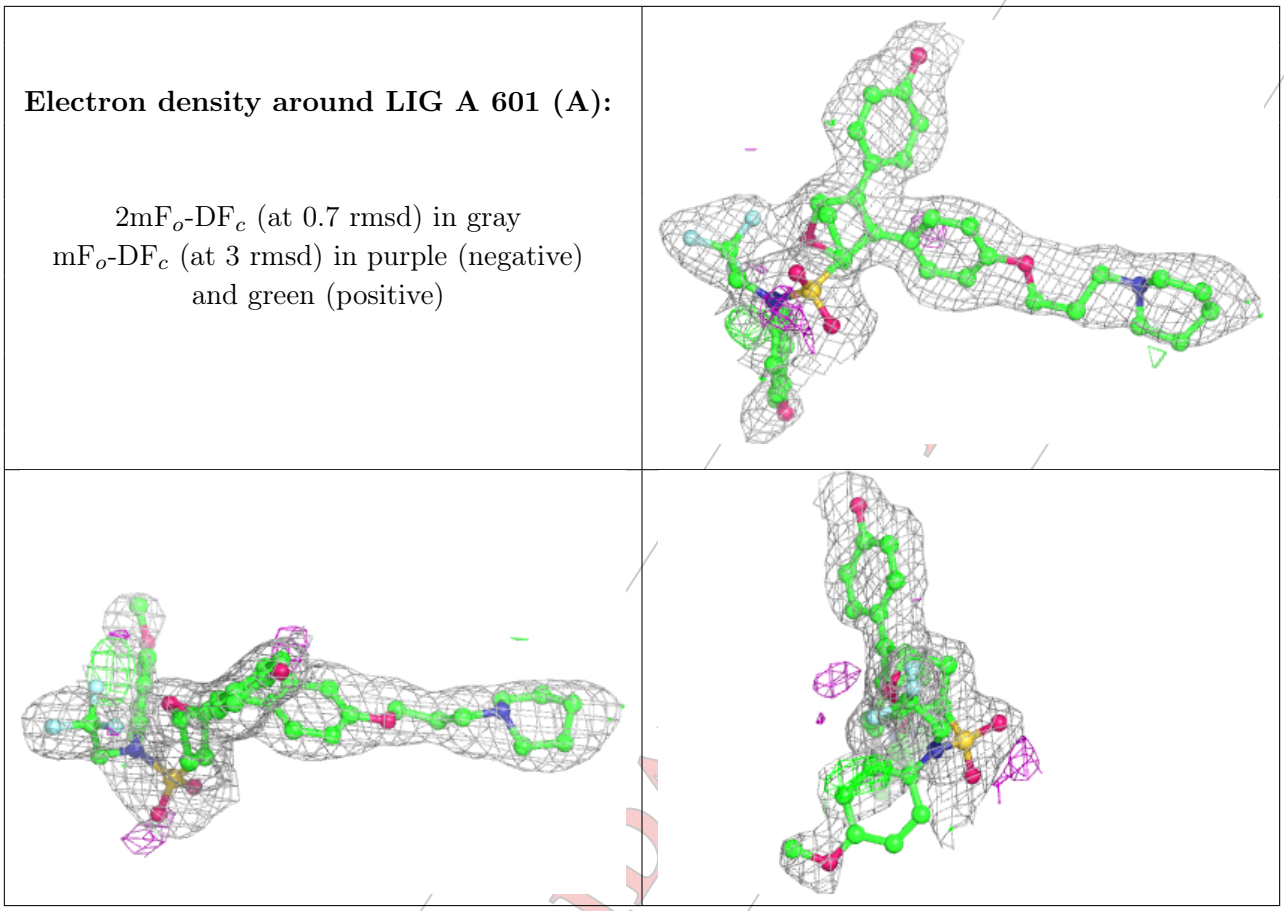
Electron density around LIG A 601 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



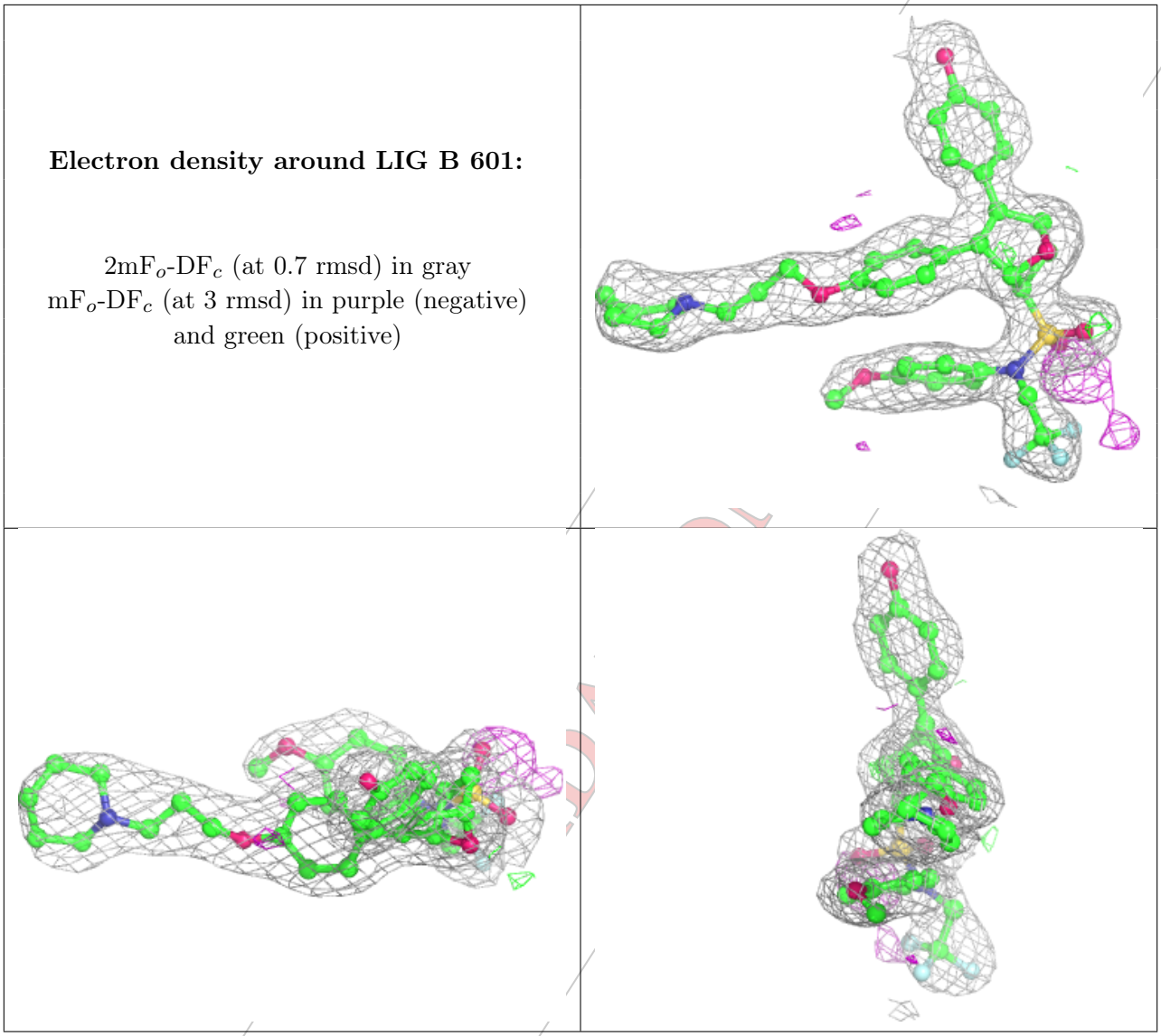
Electron density around LIG A 601 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



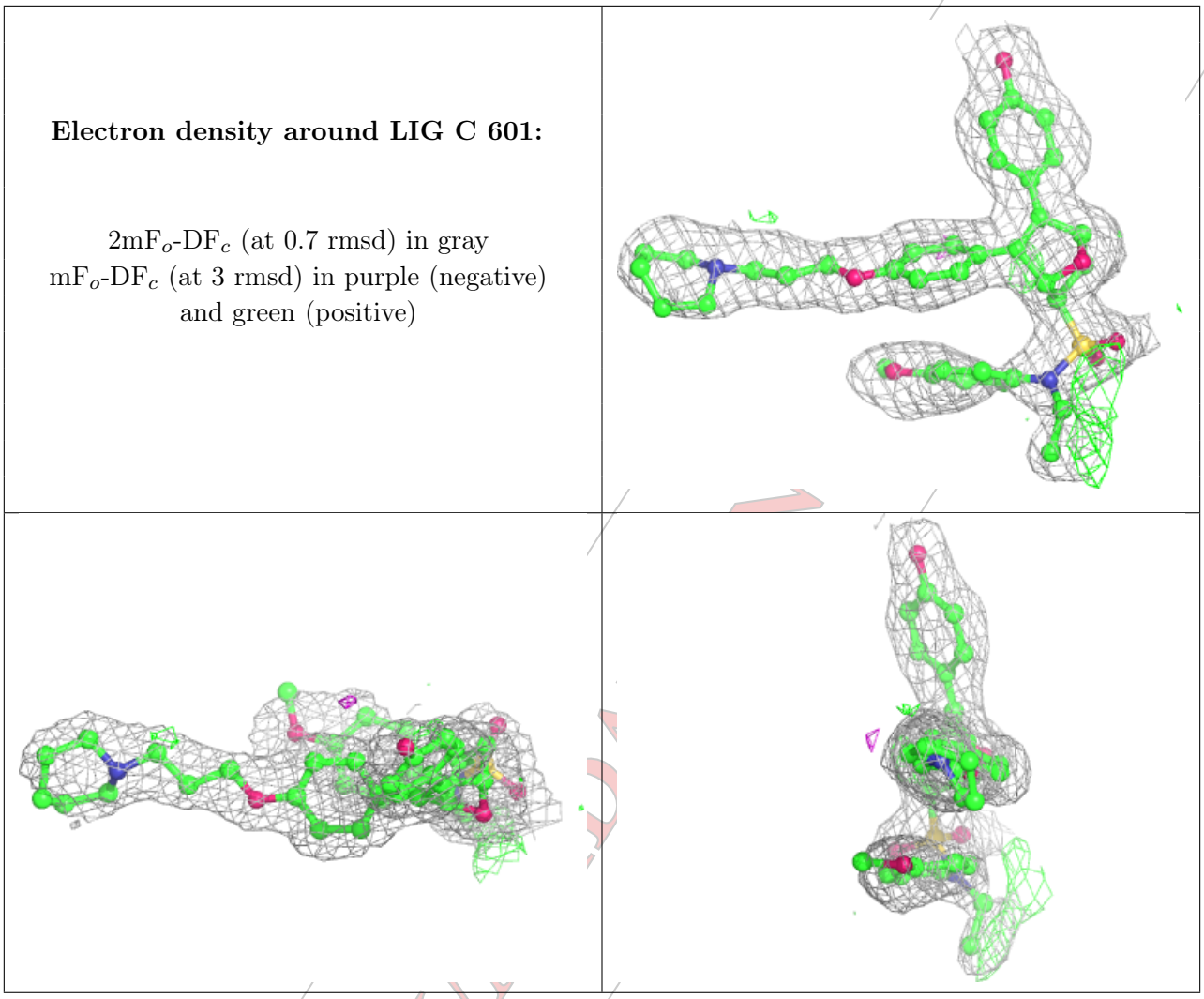
Electron density around LIG B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 09:51 PM EDT

Deposition ID : D_1000251196

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

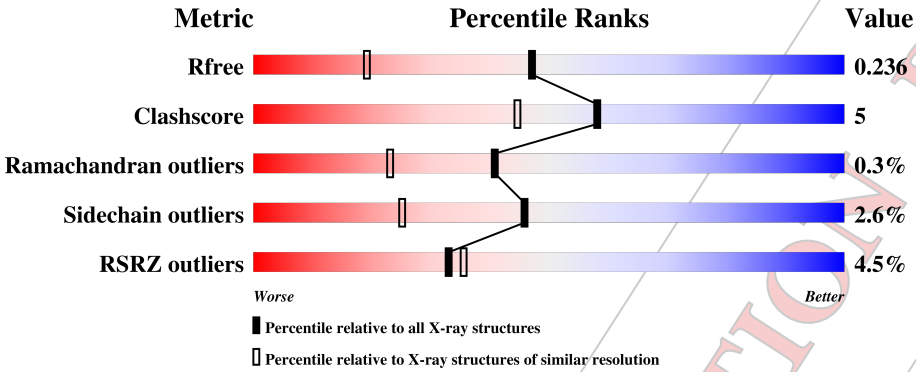
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	7% 81% 11% • 6%
1	B	257	2% 77% 9% 14%
1	C	257	5% 84% 7% • 8%
1	D	257	2% 77% 5% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LIG	A	601	-	-	X	-
2	LIG	B	601	-	-	X	-
2	LIG	C	601	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7689 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1937	1237	327	354	19			
1	B	221	Total	C	N	O	S	0	0	0
			1755	1123	299	316	17			
1	C	236	Total	C	N	O	S	0	1	0
			1890	1208	318	347	17			
1	D	210	Total	C	N	O	S	0	0	0
			1678	1076	286	301	15			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	S		0	0
			26	19	1	5	1			
2	B	1	Total	C	F	N	O	S	0	0
			34	24	3	1	5	1		
2	C	1	Total	C	N	O	S		0	0
			28	21	1	5	1			
2	D	1	Total	C	F	N	O	S	0	0
			33	23	3	1	5	1		

- Molecule 3 is water.

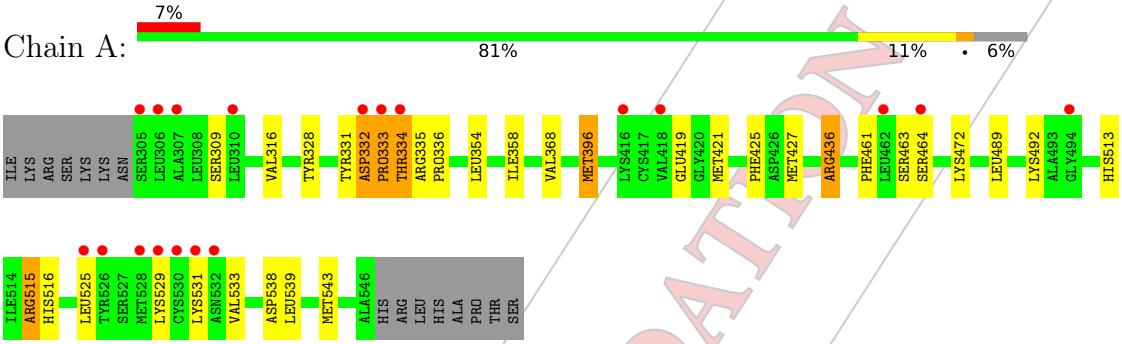
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	308	Total	O	0	0
			308	308		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

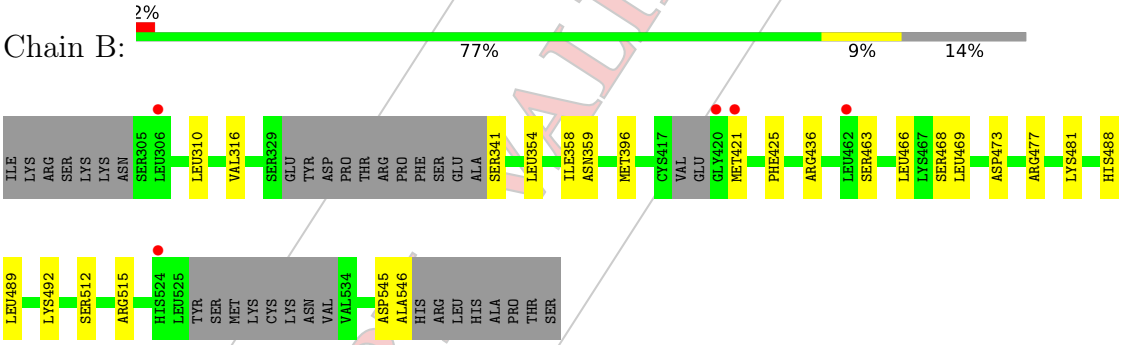
• Molecule 1: Estrogen Receptor

Chain A:



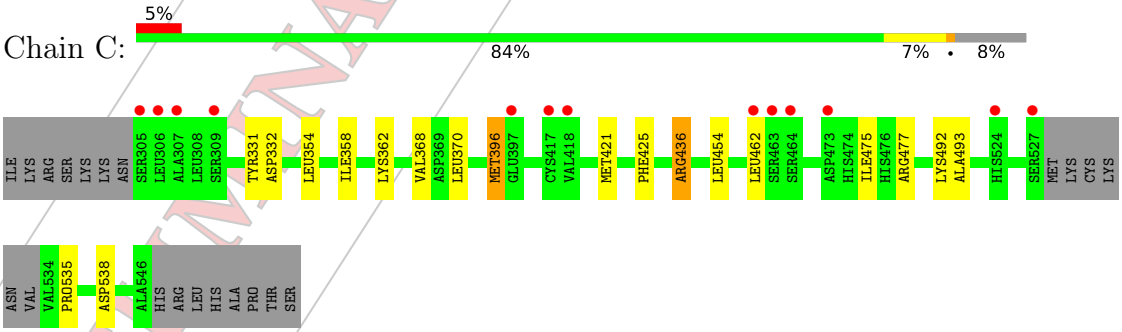
• Molecule 1: Estrogen Receptor

Chain B:



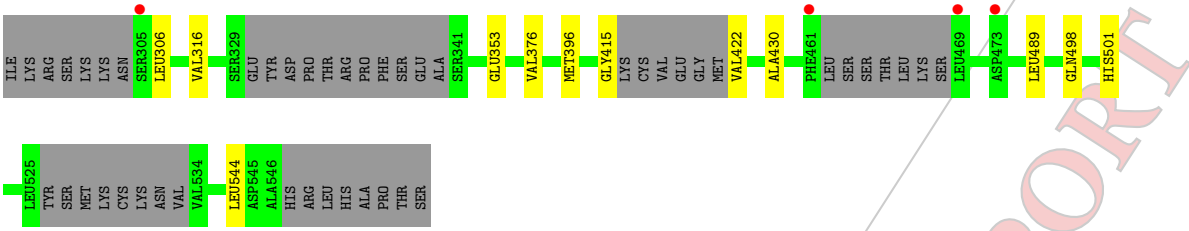
• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.27Å 58.80Å 92.67Å 79.95° 75.46° 63.10°	Depositor
Resolution (Å)	89.48 – 1.67 89.48 – 1.67	Depositor EDS
% Data completeness (in resolution range)	57.1 (89.48-1.67) 57.1 (89.48-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.227 0.202 , 0.236	Depositor DCC
R_{free} test set	3158 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.084 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7689	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	0/1962	0.64	1/2649 (0.0%)
1	B	0.44	0/1772	0.66	1/2387 (0.0%)
1	C	0.47	0/1914	0.66	1/2585 (0.0%)
1	D	0.48	0/1694	0.65	0/2283
All	All	0.46	0/7342	0.65	3/9904 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	436	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	436	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	436	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	TYR	Peptide
1	A	333	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1937	0	1977	22	1
1	B	1755	0	1807	14	1
1	C	1890	0	1921	13	0
1	D	1678	0	1719	8	0
2	A	26	0	0	6	0
2	B	34	0	0	7	0
2	C	28	0	0	6	0
2	D	33	0	0	5	0
3	S	308	0	0	7	0
All	All	7689	0	7424	71	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:LIG:C01	2:C:601:LIG:C05	1.75	1.42
2:B:601:LIG:C05	2:B:601:LIG:C01	1.75	1.41
2:A:601:LIG:C01	2:A:601:LIG:C05	1.75	1.38
2:C:601:LIG:S42	2:C:601:LIG:C03	2.11	1.38
2:D:601:LIG:C05	2:D:601:LIG:C01	1.75	1.37
2:D:601:LIG:S42	2:D:601:LIG:C03	2.12	1.36
2:B:601:LIG:S42	2:B:601:LIG:C03	2.12	1.36
2:A:601:LIG:C03	2:A:601:LIG:S42	2.12	1.35
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.57	0.84
1:A:515:ARG:NH1	1:B:512:SER:OG	2.15	0.80
1:B:473:ASP:OD2	1:B:477:ARG:NH1	2.17	0.78
2:A:601:LIG:C02	2:A:601:LIG:S42	2.75	0.74
2:D:601:LIG:S42	2:D:601:LIG:C04	2.75	0.74
1:B:546:ALA:O	3:S:34:HOH:O	2.08	0.71
2:B:601:LIG:S42	2:B:601:LIG:C04	2.77	0.70
2:C:601:LIG:S42	2:C:601:LIG:C02	2.80	0.68
1:A:533:VAL:HG12	2:A:601:LIG:O21	1.93	0.68
2:C:601:LIG:S42	2:C:601:LIG:C04	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PRO:O	1:A:335:ARG:HG3	1.96	0.64
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.81	0.62
1:B:488:HIS:NE2	1:B:492:LYS:HD2	2.16	0.61
2:A:601:LIG:S42	2:A:601:LIG:C04	2.84	0.60
1:A:332:ASP:O	3:S:242:HOH:O	2.17	0.60
1:A:515:ARG:NE	3:S:238:HOH:O	2.33	0.59
2:B:601:LIG:C02	2:B:601:LIG:S42	2.88	0.58
1:D:415:GLY:C	1:D:422:VAL:HG22	2.24	0.58
1:B:310:LEU:O	1:B:481:LYS:CE	2.54	0.56
1:B:477:ARG:NH2	3:S:97:HOH:O	2.28	0.55
1:A:461:PHE:HB2	1:A:472:LYS:HE3	1.90	0.53
2:C:601:LIG:C08	2:C:601:LIG:C01	2.76	0.53
1:C:462:LEU:CD2	1:D:430:ALA:HB2	2.39	0.53
2:D:601:LIG:S42	2:D:601:LIG:C02	2.90	0.53
1:A:427:MET:CE	1:A:516:HIS:HD2	2.22	0.53
1:C:462:LEU:HD21	1:D:430:ALA:HB2	1.91	0.53
1:B:463:SER:HB3	1:B:468:SER:OG	2.10	0.51
1:A:539:LEU:HG	1:A:543:MET:CE	2.41	0.50
1:A:427:MET:HE1	1:A:516:HIS:CD2	2.48	0.49
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.95	0.48
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.94	0.48
1:C:396:MET:O	1:C:436:ARG:HD3	2.13	0.48
1:C:454:LEU:HD22	1:C:475:ILE:HD12	1.96	0.47
1:A:396:MET:O	1:A:436:ARG:HD3	2.15	0.47
1:B:354:LEU:O	1:B:358:ILE:HD13	2.16	0.46
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.45	0.46
1:A:515:ARG:NH2	3:S:238:HOH:O	2.49	0.45
1:C:421:MET:SD	2:C:601:LIG:N22	2.89	0.45
1:B:469:LEU:HD13	1:C:493:ALA:O	2.16	0.45
1:B:310:LEU:O	1:B:481:LYS:HE3	2.17	0.45
1:A:525:LEU:HD23	1:A:525:LEU:C	2.37	0.44
1:C:362:LYS:HD2	1:C:368:VAL:HG12	1.99	0.44
1:A:427:MET:HE2	1:A:513:HIS:CE1	2.52	0.44
1:A:354:LEU:O	1:A:358:ILE:HD13	2.17	0.44
1:C:331:TYR:CE2	1:C:332:ASP:HB2	2.53	0.43
1:D:353:GLU:OE1	2:D:601:LIG:O20	2.37	0.43
1:A:539:LEU:HG	1:A:543:MET:HE1	1.99	0.43
1:C:492:LYS:HE2	1:C:492:LYS:HB3	1.85	0.43
1:A:427:MET:CE	1:A:516:HIS:CD2	3.01	0.43
1:A:427:MET:HE1	1:A:516:HIS:HD2	1.83	0.43
1:A:334:THR:O	1:A:334:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:MET:HG3	2:B:601:LIG:C24	2.50	0.42
1:C:354:LEU:O	1:C:358:ILE:HD13	2.19	0.42
1:A:421:MET:SD	2:A:601:LIG:N22	2.93	0.42
1:A:368:VAL:HG22	3:S:75:HOH:O	2.20	0.41
2:B:601:LIG:C08	2:B:601:LIG:C01	2.81	0.41
1:B:421:MET:HG3	2:B:601:LIG:F47	2.11	0.41
1:C:370:LEU:CD1	1:C:475:ILE:HD11	2.40	0.41
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.56	0.40
1:B:341:SER:N	3:S:278:HOH:O	2.54	0.40
1:C:354:LEU:HD21	1:C:535:PRO:HB3	2.04	0.40
1:A:316:VAL:HG21	1:A:489:LEU:HD21	2.03	0.40
1:A:335:ARG:HA	1:A:336:PRO:C	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:OH	1:B:359:ASN:ND2[1_545]	1.84	0.36

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	240/257 (93%)	233 (97%)	4 (2%)	3 (1%)	12 2
1	B	212/257 (82%)	210 (99%)	2 (1%)	0	100 100
1	C	232/257 (90%)	230 (99%)	2 (1%)	0	100 100
1	D	199/257 (77%)	198 (100%)	1 (0%)	0	100 100
All	All	883/1028 (86%)	871 (99%)	9 (1%)	3 (0%)	41 23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	SER
1	A	529	LYS
1	A	332	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/232 (94%)	208 (95%)	10 (5%)	27	9
1	B	197/232 (85%)	192 (98%)	5 (2%)	47	26
1	C	212/232 (91%)	208 (98%)	4 (2%)	57	38
1	D	187/232 (81%)	185 (99%)	2 (1%)	73	61
All	All	814/928 (88%)	793 (97%)	21 (3%)	46	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	SER
1	A	334	THR
1	A	396	MET
1	A	419	GLU
1	A	425	PHE
1	A	464	SER
1	A	492	LYS
1	A	515	ARG
1	A	531	LYS
1	A	538	ASP
1	B	396	MET
1	B	425	PHE
1	B	466	LEU
1	B	515	ARG
1	B	545	ASP
1	C	396	MET
1	C	425	PHE
1	C	477	ARG
1	C	538	ASP

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Mol	Chain	Res	Type
1	D	306	LEU
1	D	396	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	502	GLN
1	A	513	HIS
1	A	516	HIS
1	B	413	ASN
1	B	513	HIS
1	B	524	HIS
1	C	413	ASN
1	C	513	HIS
1	C	519	ASN
1	D	513	HIS
1	D	519	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

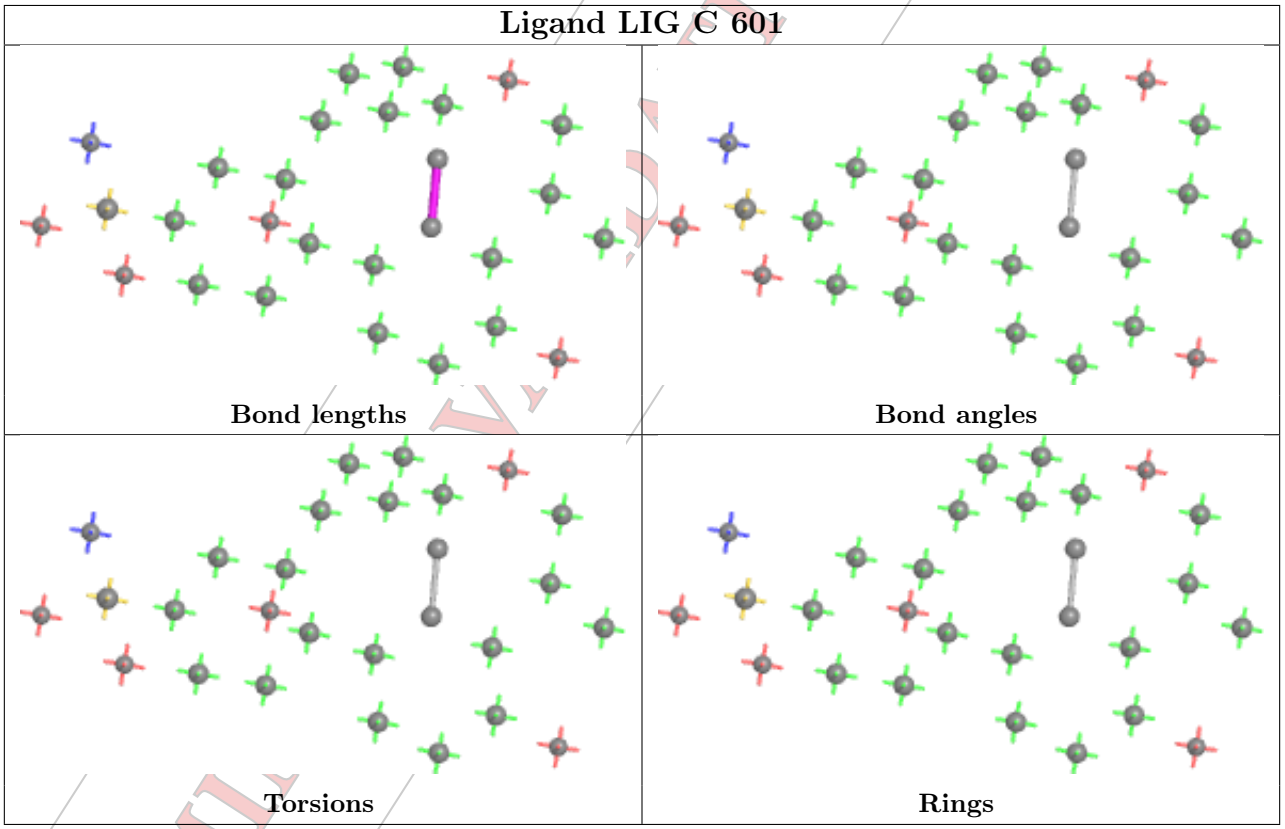
There are no torsion outliers.

There are no ring outliers.

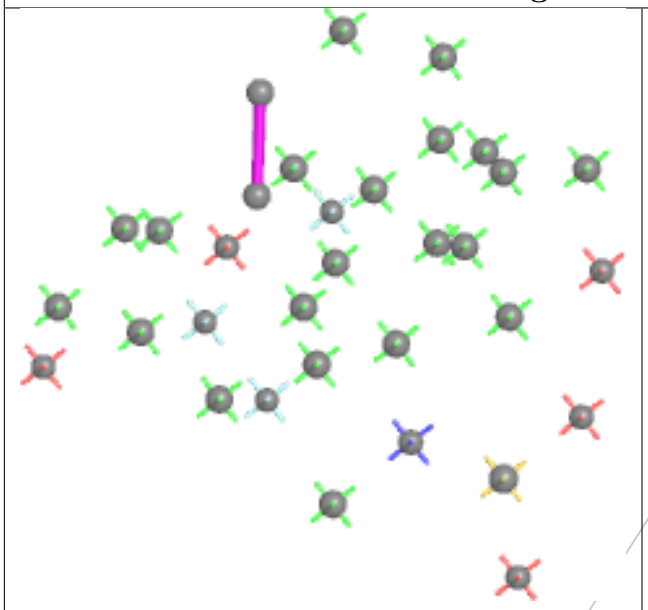
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

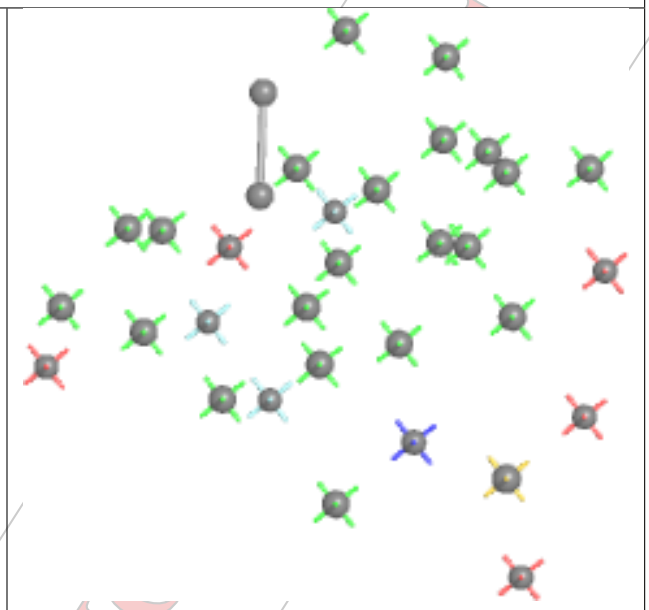
Ligand LIG C 601



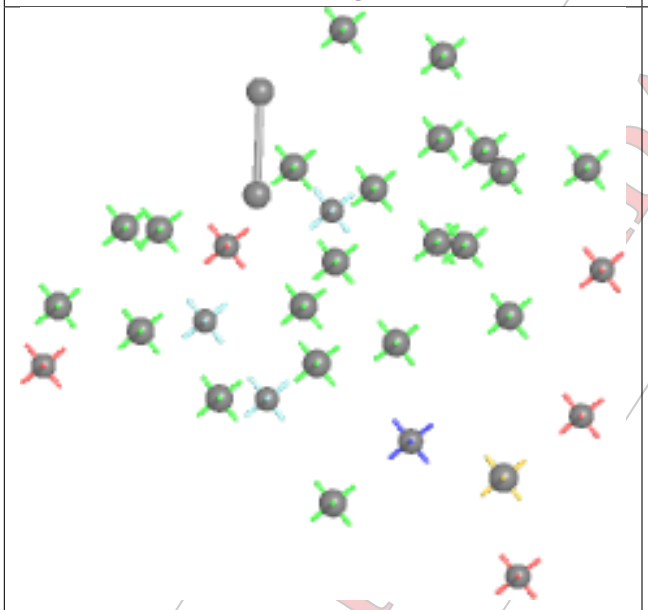
Ligand LIG D 601



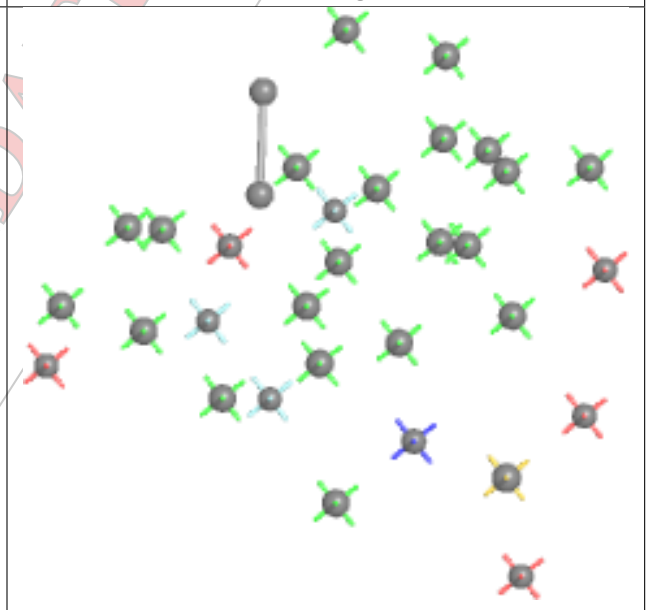
Bond lengths



Bond angles

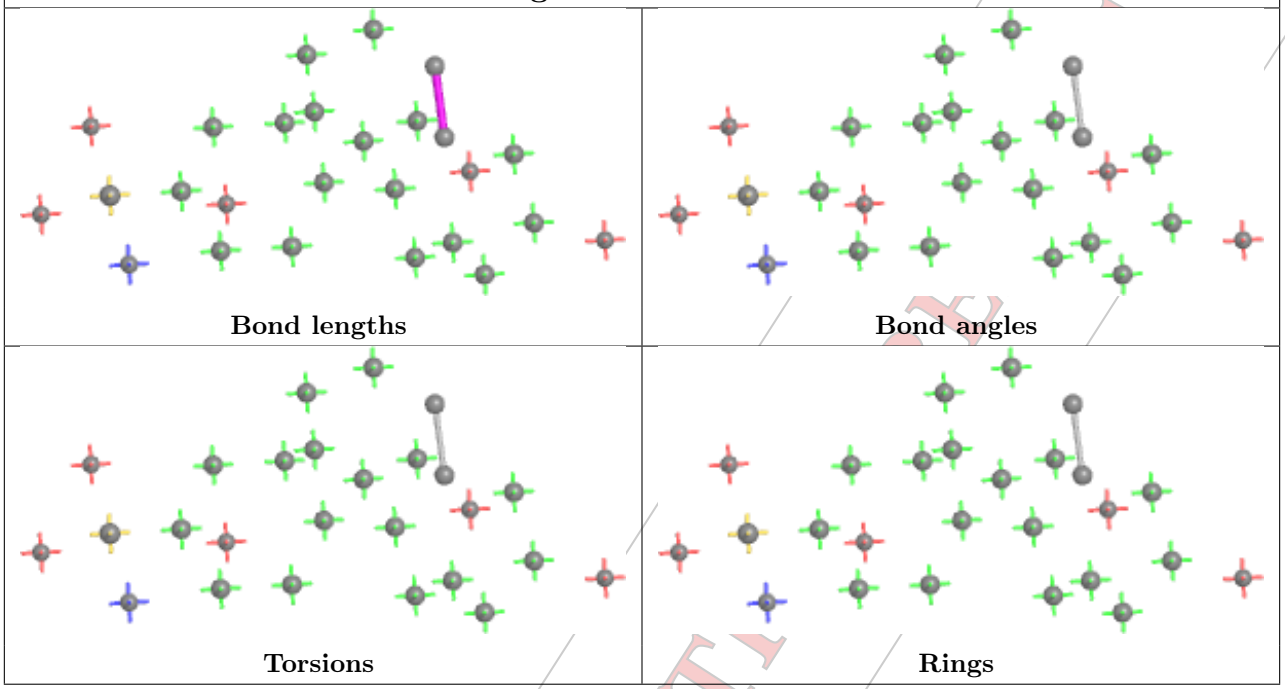


Torsions

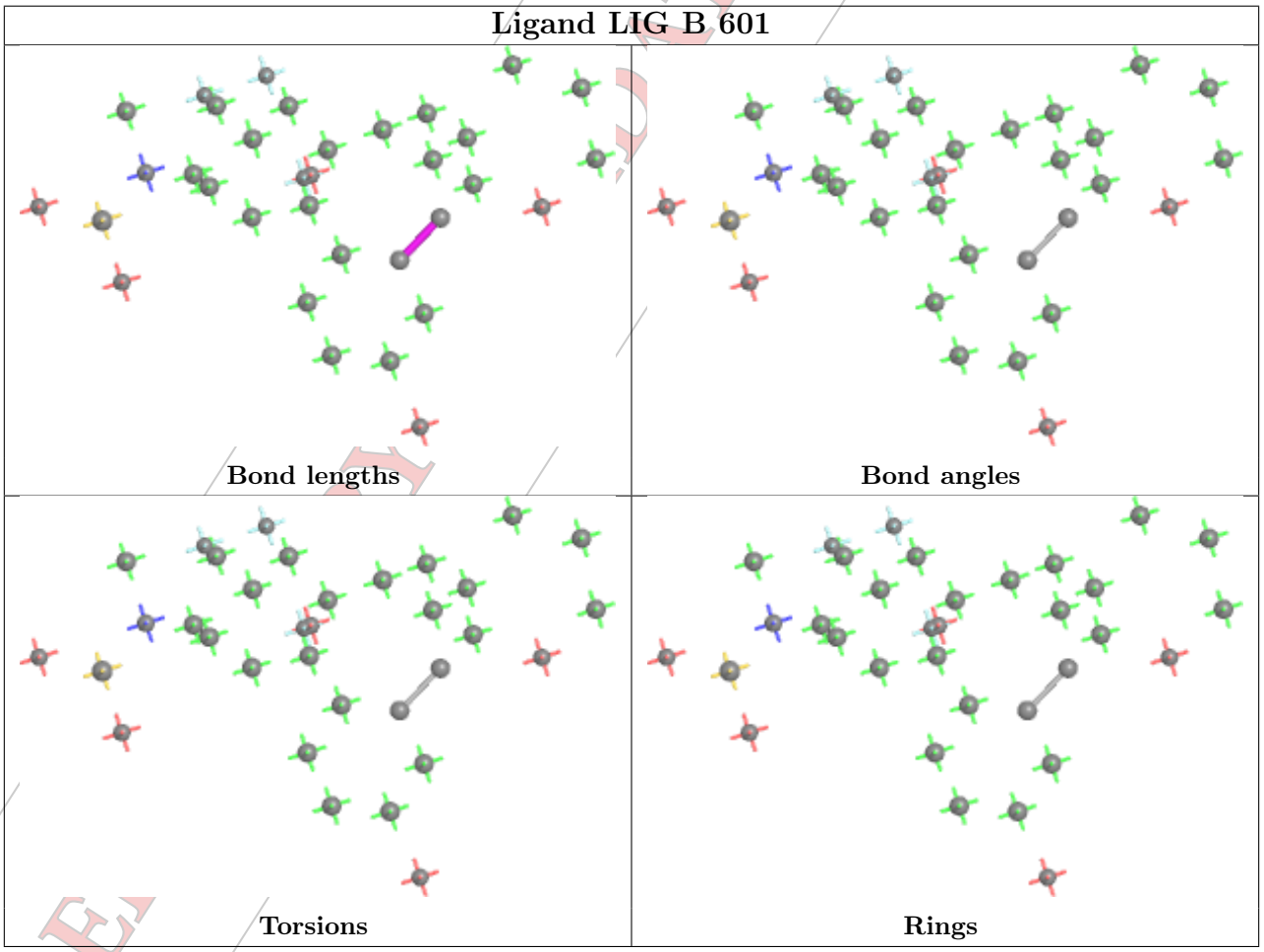


Rings

Ligand LIG A 601



Ligand LIG B 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	241/257 (93%)	0.53	19 (7%)	12	13	18, 42, 85, 131	0
1	B	220/257 (85%)	0.13	5 (2%)	60	64	18, 36, 78, 104	0
1	C	235/257 (91%)	0.37	13 (5%)	25	26	18, 36, 69, 106	0
1	D	209/257 (81%)	0.16	4 (1%)	66	70	19, 36, 75, 91	0
All	All	905/1028 (88%)	0.31	41 (4%)	33	35	18, 38, 78, 131	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	SER	8.9
1	C	305	SER	8.5
1	A	530	CYS	8.2
1	A	462	LEU	6.7
1	A	333	PRO	5.7
1	B	306	LEU	5.5
1	A	531	LYS	5.1
1	D	461	PHE	4.8
1	C	462	LEU	4.7
1	C	464	SER	4.6
1	C	527	SER	4.5
1	A	306	LEU	4.4
1	B	421	MET	4.2
1	D	469	LEU	4.2
1	A	334	THR	4.1
1	A	307	ALA	4.0
1	A	529	LYS	3.8
1	C	306	LEU	3.7
1	A	525	LEU	3.6
1	D	305	SER	3.4
1	A	332	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	309	SER	3.3
1	B	462	LEU	3.1
1	A	416	LYS	3.1
1	A	494	GLY	3.1
1	A	528	MET	3.0
1	C	524	HIS	2.9
1	A	464	SER	2.8
1	A	532	ASN	2.7
1	C	417	CYS	2.7
1	C	463	SER	2.6
1	B	420	GLY	2.5
1	A	418	VAL	2.4
1	C	307	ALA	2.3
1	D	473	ASP	2.3
1	C	418	VAL	2.2
1	B	524	HIS	2.1
1	A	310	LEU	2.1
1	C	397[A]	GLU	2.0
1	A	526	TYR	2.0
1	C	473	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	D	601	33/?	0.84	0.18	38,68,108,119	0
2	LIG	C	601	28/?	0.86	0.16	34,59,83,90	0
2	LIG	A	601	26/?	0.87	0.14	31,52,77,94	0

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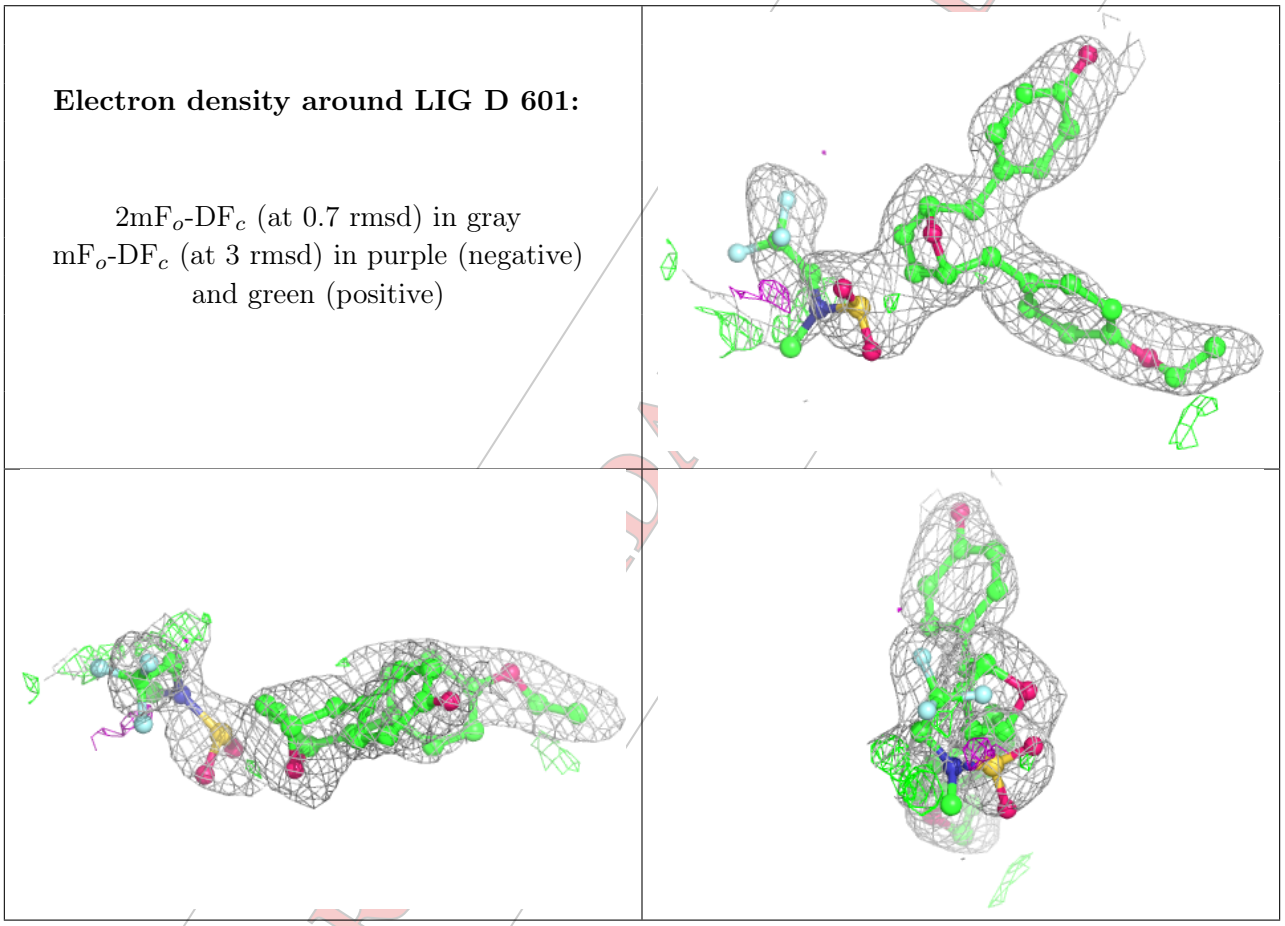
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	B	601	34/?	0.88	0.16	38,68,131,181	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

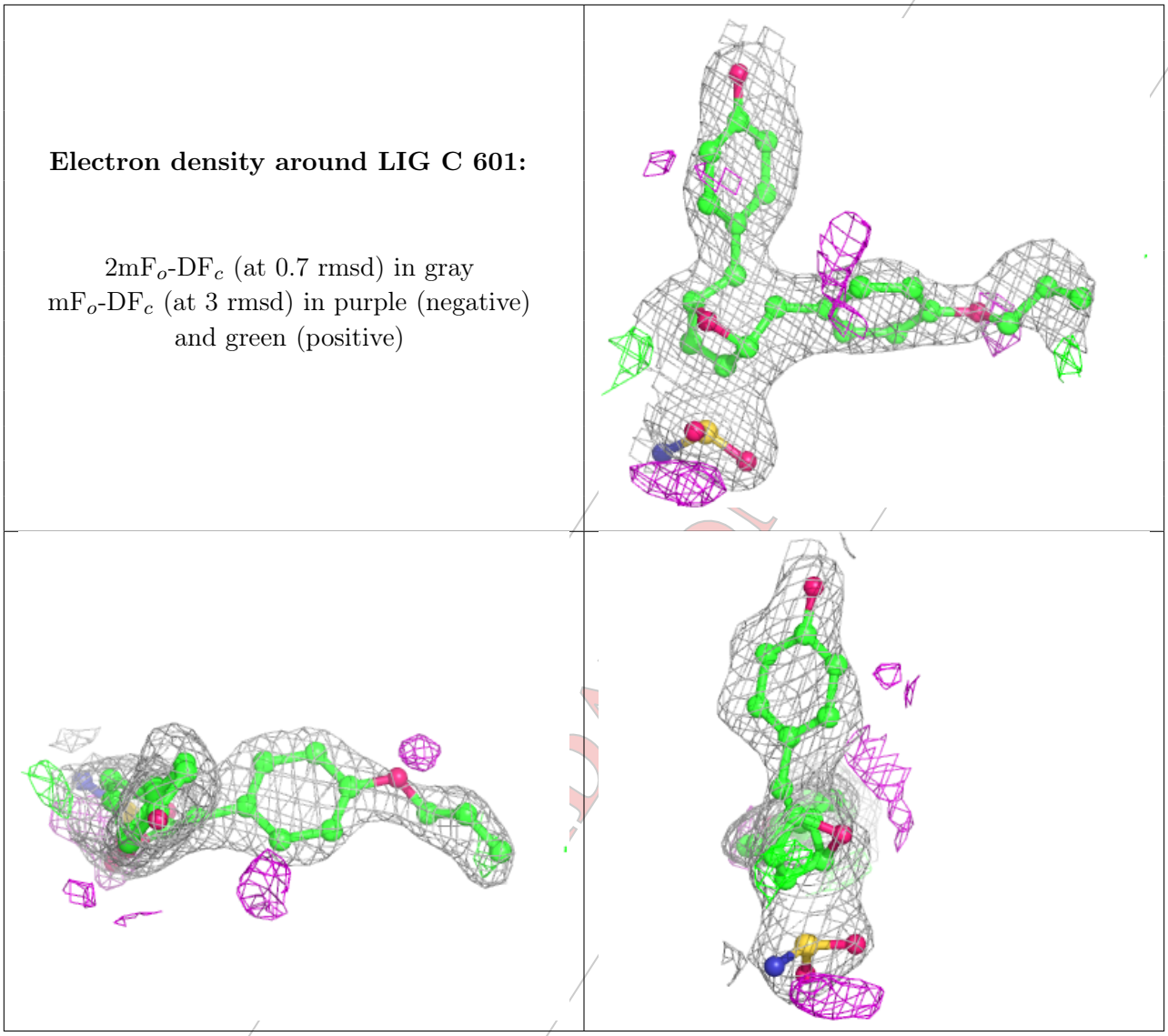
Electron density around LIG D 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



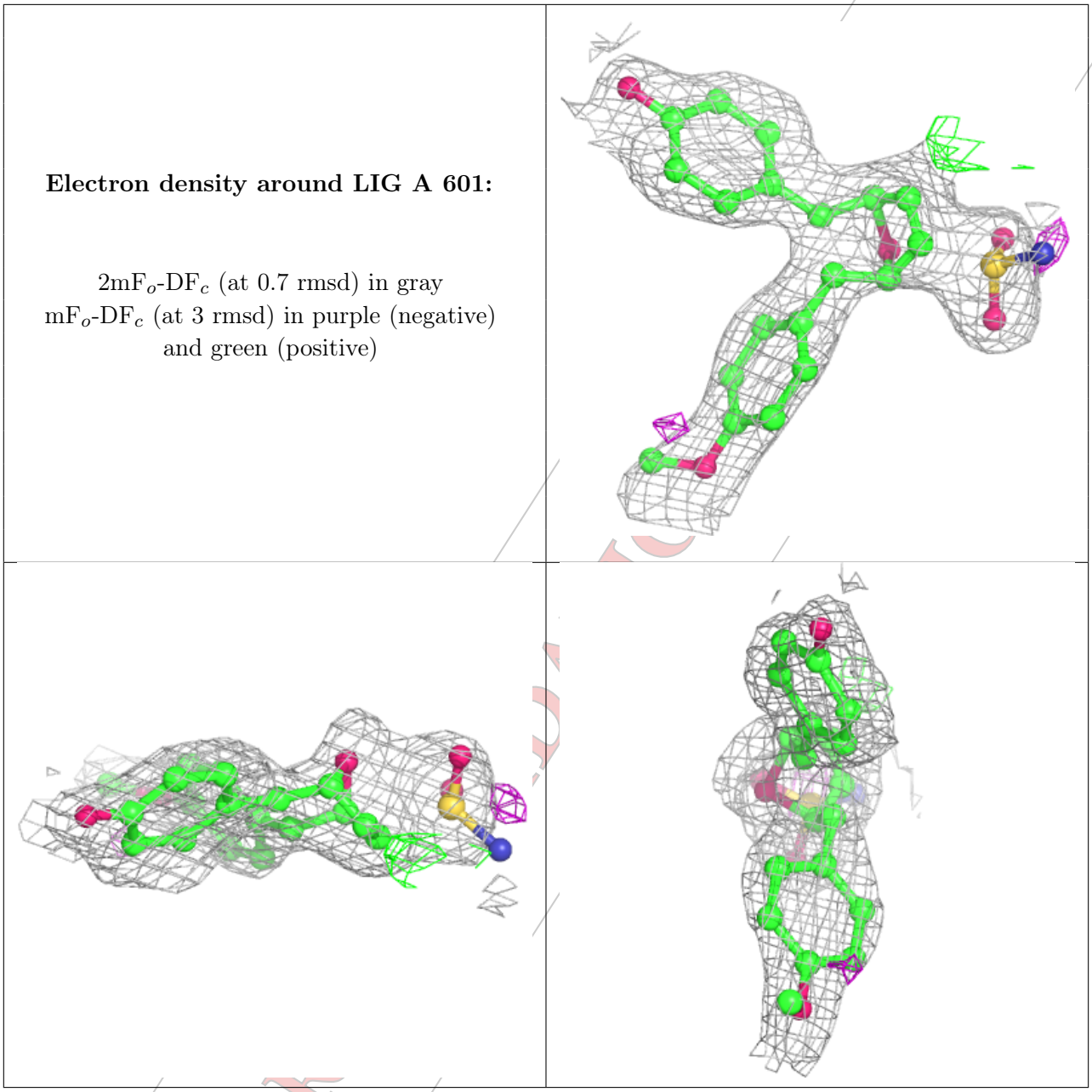
Electron density around LIG C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



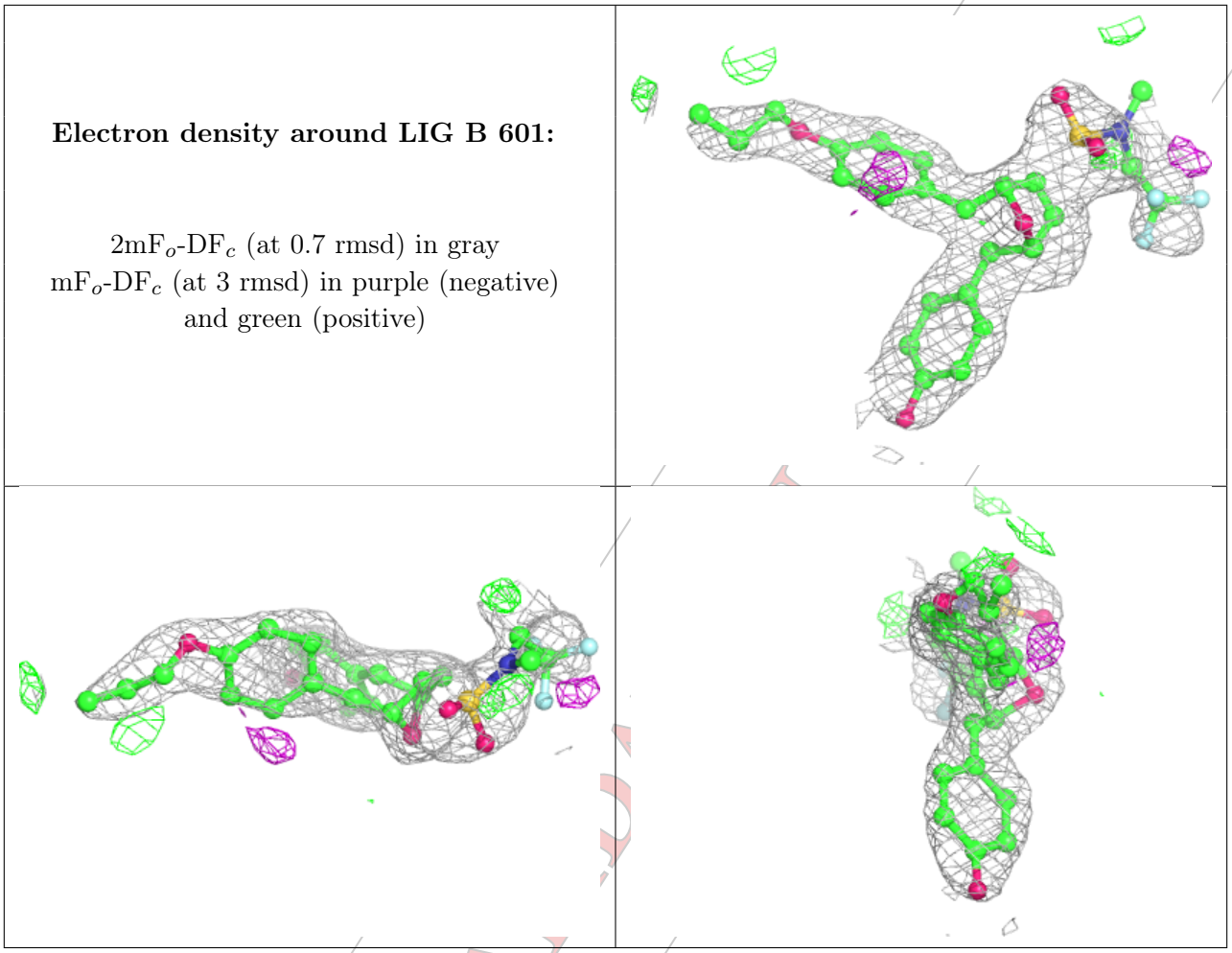
Electron density around LIG A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 10:10 PM EDT

Deposition ID : D_1000251218

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

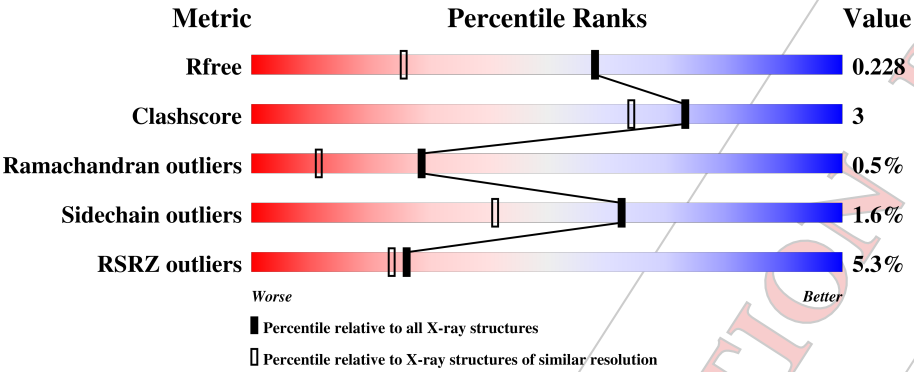
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	3% 82% 6% • 10%
1	B	257	4% 83% • 14%
1	C	257	7% 83% 7% • 9%
1	D	257	5% 85% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LIG	A	601	-	-	X	-
2	LIG	C	601	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7925 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1850	1183	313	337	17			
1	B	221	Total	C	N	O	S	0	0	0
			1765	1130	302	316	17			
1	C	233	Total	C	N	O	S	0	1	0
			1859	1186	315	341	17			
1	D	227	Total	C	N	O	S	0	0	0
			1809	1158	307	326	18			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			38	28	3	1	5	1		
2	B	1	Total	C	F	N	O	S	0	0
			42	30	3	1	7	1		
2	C	1	Total	C	F	N	O	S	0	0
			38	28	3	1	5	1		
2	D	1	Total	C	F	N	O	S	0	0
			42	30	3	1	7	1		

- Molecule 3 is water.

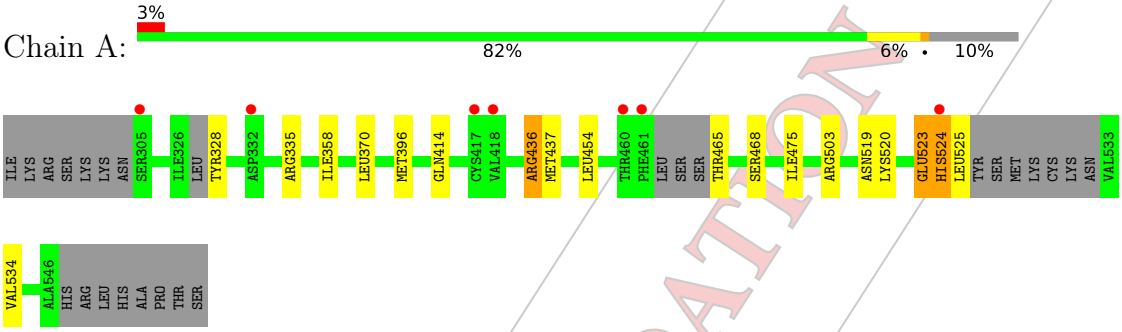
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	482	Total	O	0	0
			482	482		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

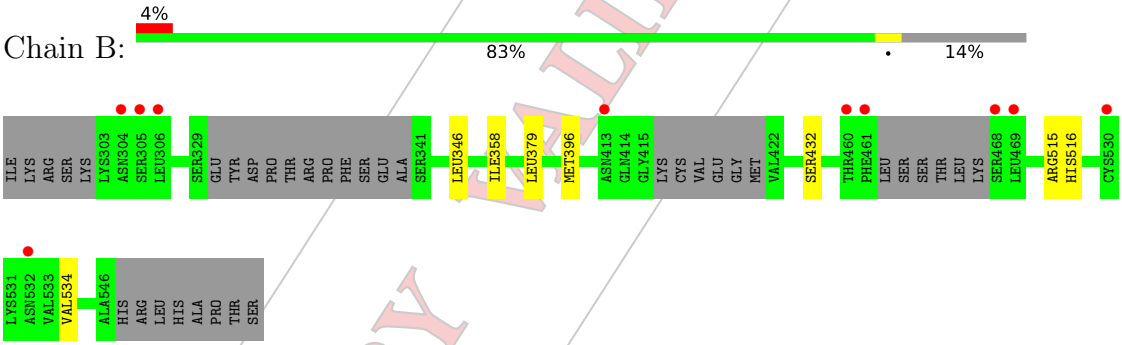
• Molecule 1: Estrogen Receptor

Chain A:



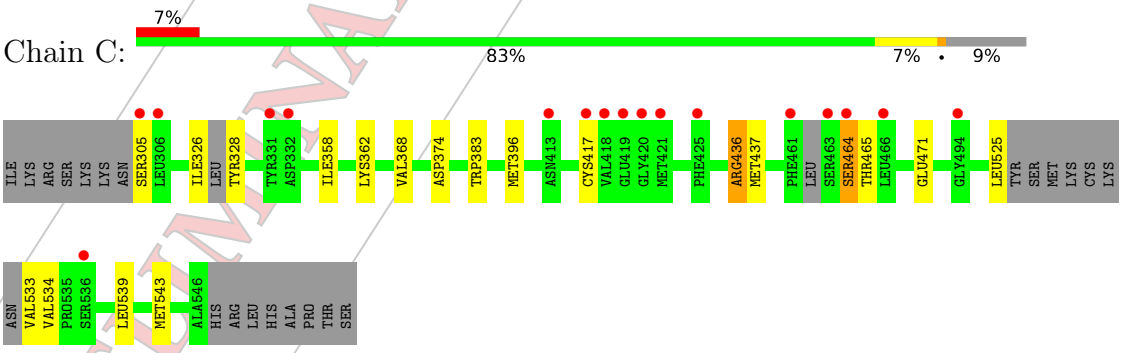
• Molecule 1: Estrogen Receptor

Chain B:



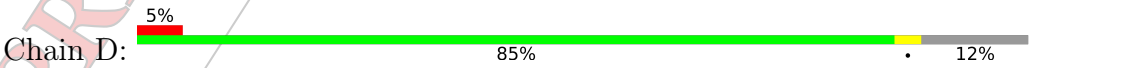
• Molecule 1: Estrogen Receptor

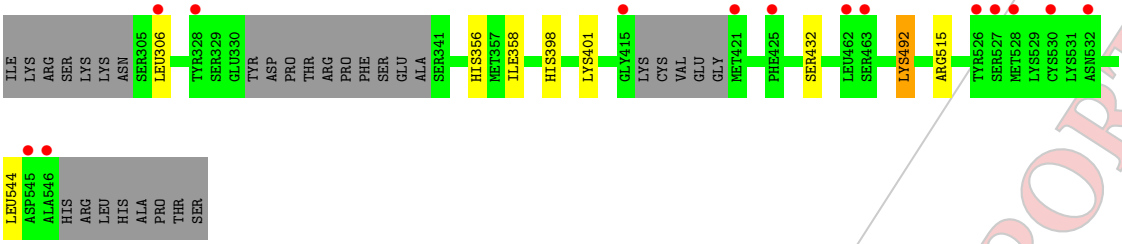
Chain C:



• Molecule 1: Estrogen Receptor

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.58Å 58.77Å 93.15Å 86.71° 75.09° 62.87°	Depositor
Resolution (Å)	89.80 – 1.59 89.80 – 1.59	Depositor EDS
% Data completeness (in resolution range)	71.0 (89.80-1.59) 71.0 (89.80-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.186 , 0.219 0.197 , 0.228	Depositor DCC
R_{free} test set	4613 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.079 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7925	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.69	0/1871	0.76	2/2525 (0.1%)
1	B	0.64	0/1783	0.76	2/2403 (0.1%)
1	C	0.59	1/1880 (0.1%)	0.71	3/2537 (0.1%)
1	D	0.58	0/1828	0.73	1/2465 (0.0%)
All	All	0.63	1/7362 (0.0%)	0.74	8/9930 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	383	TRP	CB-CG	-5.37	1.40	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	503	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	436	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	464	SER	N-CA-C	5.89	126.90	111.00
1	A	436	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	515	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	515	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	C	436	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	515	ARG	CG-CD-NE	-5.04	101.22	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1850	0	1882	14	0
1	B	1765	0	1813	3	0
1	C	1859	0	1883	18	0
1	D	1809	0	1862	3	0
2	A	38	0	1	6	0
2	B	42	0	1	4	0
2	C	38	0	1	12	0
2	D	42	0	1	3	0
3	S	482	0	0	6	2
All	All	7925	0	7444	49	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:LIG:S32	2:A:601:LIG:C03	2.11	1.39
2:B:601:LIG:S32	2:B:601:LIG:C03	2.11	1.39
2:D:601:LIG:S32	2:D:601:LIG:C03	2.12	1.38
2:C:601:LIG:C03	2:C:601:LIG:S32	2.10	1.37
1:C:525:LEU:CB	2:C:601:LIG:C27	2.31	1.08
1:C:328:TYR:N	3:S:13:HOH:O	2.03	0.92
1:C:305:SER:N	3:S:172:HOH:O	2.04	0.87
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.58	0.86
1:A:328:TYR:N	3:S:6:HOH:O	2.11	0.84
1:C:326:ILE:C	3:S:287:HOH:O	2.16	0.82
2:B:601:LIG:S32	2:B:601:LIG:C02	2.68	0.81
1:C:525:LEU:CB	2:C:601:LIG:C31	2.60	0.80
1:C:525:LEU:CB	2:C:601:LIG:C26	2.60	0.79
2:C:601:LIG:C04	2:C:601:LIG:S32	2.71	0.79
2:A:601:LIG:S32	2:A:601:LIG:C02	2.72	0.77
2:D:601:LIG:S32	2:D:601:LIG:C02	2.74	0.76
2:B:601:LIG:S32	2:B:601:LIG:C04	2.75	0.74
2:A:601:LIG:S32	2:A:601:LIG:C04	2.74	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:LIG:C02	2:C:601:LIG:S32	2.78	0.72
1:A:523:GLU:O	1:A:525:LEU:C	2.30	0.70
1:A:534:VAL:HG22	2:A:601:LIG:C31	2.22	0.69
2:D:601:LIG:S32	2:D:601:LIG:C04	2.79	0.63
1:A:465:THR:HG23	1:A:468:SER:H	1.63	0.63
1:C:525:LEU:CB	2:C:601:LIG:C30	2.78	0.62
1:A:523:GLU:O	1:A:525:LEU:N	2.33	0.61
1:A:335:ARG:NH2	1:A:414:GLN:HE22	1.99	0.60
1:C:533:VAL:CG2	2:C:601:LIG:C31	2.78	0.60
1:C:539:LEU:HG	1:C:543:MET:HE3	1.85	0.58
1:C:396:MET:O	1:C:436:ARG:HD3	2.07	0.55
1:C:533:VAL:HG23	2:C:601:LIG:C31	2.37	0.54
1:A:525:LEU:HD22	2:A:601:LIG:C27	2.38	0.54
1:A:396:MET:O	1:A:436:ARG:HD3	2.08	0.53
1:C:539:LEU:HD11	1:C:543:MET:HE2	1.91	0.51
1:D:356:HIS:HE1	3:S:20:HOH:O	1.95	0.49
1:C:525:LEU:CB	2:C:601:LIG:C28	2.90	0.48
1:D:492:LYS:HE2	1:D:492:LYS:HA	1.96	0.48
1:A:525:LEU:HD22	2:A:601:LIG:C30	2.44	0.47
1:B:346:LEU:HD12	2:B:601:LIG:HC26	1.97	0.47
1:A:523:GLU:O	1:A:524:HIS:C	2.54	0.46
1:C:533:VAL:HG22	2:C:601:LIG:C31	2.46	0.46
1:C:534:VAL:HG23	2:C:601:LIG:C31	2.45	0.46
1:D:398:HIS:HB3	1:D:401:LYS:HE2	1.99	0.44
1:A:519:ASN:HD21	1:B:516:HIS:HA	1.83	0.43
1:A:454:LEU:HD22	1:A:475:ILE:HD12	2.00	0.43
1:C:362:LYS:HD2	1:C:368:VAL:HG12	2.01	0.42
1:B:358:ILE:CD1	1:B:379:LEU:HD13	2.49	0.41
1:C:328:TYR:N	3:S:287:HOH:O	2.54	0.41
1:A:520:LYS:HD2	1:A:520:LYS:HA	1.84	0.41
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.39	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:399:HOH:O	3:S:438:HOH:O[1_545]	2.04	0.16
3:S:435:HOH:O	3:S:442:HOH:O[1_545]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	223/257 (87%)	219 (98%)	2 (1%)	2 (1%)	17 4
1	B	212/257 (82%)	211 (100%)	1 (0%)	0	100 100
1	C	225/257 (88%)	222 (99%)	1 (0%)	2 (1%)	17 4
1	D	220/257 (86%)	219 (100%)	1 (0%)	0	100 100
All	All	880/1028 (86%)	871 (99%)	5 (1%)	4 (0%)	29 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	464	SER
1	A	523	GLU
1	A	524	HIS
1	C	465	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	207/232 (89%)	205 (99%)	2 (1%)	76 61
1	B	198/232 (85%)	195 (98%)	3 (2%)	65 44
1	C	208/232 (90%)	205 (99%)	3 (1%)	67 47
1	D	204/232 (88%)	199 (98%)	5 (2%)	47 22
All	All	817/928 (88%)	804 (98%)	13 (2%)	62 41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	ILE
1	A	437	MET
1	B	396	MET
1	B	432	SER
1	B	534	VAL
1	C	358	ILE
1	C	417	CYS
1	C	437	MET
1	D	306	LEU
1	D	358	ILE
1	D	432	SER
1	D	492	LYS
1	D	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	413	ASN
1	A	500	GLN
1	A	513	HIS
1	A	519	ASN
1	B	304	ASN
1	B	519	ASN
1	C	519	ASN
1	D	356	HIS
1	D	519	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

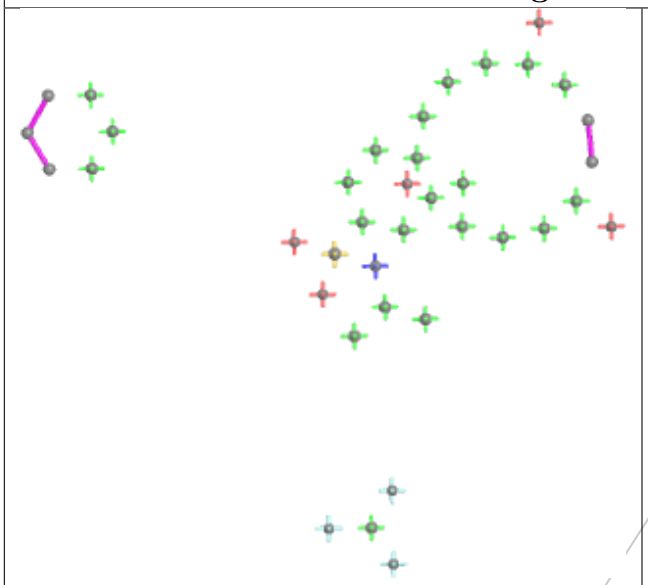
There are no torsion outliers.

There are no ring outliers.

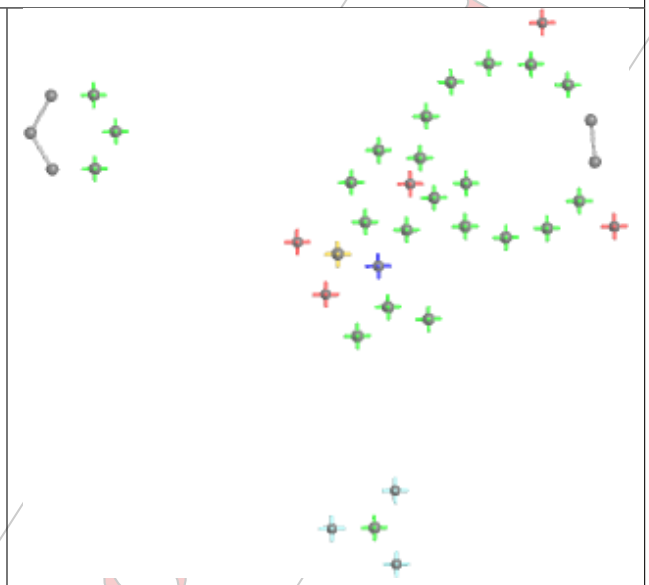
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

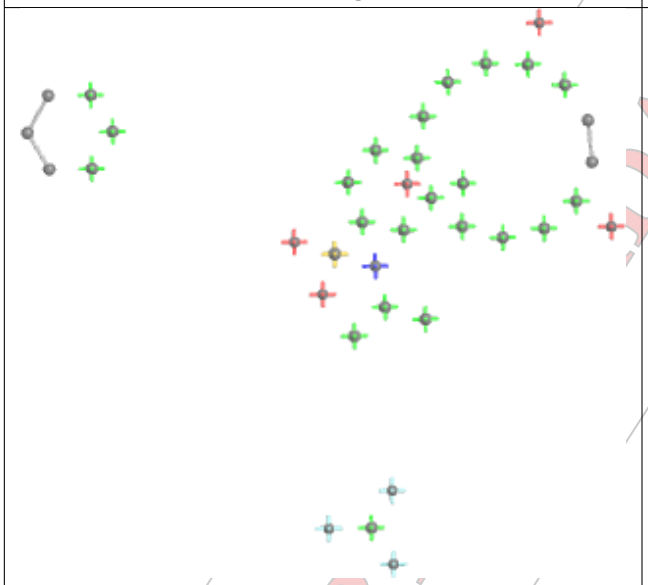
Ligand LIG C 601



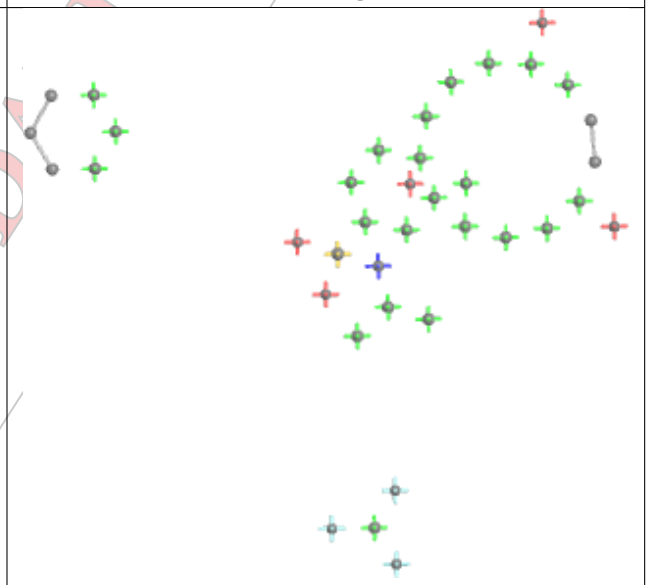
Bond lengths



Bond angles

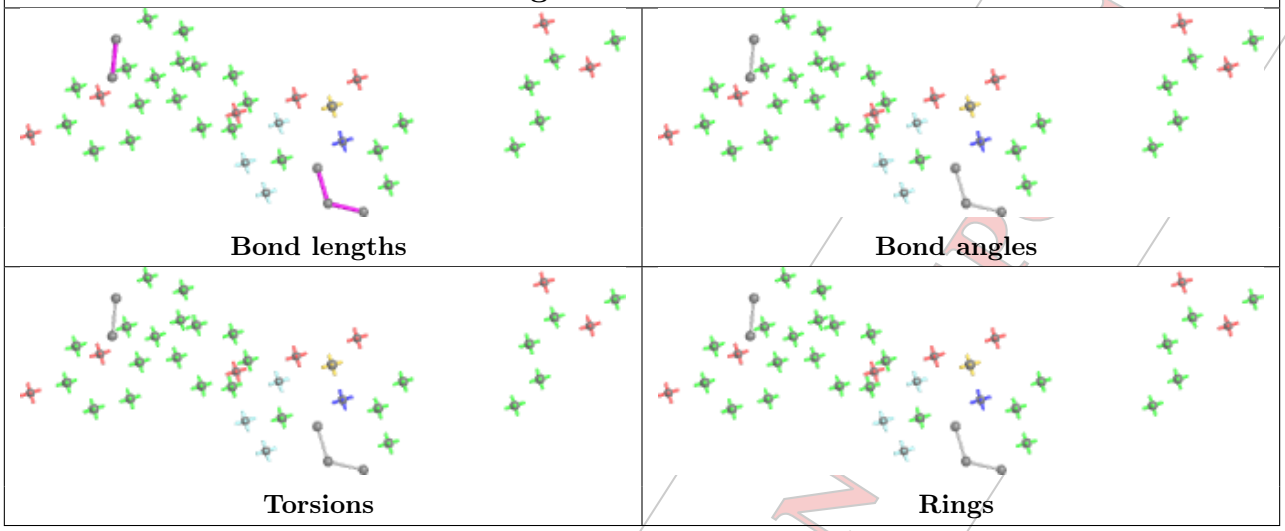


Torsions

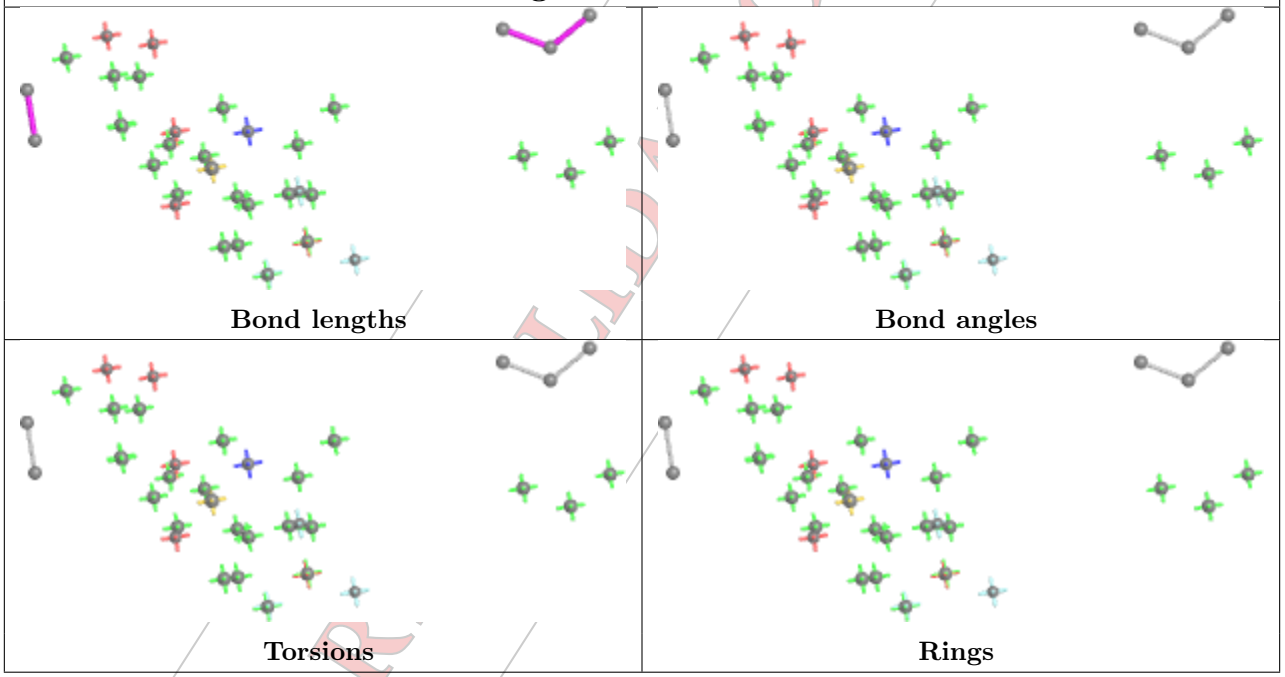


Rings

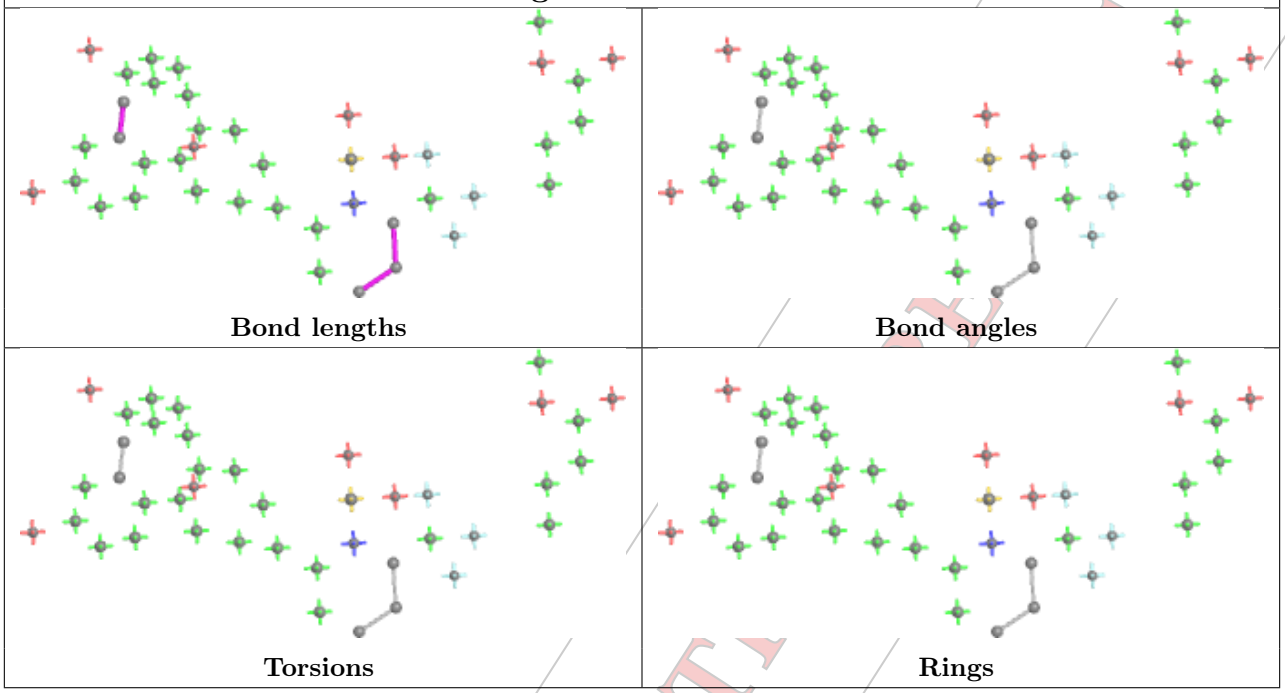
Ligand LIG D 601



Ligand LIG A 601



Ligand LIG B 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/257 (89%)	0.04	7 (3%)	50	48	15, 28, 54, 72	0
1	B	220/257 (85%)	0.09	10 (4%)	33	30	17, 28, 63, 106	0
1	C	232/257 (90%)	0.26	17 (7%)	15	13	16, 35, 65, 98	0
1	D	226/257 (87%)	0.09	14 (6%)	20	18	17, 31, 66, 83	0
All	All	908/1028 (88%)	0.12	48 (5%)	26	24	15, 30, 64, 106	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	417	CYS	6.0
1	B	469	LEU	5.7
1	D	528	MET	5.2
1	C	464	SER	4.7
1	D	530	CYS	4.6
1	C	305	SER	4.5
1	B	304	ASN	4.4
1	B	468	SER	4.3
1	B	530	CYS	4.2
1	A	524	HIS	4.2
1	B	461	PHE	4.1
1	A	332	ASP	3.9
1	C	332	ASP	3.9
1	D	462	LEU	3.8
1	D	306	LEU	3.6
1	A	418	VAL	3.6
1	C	306	LEU	3.5
1	C	463	SER	3.5
1	C	466	LEU	3.4
1	C	420	GLY	3.4
1	A	461	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	418	VAL	3.4
1	B	305	SER	3.4
1	D	526	TYR	3.1
1	D	425	PHE	3.0
1	C	425	PHE	3.0
1	A	305	SER	3.0
1	A	460	THR	2.7
1	B	460	THR	2.7
1	D	527	SER	2.6
1	B	532	ASN	2.6
1	D	532	ASN	2.6
1	C	413	ASN	2.4
1	B	413	ASN	2.4
1	C	331	TYR	2.4
1	D	328	TYR	2.4
1	D	546	ALA	2.3
1	B	306	LEU	2.3
1	A	417	CYS	2.3
1	D	545	ASP	2.3
1	C	536	SER	2.2
1	D	415	GLY	2.2
1	C	461	PHE	2.2
1	D	463	SER	2.1
1	C	421	MET	2.1
1	C	419	GLU	2.1
1	D	421	MET	2.0
1	C	494	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

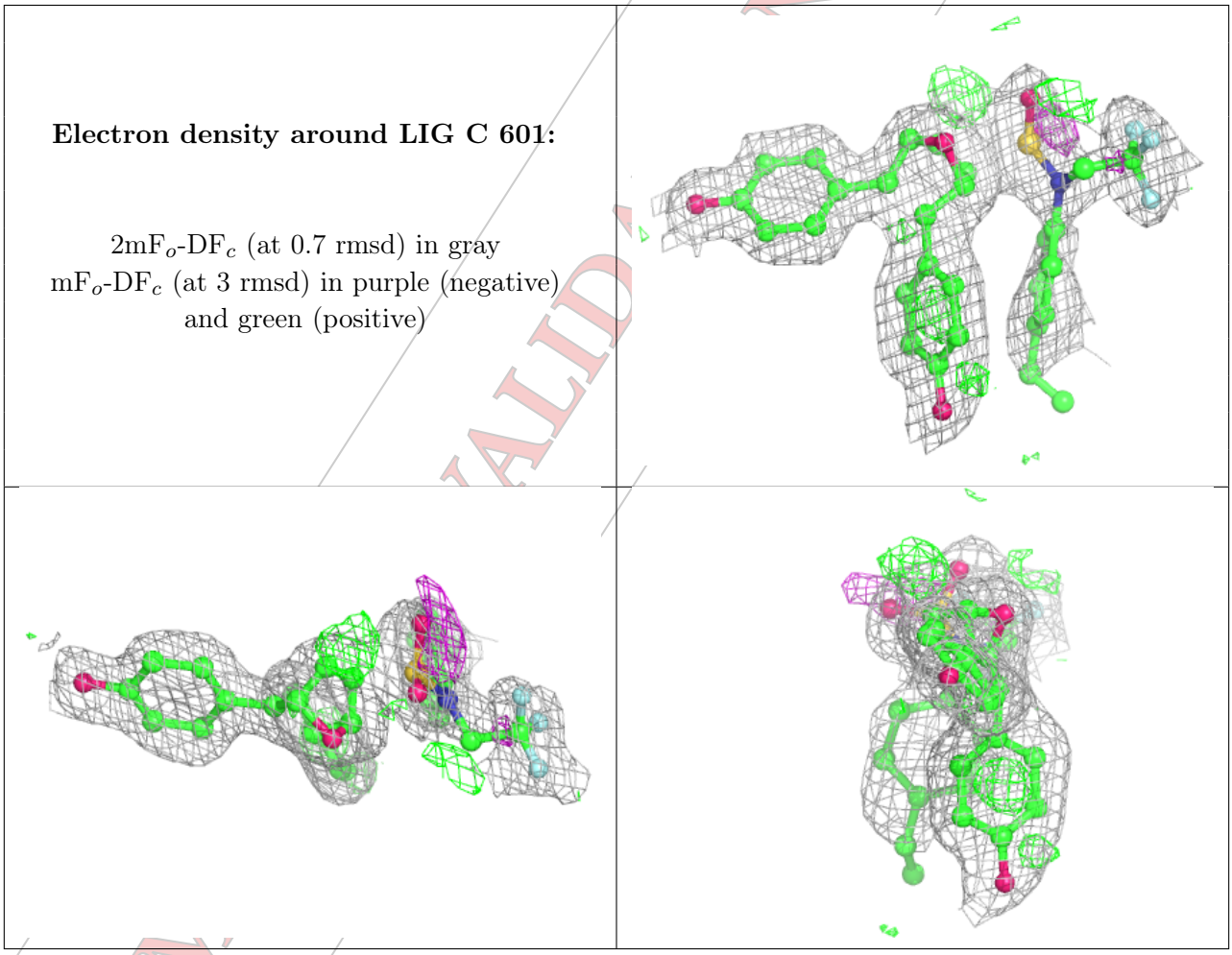
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	C	601	38/?	0.89	0.14	17,31,70,85	0
2	LIG	D	601	42/?	0.89	0.14	23,44,106,128	0
2	LIG	A	601	38/?	0.89	0.15	18,28,83,88	0
2	LIG	B	601	42/?	0.90	0.15	21,43,77,82	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

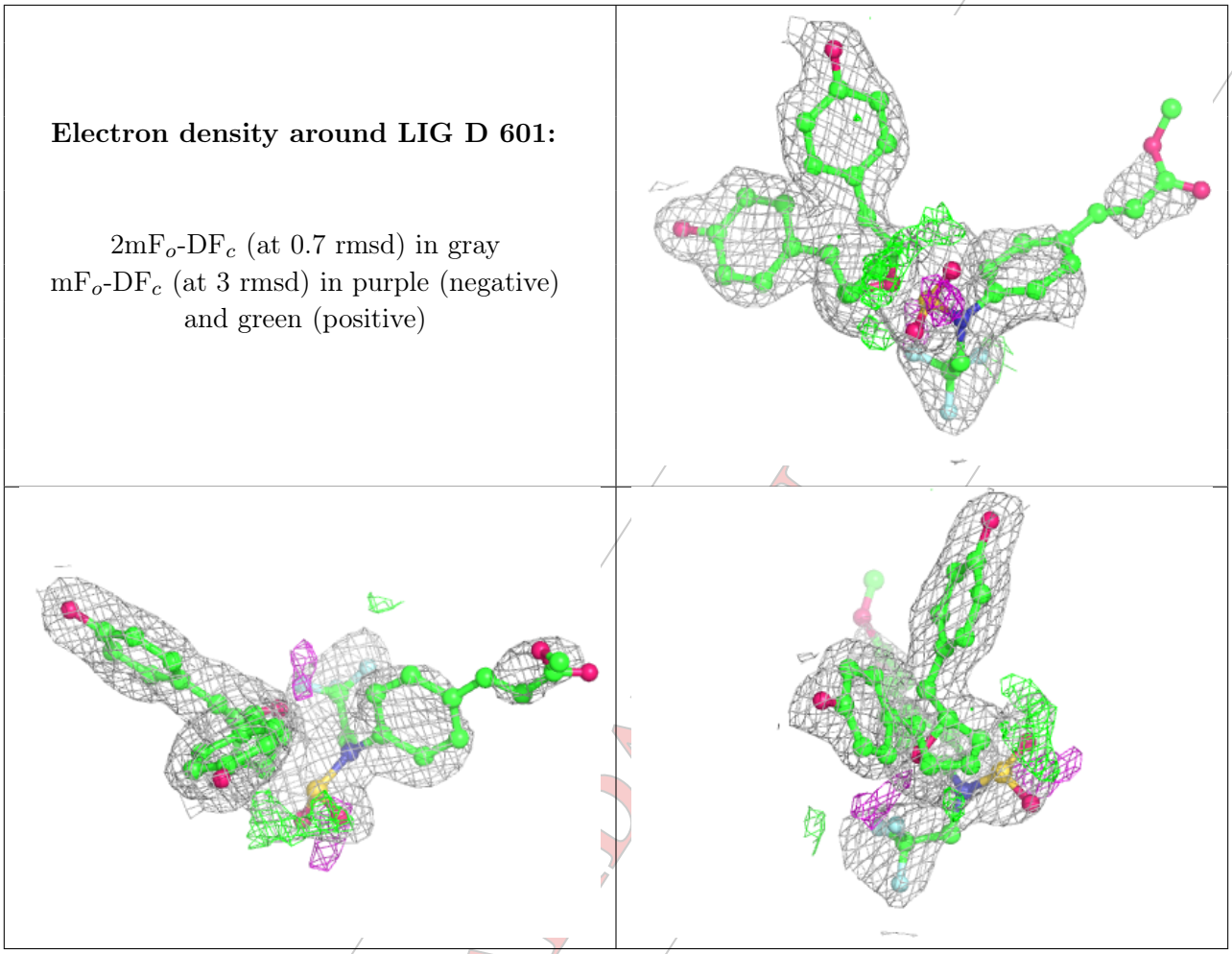
Electron density around LIG C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



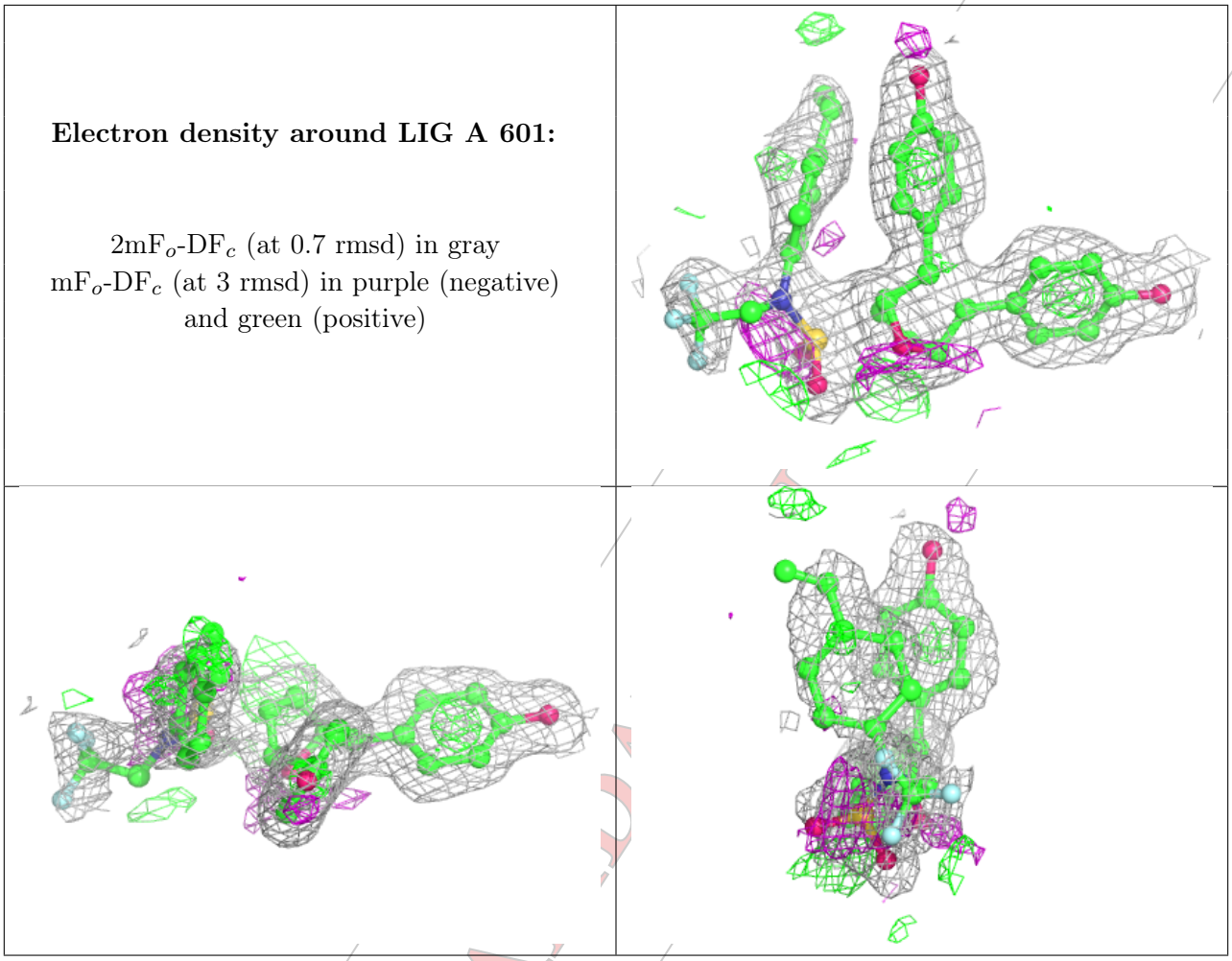
Electron density around LIG D 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



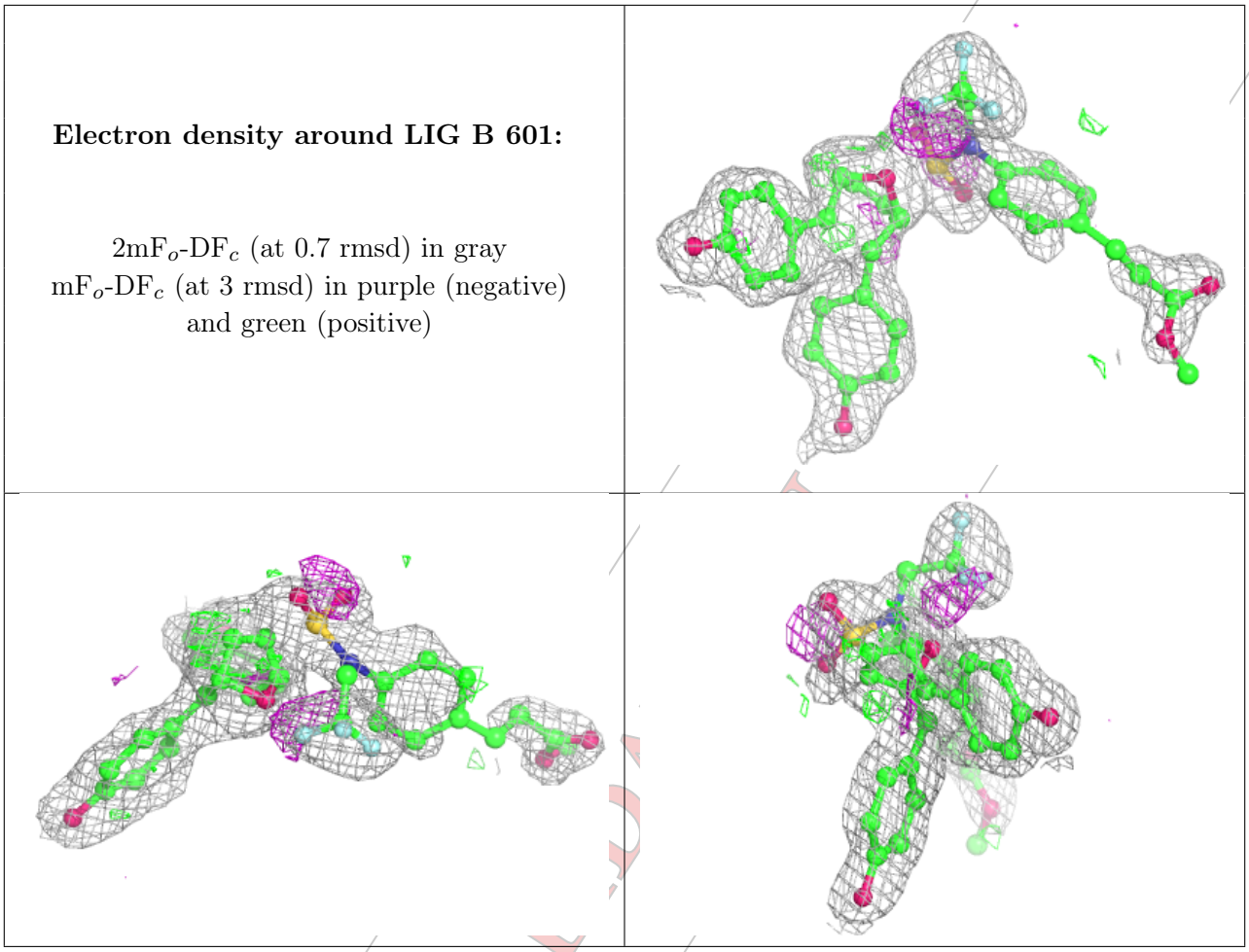
Electron density around LIG A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 10:26 PM EDT

Deposition ID : D_1000251219

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

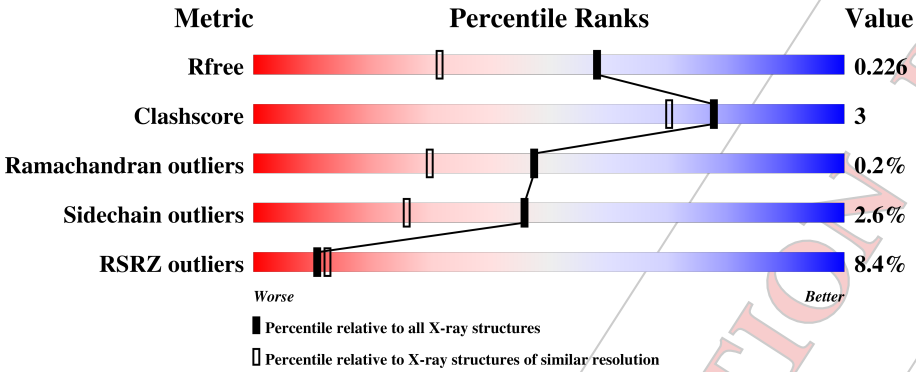
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	7%, 87%, 6% • 6%
1	B	260	5%, 84% • 12%
1	C	260	12%, 88%, 6% • 5%
1	D	260	7%, 84%, 6% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8127 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	1	0
			1962	1252	335	358	17			
1	B	230	Total	C	N	O	S	0	0	0
			1842	1178	314	331	19			
1	C	247	Total	C	N	O	S	0	1	0
			1965	1252	337	360	16			
1	D	234	Total	C	N	O	S	0	0	0
			1865	1191	318	337	19			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	N	O	S		0	0
			33	26	1	5	1			
2	E	1	Total	C	F	N	O	S	0	0
			41	29	3	1	7	1		
2	E	1	Total	C	N	O	S		0	0
			33	26	1	5	1			
2	E	1	Total	C	F	N	O	S	0	0
			41	29	3	1	7	1		

- Molecule 3 is water.

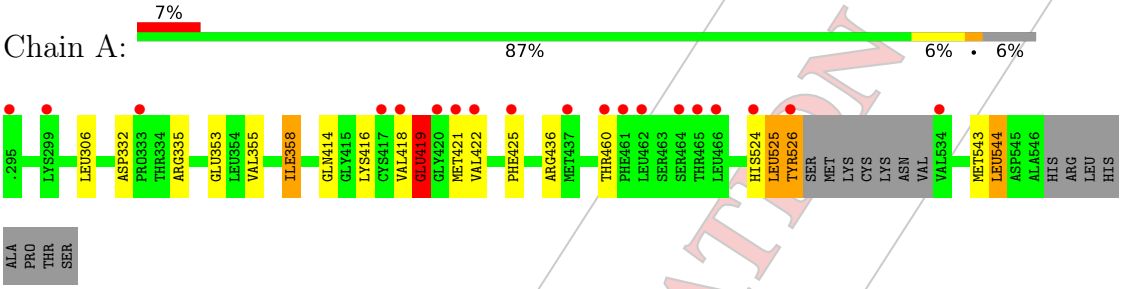
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	345	Total	O	0	0
			345	345		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

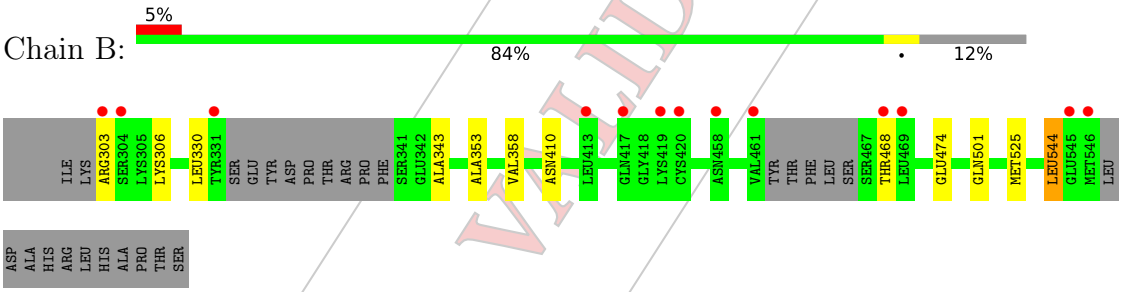
• Molecule 1: Estrogen Receptor

Chain A:



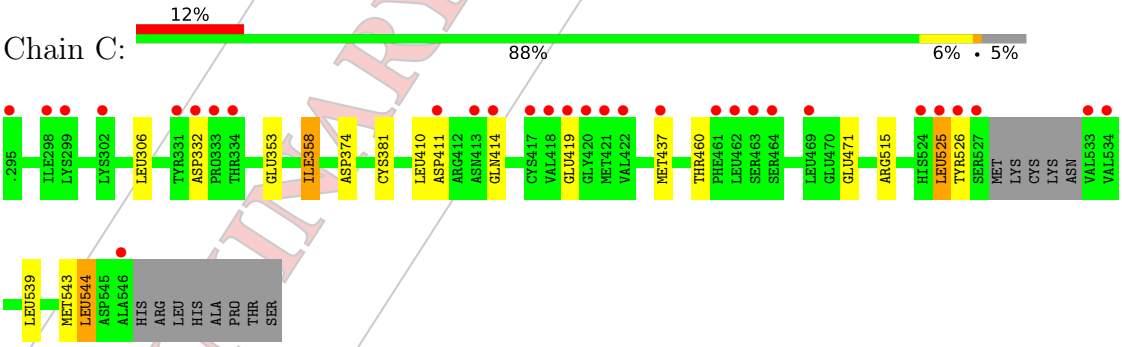
• Molecule 1: Estrogen Receptor

Chain B:



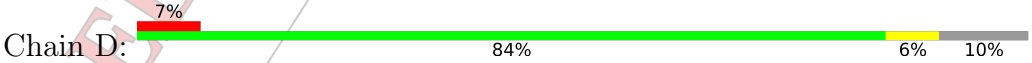
• Molecule 1: Estrogen Receptor

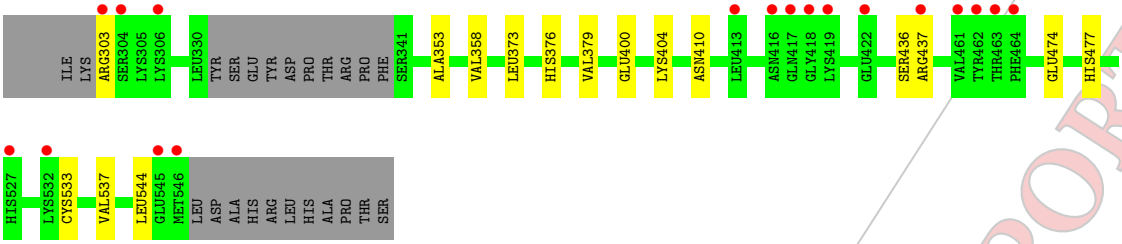
Chain C:



• Molecule 1: Estrogen Receptor

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.86Å 58.76Å 93.70Å 86.45° 75.11° 62.82°	Depositor
Resolution (Å)	90.36 – 1.72 90.36 – 1.72	Depositor EDS
% Data completeness (in resolution range)	72.8 (90.36-1.72) 72.8 (90.36-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194 , 0.221 0.203 , 0.226	Depositor DCC
R_{free} test set	3761 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.107 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8127	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.71	0/1986	0.73	0/2680
1	B	0.69	0/1851	0.76	0/2492
1	C	0.70	0/1989	0.73	0/2684
1	D	0.70	0/1874	0.76	0/2525
All	All	0.70	0/7700	0.74	0/10381

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	THR	Peptide
1	C	460	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1962	0	2006	19	0
1	B	1842	0	1889	5	1
1	C	1965	0	2001	9	0
1	D	1865	0	1920	12	0
2	E	148	0	4	8	0
3	S	345	0	0	4	1
All	All	8127	0	7820	45	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:VAL:HG11	2:E:4:LIG:O21	1.78	0.82
1:D:533:VAL:CG1	2:E:4:LIG:O21	2.34	0.74
1:A:416:LYS:HG2	1:A:422:VAL:HG21	1.69	0.73
1:C:411:ASP:H	1:C:414:GLN:HE21	1.35	0.73
1:A:525:LEU:HD12	2:E:1:LIG:C27	2.24	0.67
1:A:355:VAL:HA	1:A:543:MET:CE	2.26	0.66
1:C:525:LEU:HD13	1:C:526:TYR:N	2.13	0.64
1:A:525:LEU:CD2	1:A:525:LEU:C	2.71	0.59
1:A:525:LEU:HD12	2:E:1:LIG:C30	2.32	0.58
1:D:400:GLY:O	3:S:208:HOH:O	2.17	0.58
1:D:477:ARG:NH2	3:S:94:HOH:O	2.37	0.57
1:A:526:TYR:CD1	1:A:526:TYR:C	2.82	0.53
1:A:355:VAL:HA	1:A:543:MET:HE2	1.89	0.52
1:A:335:ARG:NH1	1:A:414:GLN:HE22	2.06	0.52
1:A:525:LEU:HD23	1:A:525:LEU:C	2.30	0.52
1:A:525:LEU:HD23	1:A:525:LEU:O	2.10	0.52
1:C:525:LEU:C	1:C:525:LEU:HD13	2.31	0.51
1:D:353:GLU:OE1	2:E:4:LIG:O20	2.29	0.51
1:B:353:GLU:OE1	2:E:2:LIG:O20	2.29	0.50
1:D:373:HIS:HD2	1:D:537:TYR:OH	1.94	0.50
1:C:381:YCM:HD3	3:S:171:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.94	0.50
1:A:525:LEU:HD22	1:A:526:TYR:CD2	2.48	0.49
1:C:410:LEU:HA	1:C:414:GLN:NE2	2.28	0.49
1:B:358:ILE:HG23	1:B:544:LEU:HD13	1.95	0.48
1:A:353:GLU:OE1	2:E:1:LIG:O20	2.31	0.47
1:D:477:ARG:NH2	3:S:83:HOH:O	2.47	0.47
1:B:410:LEU:N	1:B:410:LEU:HD12	2.30	0.46
1:A:306:LEU:HD22	1:A:306:LEU:N	2.32	0.45
1:C:539:LEU:HG	1:C:543:MET:CE	2.46	0.45
1:C:353:GLU:OE1	2:E:3:LIG:O20	2.34	0.45
1:A:526:TYR:HD1	1:A:526:TYR:C	2.20	0.44
1:D:404:PHE:CE2	1:D:410:LEU:HD12	2.52	0.44
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.48	0.43
1:A:418:VAL:HG11	1:A:421:MET:CE	2.48	0.43
1:A:525:LEU:HD22	1:A:526:TYR:HB3	2.00	0.43
1:C:358:ILE:HG23	1:C:544:LEU:HD13	2.00	0.43
1:A:358:ILE:HG23	1:A:544:LEU:HD13	2.00	0.42
1:B:303:LYS:HG3	1:B:474:HIS:ND1	2.34	0.42
1:A:416:LYS:HA	1:A:422:VAL:CG2	2.50	0.42
1:A:418:VAL:HG12	1:A:419:GLU:HG2	2.01	0.42
1:B:343:MET:HE1	1:B:525:LEU:CD2	2.52	0.41
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.39	0.41
1:D:358:ILE:HD12	1:D:379:LEU:HD13	2.04	0.40
1:D:303:LYS:HG3	1:D:474:HIS:ND1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:GLU:OE2	3:S:275:HOH:O[1_545]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/260 (93%)	238 (99%)	2 (1%)	1 (0%)	34	18
1	B	222/260 (85%)	219 (99%)	3 (1%)	0	100	100
1	C	243/260 (94%)	240 (99%)	2 (1%)	1 (0%)	34	18
1	D	228/260 (88%)	225 (99%)	3 (1%)	0	100	100
All	All	934/1040 (90%)	922 (99%)	10 (1%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	GLU
1	C	419	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/232 (95%)	211 (96%)	9 (4%)	30	11
1	B	205/232 (88%)	201 (98%)	4 (2%)	55	37
1	C	218/232 (94%)	211 (97%)	7 (3%)	39	18
1	D	209/232 (90%)	207 (99%)	2 (1%)	76	65
All	All	852/928 (92%)	830 (97%)	22 (3%)	46	26

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ASP
1	A	358	ILE
1	A	419	GLU
1	A	425	PHE
1	A	436	ARG
1	A	524	HIS
1	A	525	LEU

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Mol	Chain	Res	Type
1	A	526	TYR
1	A	544	LEU
1	B	306	LEU
1	B	468	SER
1	B	501	HIS
1	B	544	LEU
1	C	306	LEU
1	C	332	ASP
1	C	358	ILE
1	C	437	MET
1	C	515	ARG
1	C	525	LEU
1	C	544	LEU
1	D	436	ARG
1	D	437	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	359	ASN
1	C	398	HIS
1	C	519	ASN
1	D	373	HIS
1	D	519	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

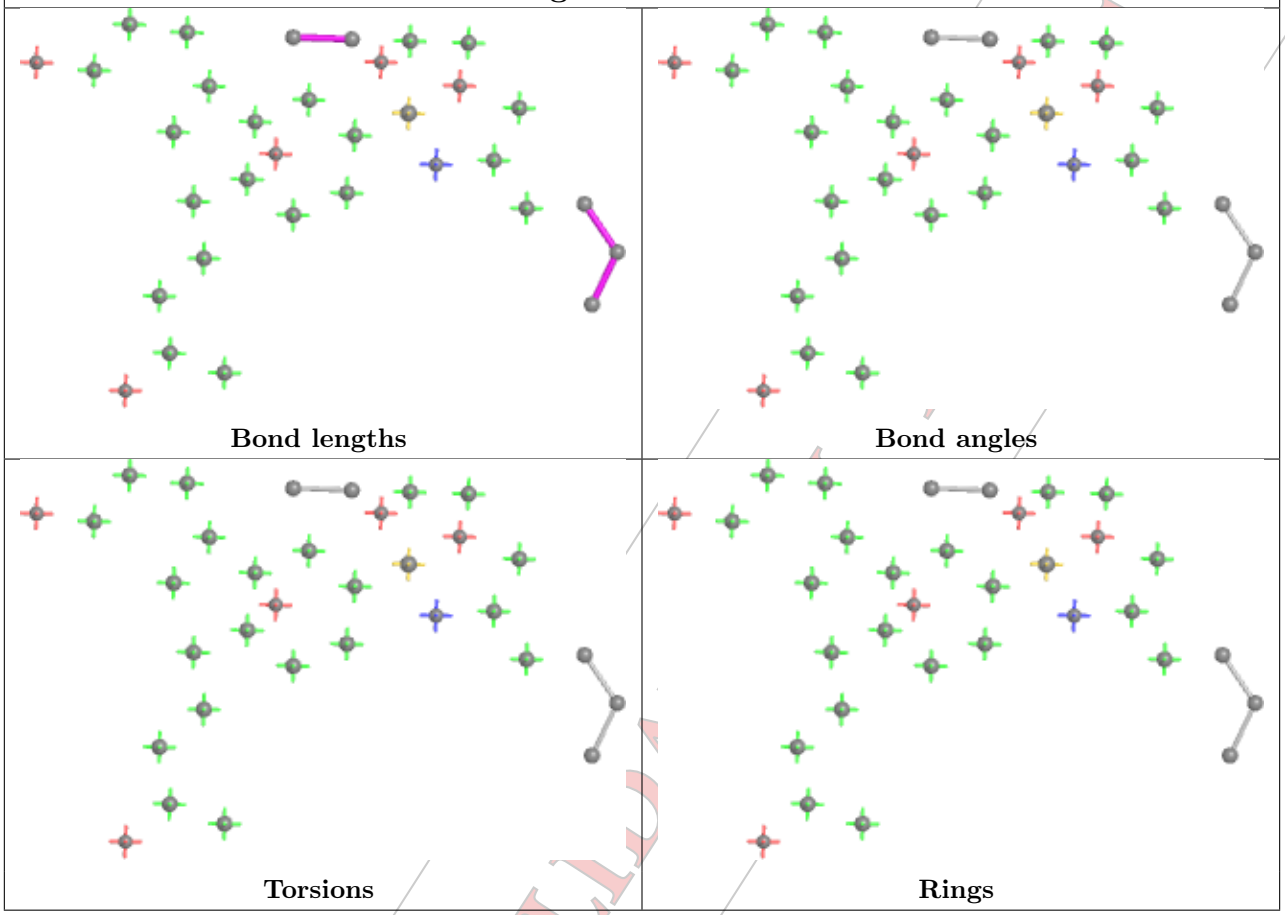
There are no torsion outliers.

There are no ring outliers.

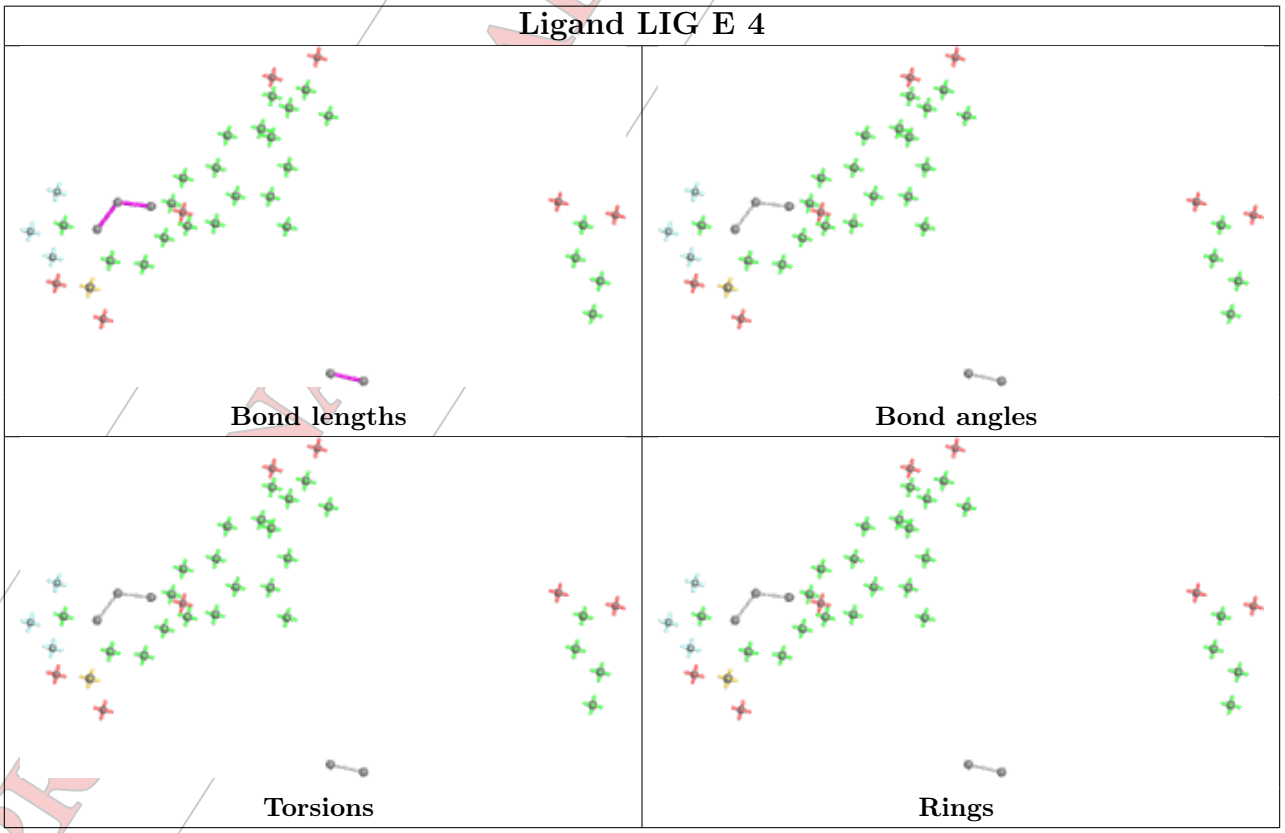
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

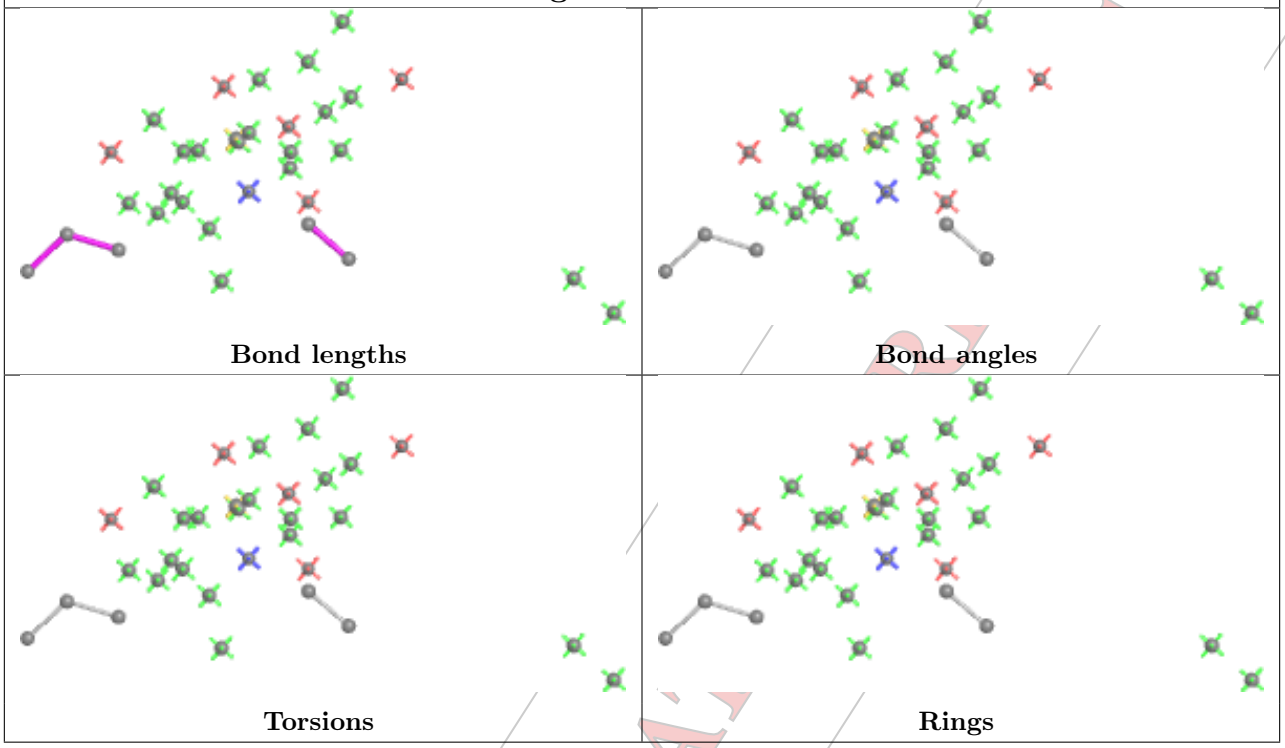
Ligand LIG E 3



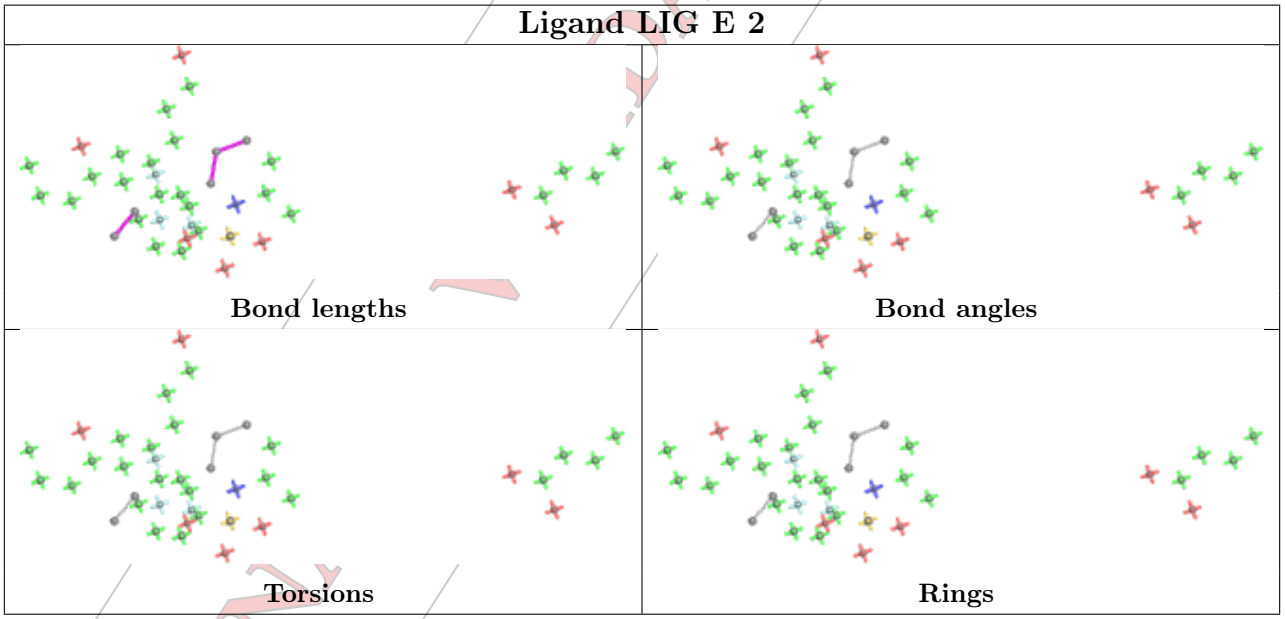
Ligand LIG E 4



Ligand LIG E 1



Ligand LIG E 2



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	244/260 (93%)	0.47	19 (7%)	13	15	14, 25, 62, 84	0
1	B	228/260 (87%)	0.45	13 (5%)	23	26	14, 26, 65, 101	0
1	C	246/260 (94%)	0.64	30 (12%)	4	4	16, 29, 67, 100	0
1	D	232/260 (89%)	0.47	18 (7%)	13	15	14, 28, 60, 104	0
All	All	950/1040 (91%)	0.51	80 (8%)	11	12	14, 27, 65, 104	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	526	TYR	9.9
1	A	418	VAL	8.6
1	D	303	LYS	8.6
1	A	420	GLY	8.2
1	C	418	VAL	7.6
1	B	304	ASN	7.1
1	B	417	CYS	6.9
1	B	468	SER	5.8
1	A	526	TYR	5.8
1	C	464	SER	5.7
1	D	304	ASN	5.6
1	D	546	ALA	5.3
1	B	303	LYS	5.3
1	A	464	SER	5.1
1	D	417	CYS	5.0
1	D	462	LEU	4.9
1	B	469	LEU	4.7
1	A	417	CYS	4.7
1	C	524	HIS	4.4
1	C	527	SER	4.3
1	C	333	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	419	GLU	4.1
1	B	461	PHE	4.0
1	C	299	LYS	3.9
1	A	462	LEU	3.8
1	C	295	SER	3.7
1	C	413	ASN	3.6
1	C	332	ASP	3.6
1	C	298	ILE	3.6
1	C	421	ALA	3.5
1	B	546	ALA	3.5
1	C	420	GLY	3.4
1	C	334	THR	3.4
1	C	461	PHE	3.3
1	C	546	ALA	3.3
1	A	524	HIS	3.3
1	C	417	CYS	3.3
1	D	306	LEU	3.2
1	C	331	TYR	3.2
1	C	414	GLN	3.1
1	A	425	PHE	3.0
1	B	331	TYR	3.0
1	D	419	GLU	3.0
1	C	469	LEU	3.0
1	C	463	SER	2.9
1	A	333	PRO	2.9
1	D	413	ASN	2.8
1	A	461	PHE	2.8
1	C	462	LEU	2.8
1	D	532	ASN	2.8
1	C	534	VAL	2.8
1	D	437	MET	2.8
1	D	461	PHE	2.8
1	C	525	LEU	2.7
1	D	463	SER	2.7
1	C	422	VAL	2.6
1	D	464	SER	2.6
1	D	416	LYS	2.6
1	B	420	GLY	2.6
1	B	413	ASN	2.6
1	C	533	ALA	2.6
1	A	299	LYS	2.5
1	A	460	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	411	ASP	2.4
1	D	422	VAL	2.3
1	A	421	MET	2.3
1	A	295	SER	2.3
1	B	419	GLU	2.3
1	A	437	MET	2.3
1	A	465	THR	2.3
1	C	302	LYS	2.2
1	D	527	SER	2.2
1	A	466	LEU	2.2
1	C	437	MET	2.2
1	A	534	VAL	2.2
1	B	458	VAL	2.2
1	B	545	ASP	2.1
1	D	545	ASP	2.1
1	A	422	VAL	2.1
1	D	418	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

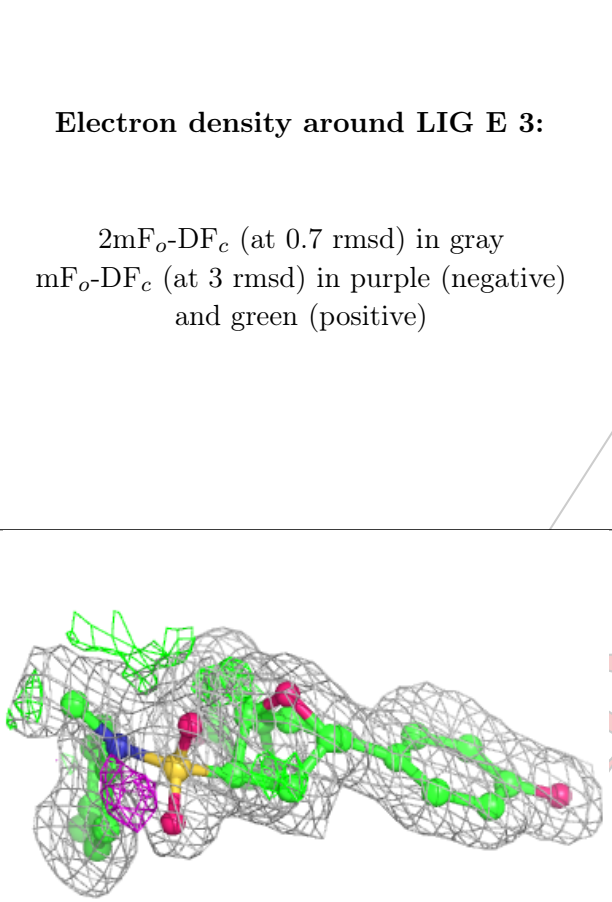
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	E	3	33/?	0.92	0.13	16,26,67,83	0
2	LIG	E	4	41/?	0.93	0.12	20,34,57,81	0
2	LIG	E	1	33/?	0.93	0.12	15,25,51,65	0
2	LIG	E	2	41/?	0.95	0.11	15,32,48,63	0

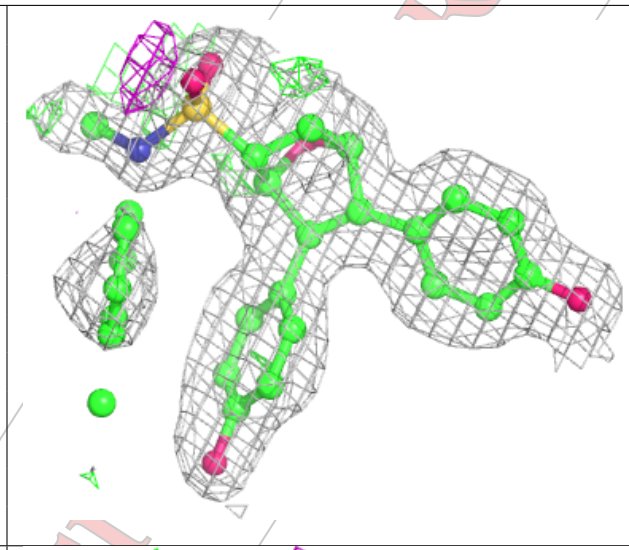
The following is a graphical depiction of the model fit to experimental electron density of all

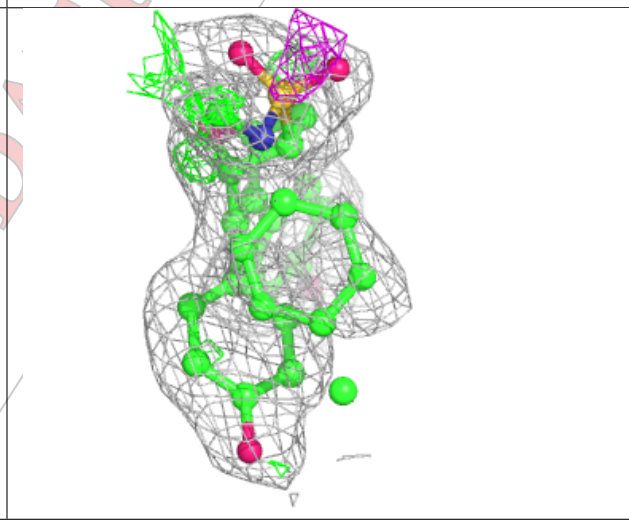
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LIG E 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

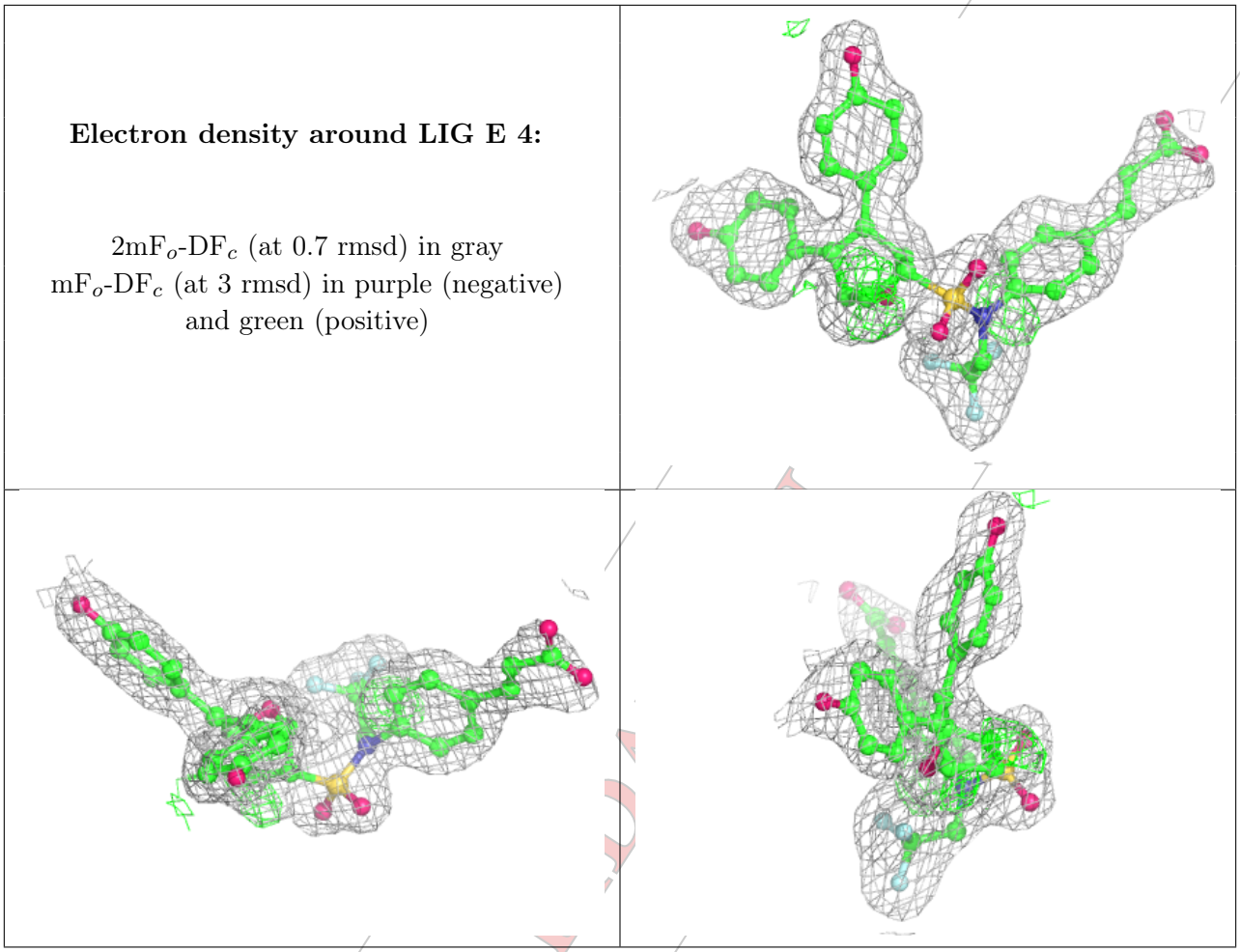






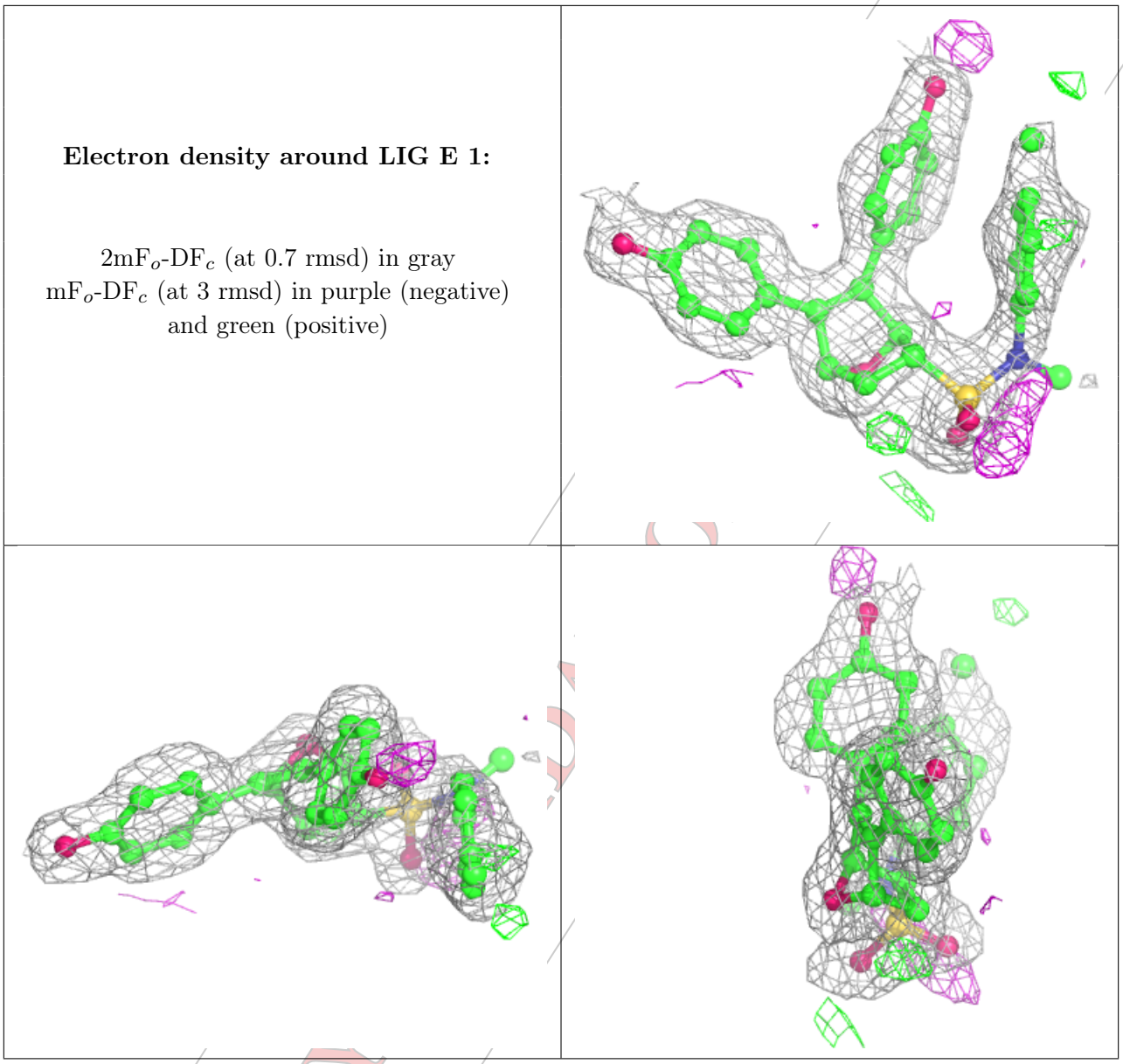
Electron density around LIG E 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



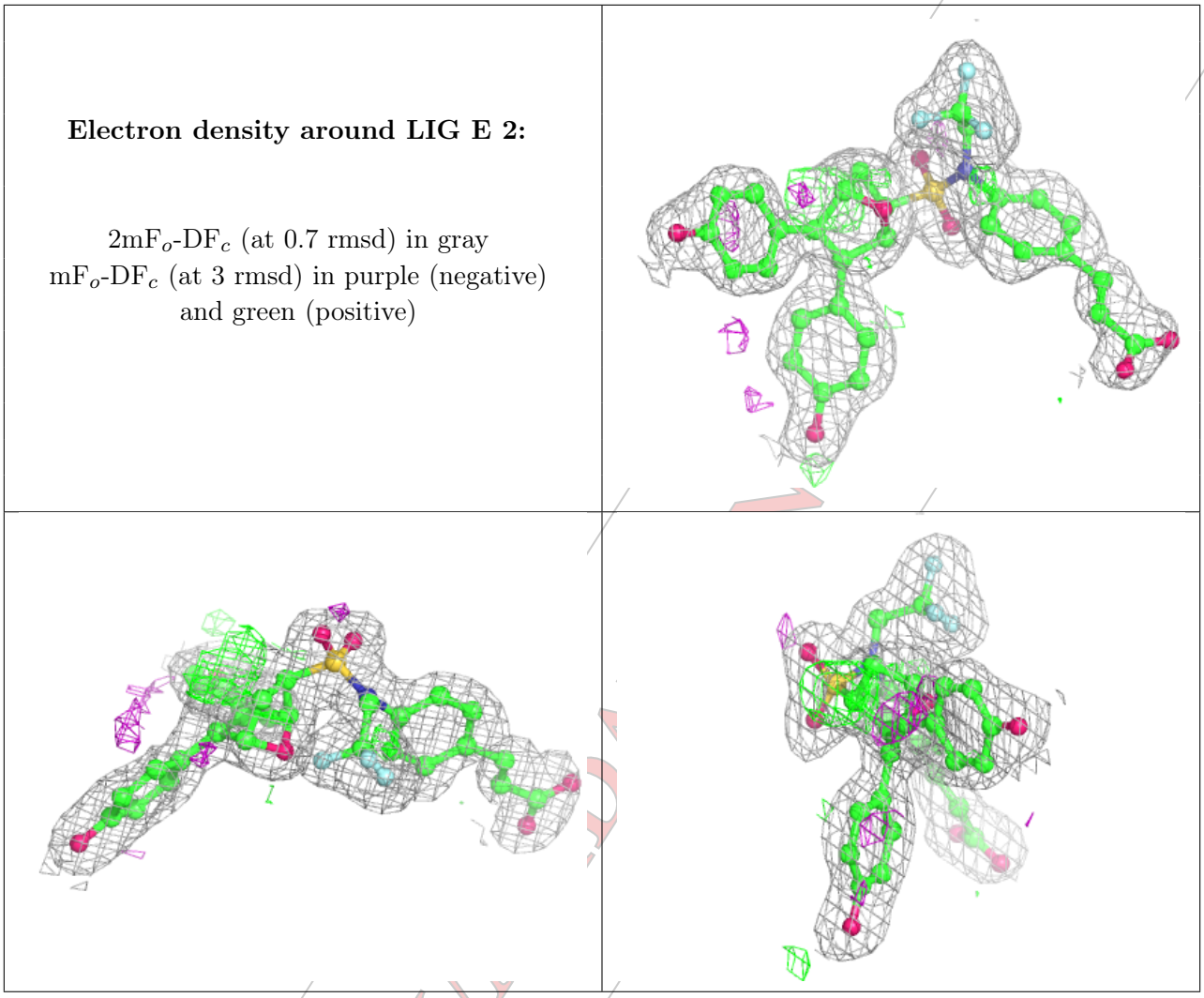
Electron density around LIG E 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG E 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 10:41 PM EDT

Deposition ID : D_1000251220

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

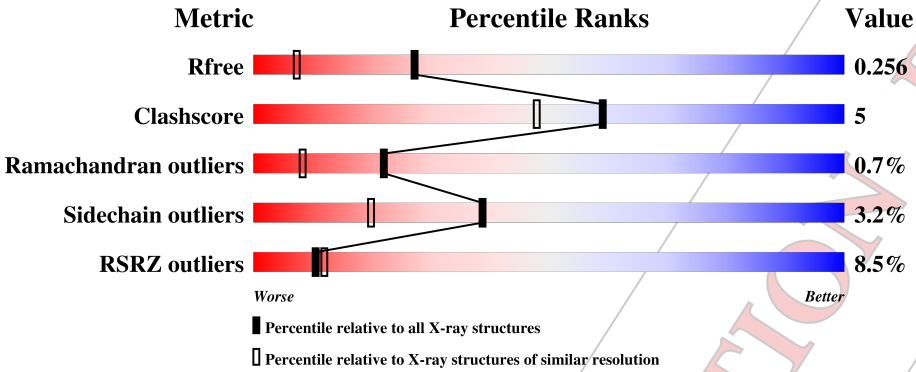
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	11% 82% 11% • 5%
1	B	257	4% 77% 10% • 12%
1	C	257	8% 79% 12% • 8%
1	D	257	7% 78% 9% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7811 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	1	0
			1939	1238	329	353	19			
1	B	226	Total	C	N	O	S	0	0	0
			1809	1160	306	326	17			
1	C	237	Total	C	N	O	S	0	1	0
			1898	1213	319	348	18			
1	D	224	Total	C	N	O	S	0	0	0
			1789	1144	304	323	18			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	F	N	O	S	0	0
			36	26	3	1	5	1		
2	E	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		
2	E	1	Total	C	F	N	O	S	0	0
			31	21	3	1	5	1		
2	E	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		

- Molecule 3 is water.

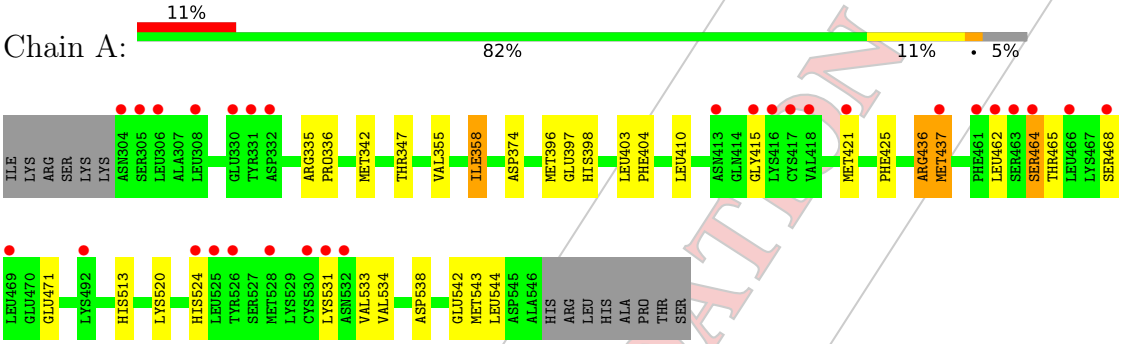
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	235	Total	O	0	0
			235	235		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

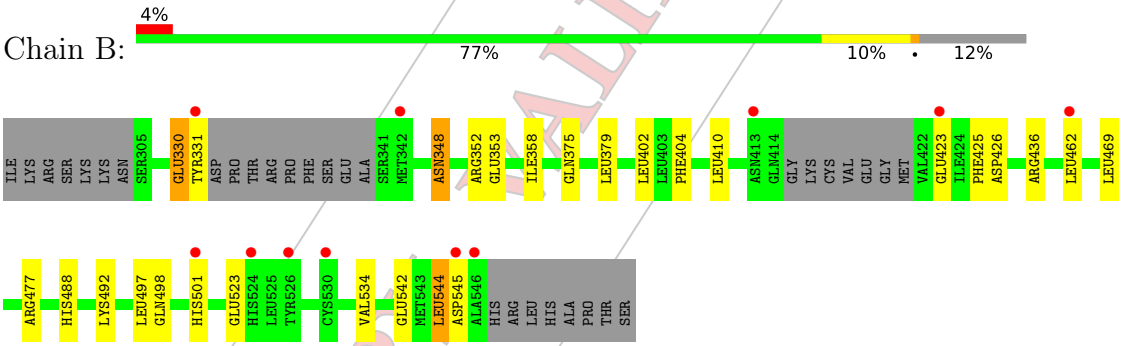
• Molecule 1: Estrogen Receptor

Chain A:



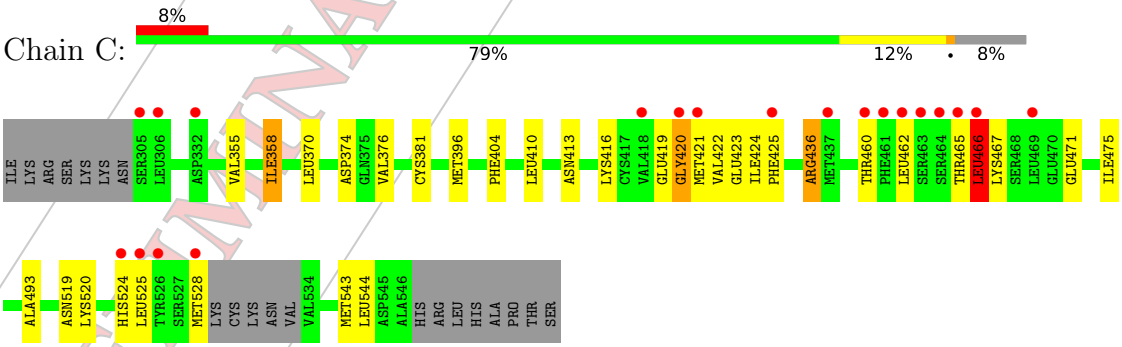
• Molecule 1: Estrogen Receptor

Chain B:



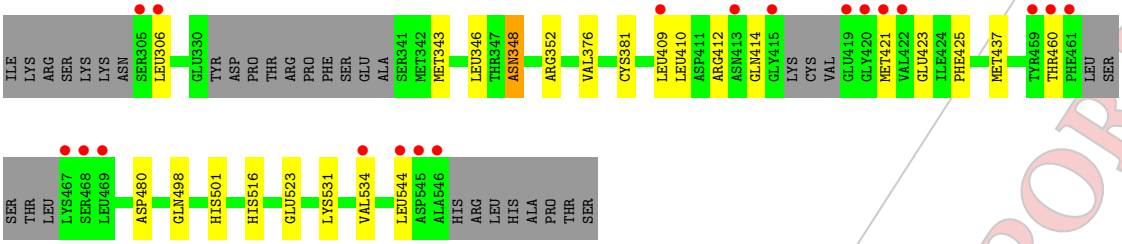
• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.57Å 58.81Å 92.86Å 86.70° 75.09° 62.91°	Depositor
Resolution (Å)	89.52 – 1.70 89.51 – 1.70	Depositor EDS
% Data completeness (in resolution range)	58.9 (89.52-1.70) 58.9 (89.51-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.252 0.225 , 0.256	Depositor DCC
R_{free} test set	3121 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.115 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7811	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.55	0/1964	0.72	1/2653 (0.0%)
1	B	0.55	0/1829	0.75	1/2468 (0.0%)
1	C	0.57	0/1922	0.75	1/2595 (0.0%)
1	D	0.56	0/1796	0.74	1/2416 (0.0%)
All	All	0.56	0/7511	0.74	4/10132 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	436	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	436	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	B	436	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	480	ASP	CB-CG-OD2	-5.09	113.72	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1939	0	1978	16	1
1	B	1809	0	1859	16	0
1	C	1898	0	1930	29	1
1	D	1789	0	1832	13	0
2	E	141	0	4	7	0
3	S	235	0	0	4	0
All	All	7811	0	7603	72	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:MET:SD	1:C:423:GLU:HB2	1.92	1.10
1:D:348:ASN:ND2	3:S:119:HOH:O	1.98	0.94
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.56	0.87
1:A:397[B]:GLU:OE1	1:A:397[B]:GLU:HA	1.76	0.86
1:C:416:LYS:HG2	1:C:422:VAL:HG21	1.60	0.84
1:A:513:HIS:ND1	3:S:86:HOH:O	2.17	0.77
1:A:355:VAL:HG22	1:A:543:MET:CE	2.17	0.75
1:A:355:VAL:HG22	1:A:543:MET:HE1	1.69	0.73
1:C:413:ASN:OD1	3:S:135:HOH:O	2.09	0.71
1:C:421:MET:SD	1:C:423:GLU:CB	2.78	0.67
1:A:464:SER:O	1:A:468:SER:HB2	1.97	0.65
1:C:355:VAL:HG22	1:C:543:MET:CE	2.28	0.64
1:A:404:PHE:CE2	1:A:410:LEU:HD12	2.39	0.58
1:C:421:MET:CE	1:C:524:HIS:CE1	2.88	0.57
1:B:469:LEU:HD13	1:C:493:ALA:O	2.06	0.56
1:B:404:PHE:CE2	1:B:410:LEU:HD12	2.41	0.56
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.41	0.56
1:D:343:MET:HE1	2:E:4:LIG:C18	2.37	0.55
1:A:347:THR:HG23	1:A:533:VAL:HG22	1.88	0.55
1:B:542:GLU:HA	1:B:545:ASP:OD1	2.07	0.55
1:D:346:LEU:CD1	2:E:4:LIG:C16	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:HIS:NE2	1:B:492:LYS:HD2	2.24	0.52
1:D:343:MET:CE	2:E:4:LIG:C18	2.88	0.51
1:C:419:GLU:O	1:C:420:GLY:C	2.49	0.50
1:C:419:GLU:O	1:C:420:GLY:O	2.30	0.49
1:B:358:ILE:HG23	1:B:544:LEU:HD13	1.95	0.49
1:C:466:LEU:HG	1:C:467:LYS:N	2.27	0.49
1:C:462:LEU:O	1:C:462:LEU:HG	2.13	0.49
1:B:477:ARG:NH2	3:S:61:HOH:O	2.33	0.48
2:E:1:LIG:C12	2:E:1:LIG:O01	2.62	0.48
1:B:488:HIS:CD2	1:B:492:LYS:HD2	2.49	0.48
1:A:358:ILE:HG23	1:A:544:LEU:HD23	1.97	0.47
1:C:355:VAL:HG22	1:C:543:MET:HE3	1.97	0.47
1:C:465:THR:O	1:C:467:LYS:N	2.47	0.47
1:C:421:MET:HE2	1:C:524:HIS:CE1	2.51	0.46
1:A:462:LEU:HG	1:B:426:ASP:HB3	1.98	0.46
1:C:355:VAL:HA	1:C:543:MET:CE	2.46	0.46
1:A:415:GLY:O	1:A:421:MET:HB3	2.15	0.46
1:C:520:LYS:O	1:C:524:HIS:CD2	2.69	0.46
1:D:346:LEU:HD12	2:E:4:LIG:C16	2.46	0.46
1:C:396:MET:O	1:C:436:ARG:HD3	2.15	0.45
1:C:519:ASN:HD21	1:D:516:HIS:HA	1.81	0.45
1:A:520:LYS:O	1:A:524:HIS:CD2	2.70	0.45
1:C:358:ILE:HG23	1:C:544:LEU:HD23	1.99	0.45
1:B:375:GLN:HB3	1:B:544:LEU:HD21	1.98	0.45
1:B:330:GLU:HA	1:B:330:GLU:OE1	2.18	0.44
1:D:348:ASN:HD21	1:D:352:ARG:HH21	1.63	0.44
1:B:353:GLU:OE2	2:E:2:LIG:O03	2.35	0.44
1:A:396:MET:O	1:A:436:ARG:HD3	2.18	0.43
1:B:542:GLU:O	1:B:545:ASP:OD1	2.36	0.43
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.53	0.43
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.53	0.43
1:C:525:LEU:O	1:C:528:MET:HG3	2.18	0.43
1:D:412:ARG:HA	1:D:425:PHE:CE1	2.54	0.42
1:C:421:MET:HB3	1:C:424:ILE:H	1.84	0.42
1:C:421:MET:HE1	1:C:524:HIS:CE1	2.54	0.42
1:B:402:LEU:HD12	1:B:425:PHE:CE2	2.55	0.42
1:C:374:ASP:OD2	1:C:471:GLU:OE2	2.37	0.42
1:D:409:LEU:C	1:D:410:LEU:HD12	2.40	0.42
1:A:437:MET:HE3	1:A:437:MET:O	2.20	0.42
1:B:348:ASN:HD21	1:B:352:ARG:HH21	1.66	0.42
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:VAL:HA	1:C:543:MET:HE2	2.03	0.41
1:A:398:HIS:CE1	1:A:403:LEU:HD12	2.55	0.41
1:C:466:LEU:HG	1:C:467:LYS:H	1.84	0.41
1:D:348:ASN:ND2	1:D:352:ARG:HH21	2.19	0.41
1:A:533:VAL:HG13	2:E:1:LIG:O06	2.21	0.41
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.39	0.40
1:C:376:VAL:CG2	1:C:544:LEU:HD12	2.52	0.40
1:D:381:YCM:NZ2	1:D:460:THR:HG21	2.37	0.40
1:C:381:YCM:NZ2	1:C:460:THR:HG21	2.36	0.40
1:B:358:ILE:CD1	1:B:379:LEU:HD13	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:OE2	1:C:465:THR:OG1[1_556]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	241/257 (94%)	234 (97%)	4 (2%)	3 (1%)	13 3
1	B	219/257 (85%)	217 (99%)	2 (1%)	0	100 100
1	C	233/257 (91%)	226 (97%)	5 (2%)	2 (1%)	17 5
1	D	214/257 (83%)	210 (98%)	3 (1%)	1 (0%)	29 13
All	All	907/1028 (88%)	887 (98%)	14 (2%)	6 (1%)	22 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	PRO
1	C	466	LEU
1	D	421	MET
1	A	465	THR
1	C	420	GLY
1	A	464	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/232 (94%)	211 (97%)	7 (3%)	39	20
1	B	204/232 (88%)	195 (96%)	9 (4%)	28	11
1	C	213/232 (92%)	210 (99%)	3 (1%)	67	53
1	D	198/232 (85%)	190 (96%)	8 (4%)	31	13
All	All	833/928 (90%)	806 (97%)	27 (3%)	39	20

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	MET
1	A	358	ILE
1	A	425	PHE
1	A	437	MET
1	A	531	LYS
1	A	534	VAL
1	A	538	ASP
1	B	330	GLU
1	B	331	TYR
1	B	348	ASN
1	B	423	GLU
1	B	462	LEU
1	B	497	LEU
1	B	523	GLU
1	B	534	VAL
1	B	544	LEU

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Mol	Chain	Res	Type
1	C	358	ILE
1	C	425	PHE
1	C	466	LEU
1	D	306	LEU
1	D	348	ASN
1	D	414	GLN
1	D	423	GLU
1	D	437	MET
1	D	523	GLU
1	D	531	LYS
1	D	534	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	519	ASN
1	A	524	HIS
1	B	373	HIS
1	B	519	ASN
1	C	398	HIS
1	C	488	HIS
1	C	519	ASN
1	C	524	HIS
1	D	519	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

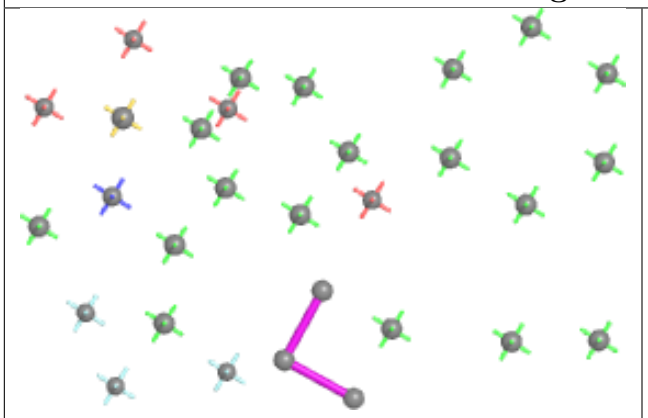
There are no torsion outliers.

There are no ring outliers.

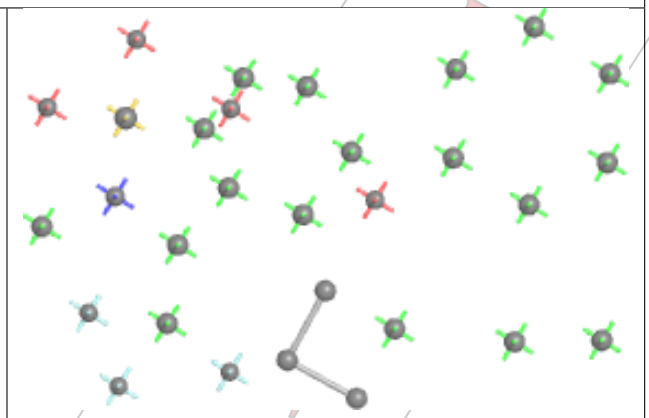
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

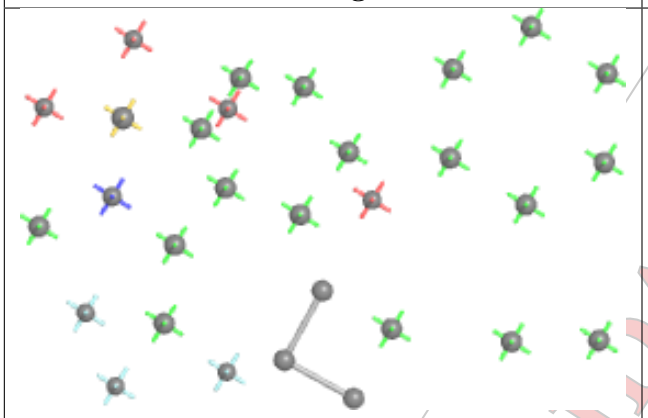
Ligand LIG E 3



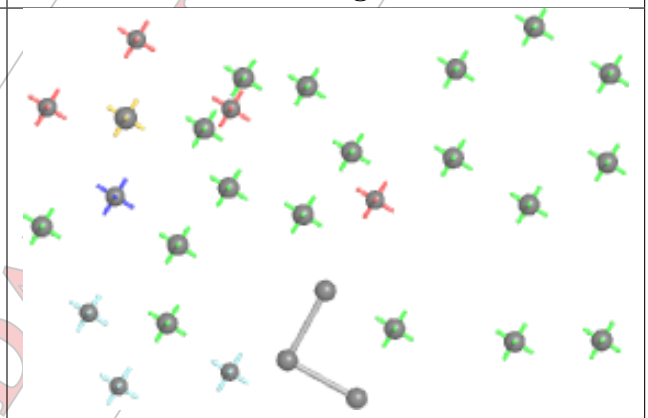
Bond lengths



Bond angles

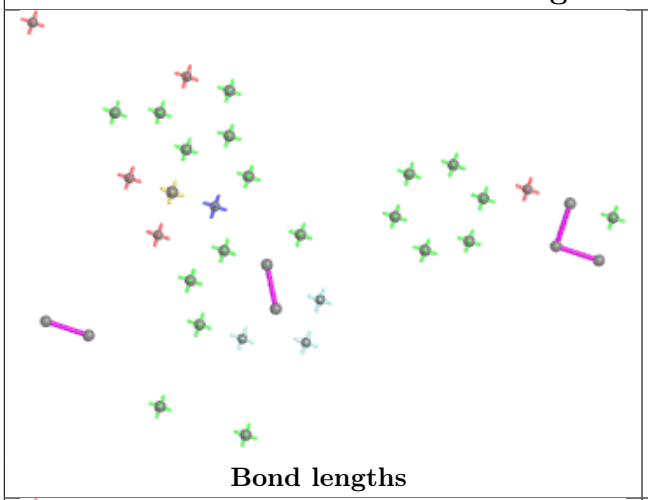


Torsions

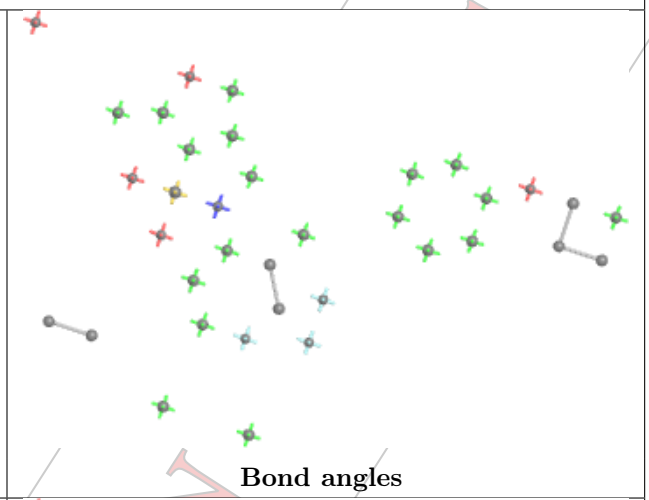


Rings

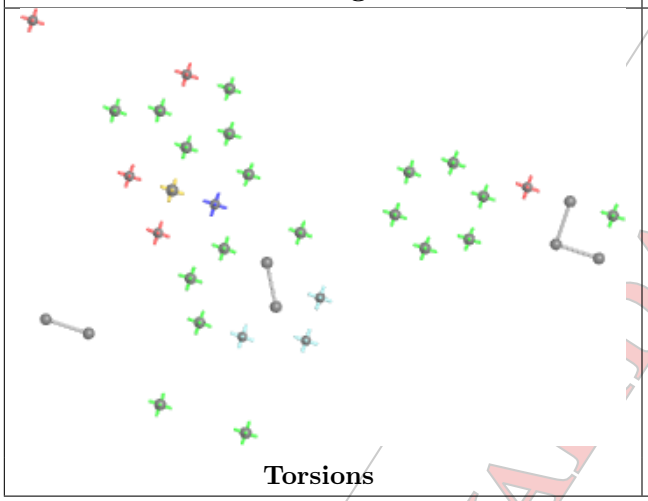
Ligand LIG E 4



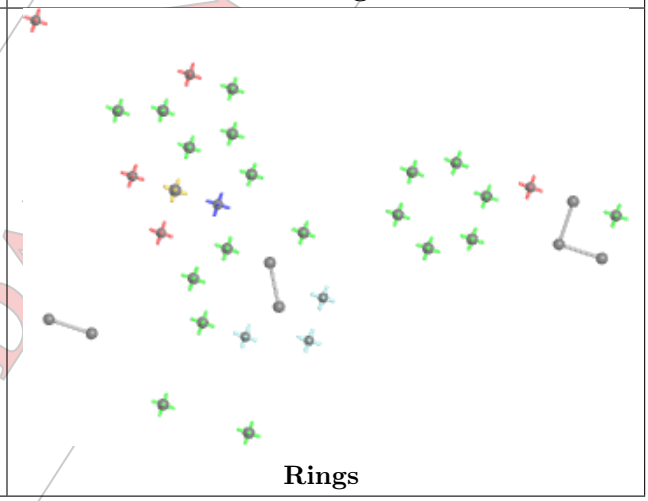
Bond lengths



Bond angles

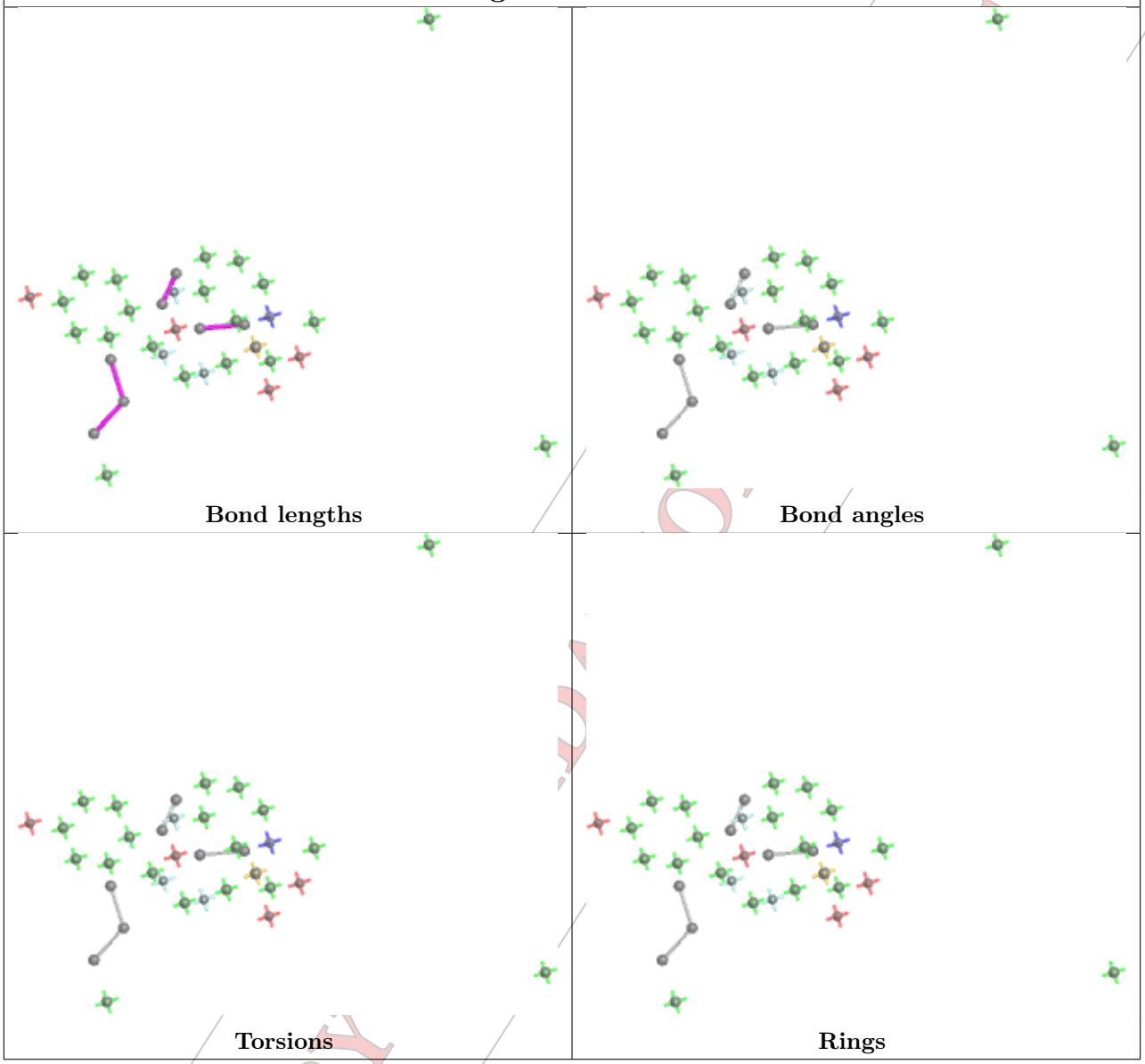


Torsions

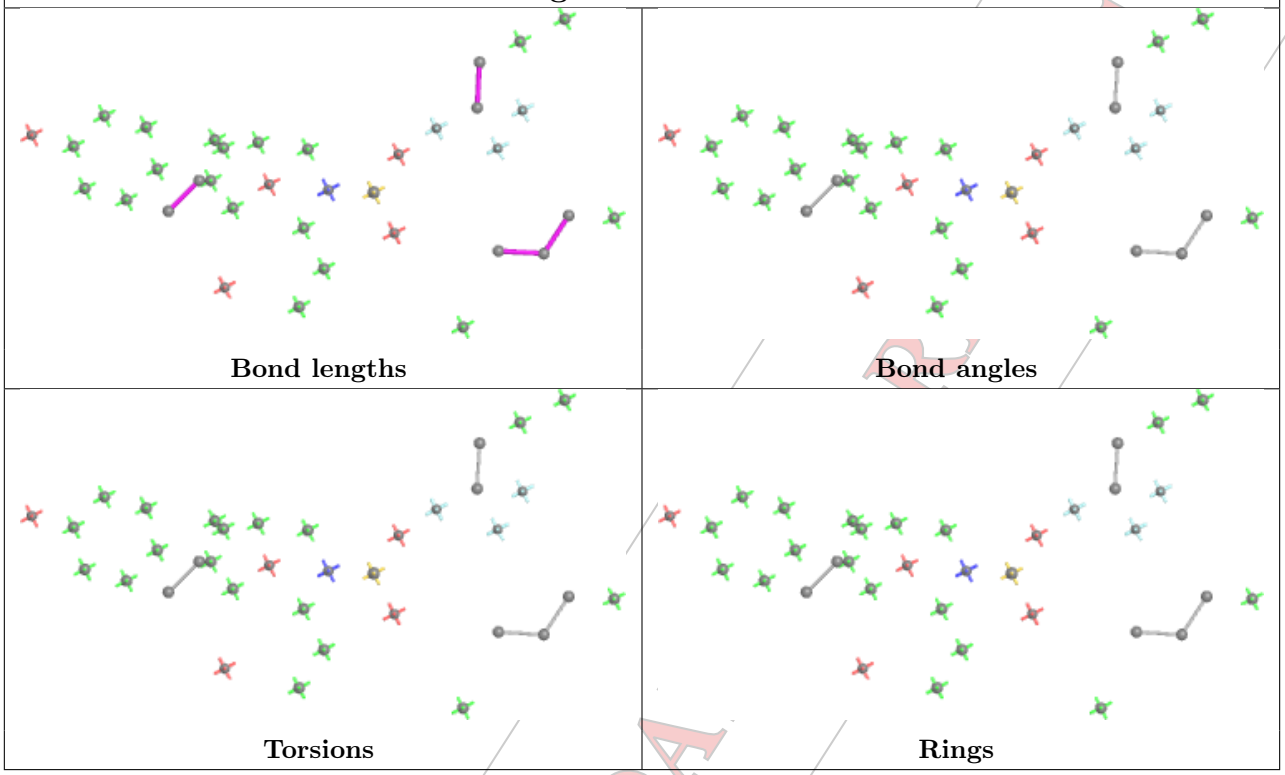


Rings

Ligand LIG E 1



Ligand LIG E 2



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	242/257 (94%)	0.68	29 (11%)	4	5	17, 36, 78, 114	0
1	B	225/257 (87%)	0.45	11 (4%)	29	33	18, 34, 68, 92	0
1	C	236/257 (91%)	0.58	20 (8%)	10	12	18, 33, 79, 126	0
1	D	222/257 (86%)	0.50	19 (8%)	10	12	19, 33, 74, 96	0
All	All	925/1028 (89%)	0.56	79 (8%)	10	12	17, 34, 77, 126	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	526	TYR	8.5
1	C	464	SER	8.2
1	C	462	LEU	7.5
1	A	462	LEU	7.1
1	A	530	CYS	6.8
1	C	420	GLY	6.4
1	A	464	SER	6.3
1	B	546	ALA	6.0
1	D	420	GLY	5.9
1	A	463	SER	5.4
1	D	546	ALA	5.4
1	D	461	PHE	5.2
1	A	305	SER	4.6
1	A	466	LEU	4.5
1	D	545	ASP	4.4
1	D	305	SER	3.9
1	B	331	TYR	3.9
1	C	463	SER	3.9
1	A	418	VAL	3.8
1	C	421	MET	3.7
1	B	413	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	304	ASN	3.6
1	D	467	LYS	3.6
1	C	305	SER	3.5
1	B	530	CYS	3.5
1	A	437	MET	3.5
1	C	461	PHE	3.5
1	A	526	TYR	3.4
1	A	332	ASP	3.4
1	A	306	LEU	3.4
1	A	417	CYS	3.4
1	A	528	MET	3.3
1	D	422	VAL	3.2
1	B	526	TYR	3.2
1	A	421	MET	3.2
1	D	534	VAL	3.1
1	B	462	LEU	3.1
1	C	524	HIS	3.1
1	D	415	GLY	3.0
1	C	528	MET	3.0
1	A	461	PHE	2.9
1	D	468	SER	2.9
1	B	545	ASP	2.9
1	D	413	ASN	2.8
1	D	421	MET	2.8
1	A	413	ASN	2.8
1	A	330	GLU	2.8
1	A	415	GLY	2.7
1	C	465	THR	2.7
1	A	524	HIS	2.7
1	A	492	LYS	2.7
1	C	460	THR	2.7
1	D	459	TYR	2.6
1	B	524	HIS	2.6
1	A	532	ASN	2.6
1	C	469	LEU	2.6
1	A	416	LYS	2.5
1	C	425	PHE	2.5
1	D	544	LEU	2.5
1	C	437	MET	2.5
1	C	332	ASP	2.4
1	A	308	LEU	2.4
1	D	460	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	531	LYS	2.3
1	A	331	TYR	2.3
1	A	469	LEU	2.3
1	C	466	LEU	2.2
1	A	468	SER	2.2
1	D	419	GLU	2.2
1	A	525	LEU	2.1
1	C	306	LEU	2.1
1	C	418	VAL	2.1
1	D	306	LEU	2.1
1	D	409	LEU	2.1
1	B	342	MET	2.1
1	B	501	HIS	2.1
1	C	525	LEU	2.0
1	B	423	GLU	2.0
1	D	469	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

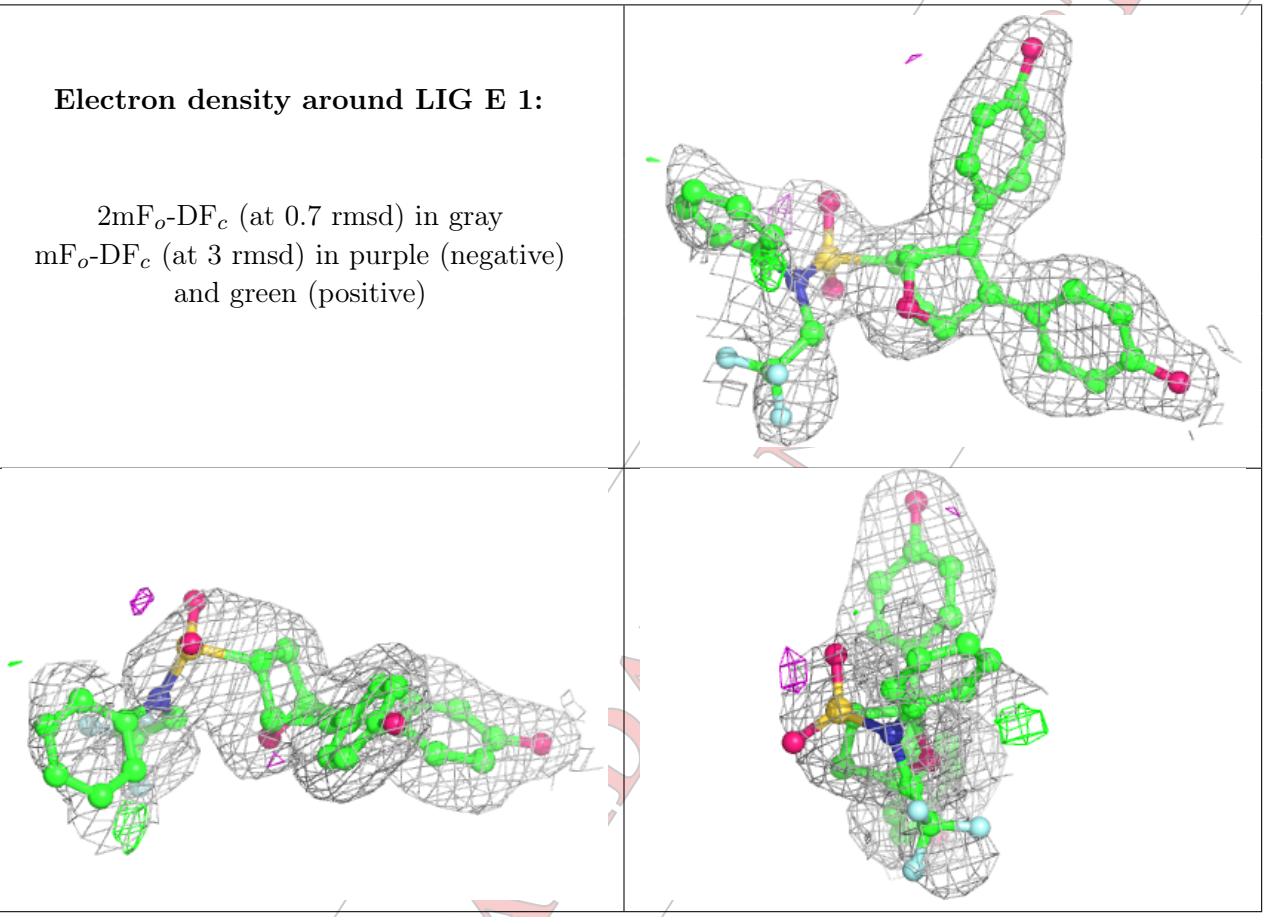
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	E	1	36/?	0.89	0.15	30,58,129,171	0
2	LIG	E	2	37/?	0.89	0.14	27,53,78,83	0
2	LIG	E	3	31/?	0.90	0.11	27,45,125,136	0
2	LIG	E	4	37/?	0.91	0.12	22,44,71,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

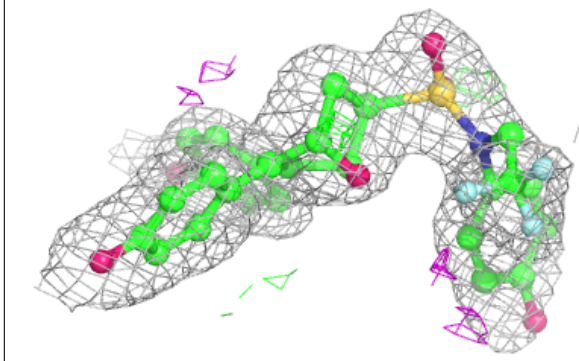
Electron density around LIG E 1:

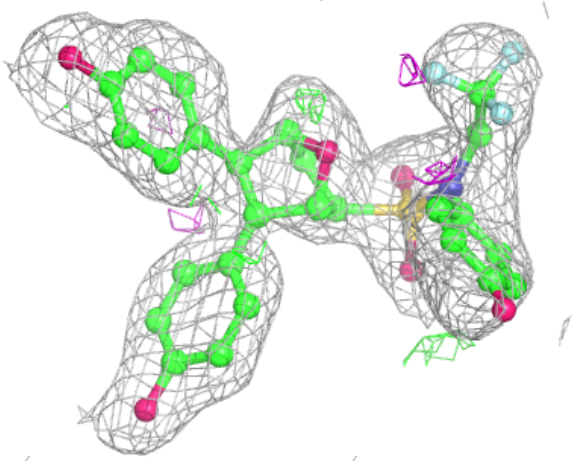
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

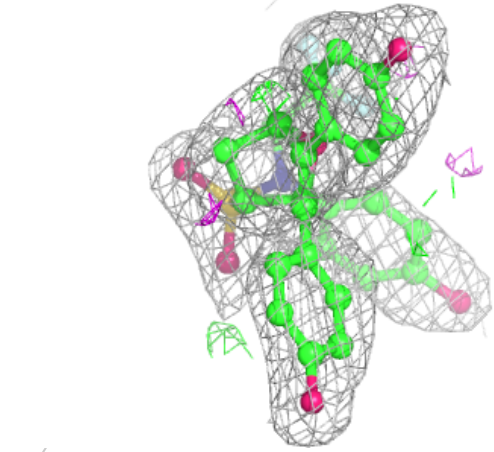


Electron density around LIG E 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

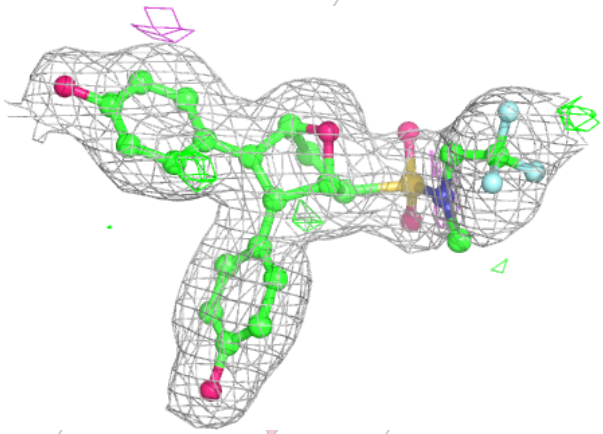


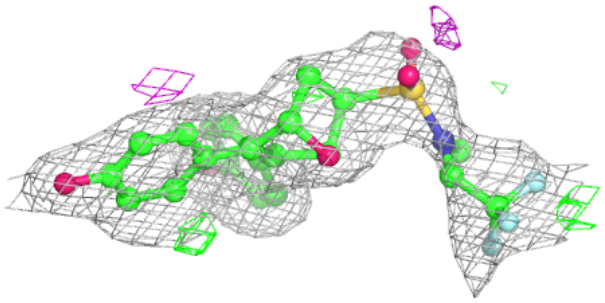


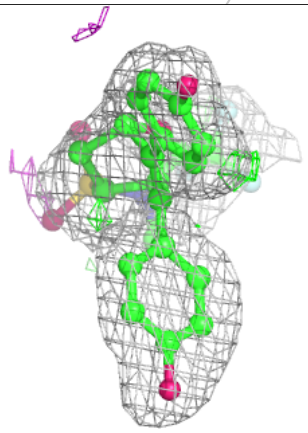


Electron density around LIG E 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

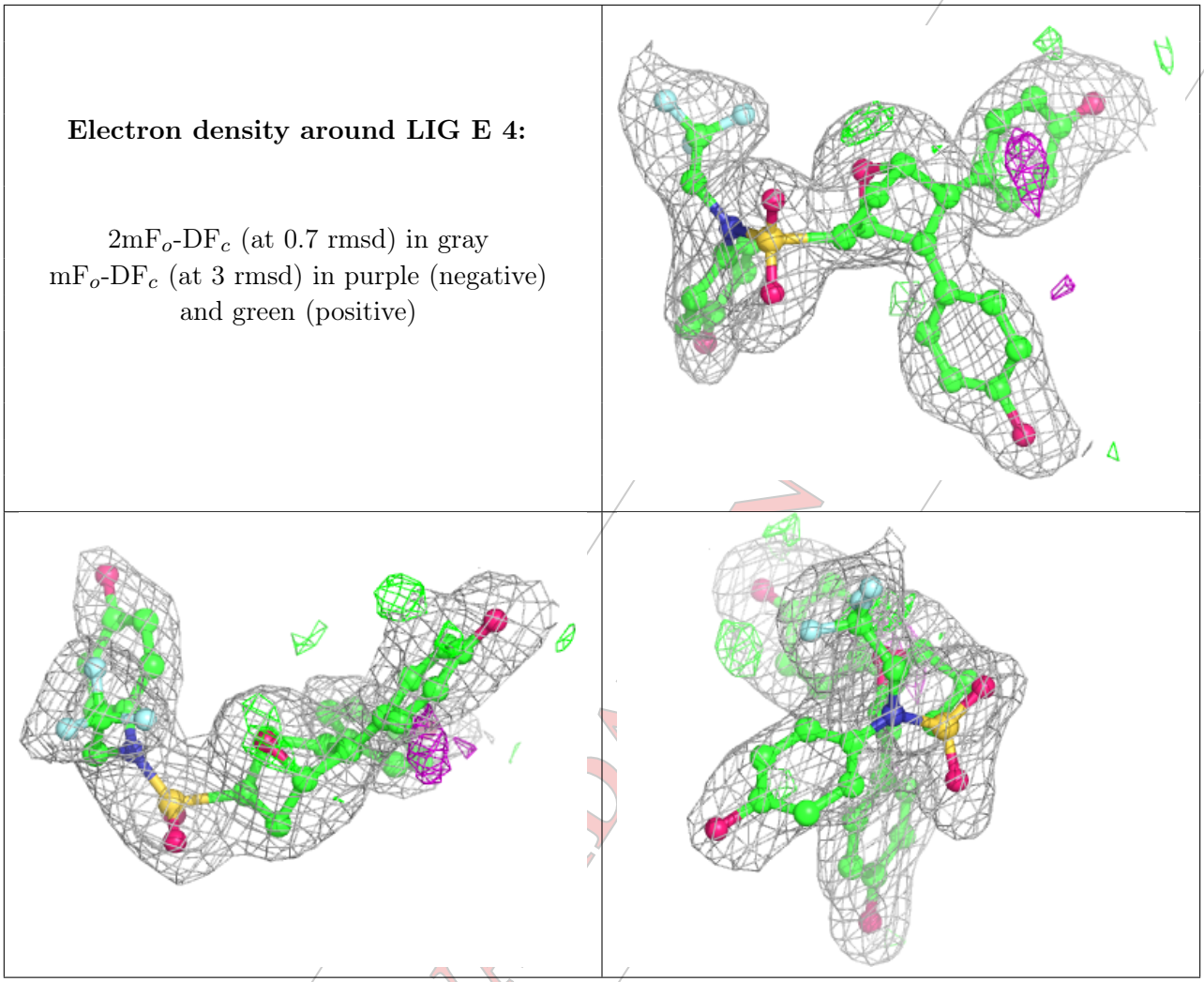






Electron density around LIG E 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 10:51 PM EDT

Deposition ID : D_1000251221

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

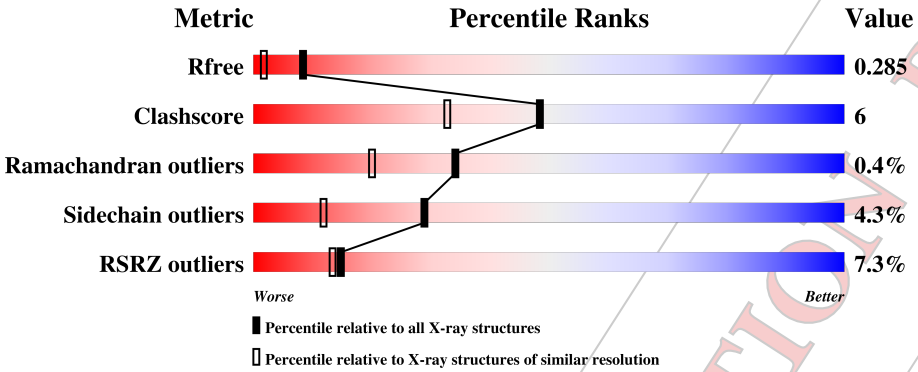
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	8% 69% 16% • 13%
1	B	257	5% 73% 9% • 18%
1	C	257	2% 71% 5% 23%
1	D	257	9% 77% 13% •• 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7212 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

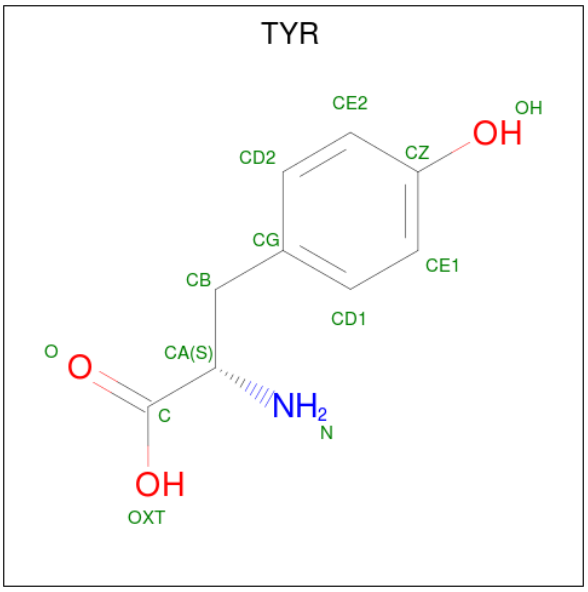
- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1779	1138	302	321	18			
1	B	212	Total	C	N	O	S	0	0	0
			1681	1074	292	299	16			
1	C	198	Total	C	N	O	S	0	1	0
			1591	1017	276	284	14			
1	D	237	Total	C	N	O	S	0	0	0
			1890	1208	321	343	18			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

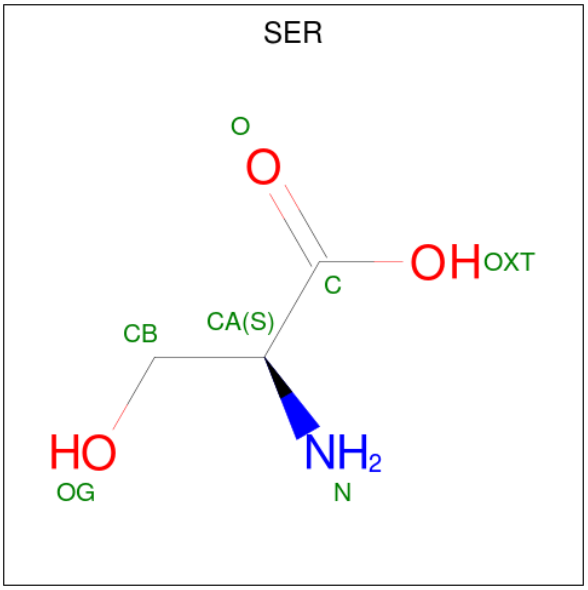
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		
2	B	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		
2	C	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		
2	D	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		

- Molecule 3 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



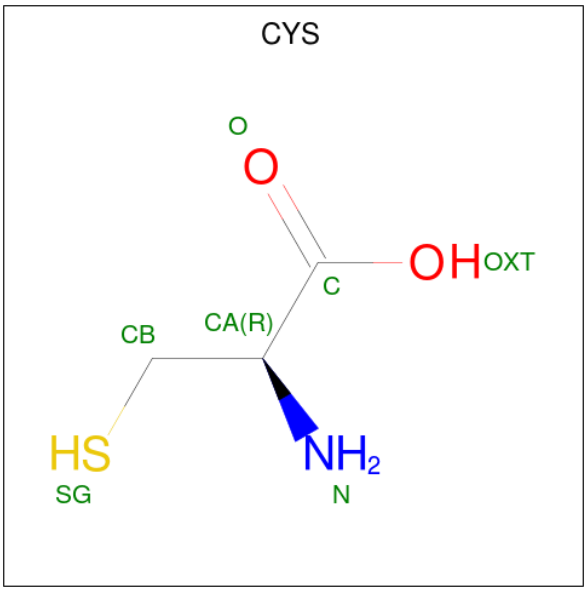
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 5 3 1 1	0	0
3	C	1	Total C N O 5 3 1 1	0	0

- Molecule 4 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 5 3 1 1	0	0

- Molecule 5 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 5 3 1 1	0	0

- Molecule 6 is water.

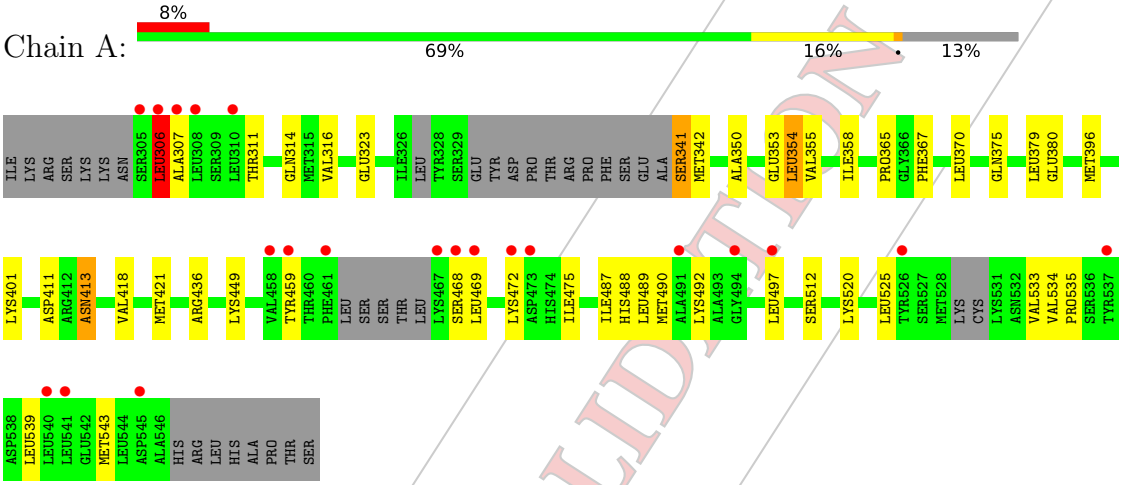
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	71	Total O 71 71	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

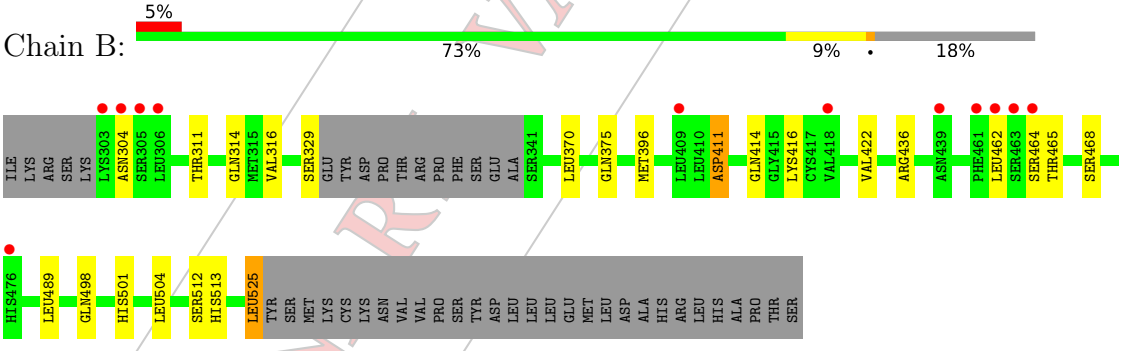
• Molecule 1: Estrogen Receptor

Chain A:



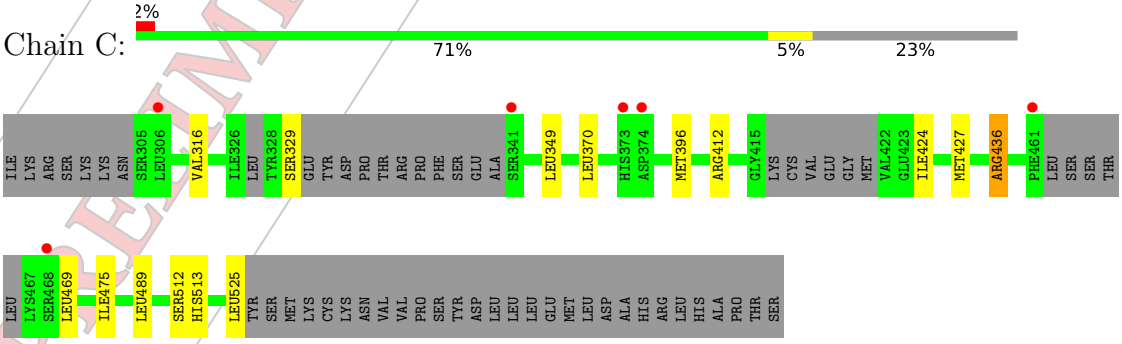
• Molecule 1: Estrogen Receptor

Chain B:

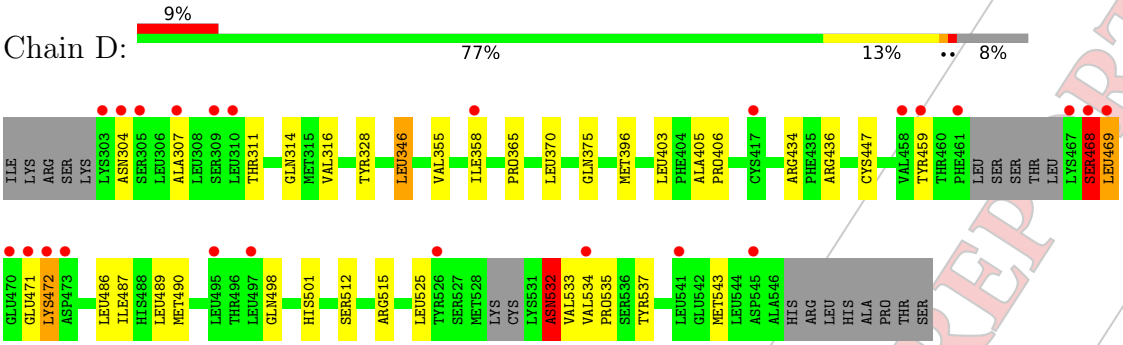


• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.56Å 58.98Å 91.67Å 89.03° 74.59° 63.60°	Depositor
Resolution (Å)	87.76 – 1.84 87.76 – 1.84	Depositor EDS
% Data completeness (in resolution range)	51.0 (87.76-1.84) 51.0 (87.76-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.283 0.243 , 0.285	Depositor DCC
R_{free} test set	2072 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.209 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7212	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.54	0/1796	0.74	1/2419 (0.0%)
1	B	0.52	0/1698	0.73	0/2289
1	C	0.52	0/1605	0.74	2/2160 (0.1%)
1	D	0.53	0/1913	0.73	0/2582
All	All	0.53	0/7012	0.73	3/9450 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	436	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	306	LEU	CA-CB-CG	6.03	129.16	115.30
1	C	349	LEU	CB-CG-CD2	-5.63	101.42	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	462	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1779	0	1812	34	0
1	B	1681	0	1737	20	0
1	C	1591	0	1629	7	0
1	D	1890	0	1921	28	0
2	A	45	0	1	2	0
2	B	45	0	1	0	0
2	C	45	0	1	0	0
2	D	45	0	1	3	0
3	B	5	0	1	0	0
3	C	5	0	1	0	0
4	B	5	0	2	0	0
5	B	5	0	2	0	0
6	S	71	0	0	2	0
All	All	7212	0	7109	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:CYS:HB3	1:D:486:LEU:HD21	1.58	0.84
1:B:311:THR:H	1:B:314:GLN:HE21	1.26	0.82
1:A:534:VAL:HG22	1:A:535:PRO:HD2	1.64	0.80
1:A:367:PHE:HZ	1:A:379:LEU:CD2	1.99	0.75
1:D:469:LEU:O	1:D:472:LYS:HG3	1.87	0.75
1:A:367:PHE:CZ	1:A:379:LEU:CD2	2.70	0.74
1:B:311:THR:H	1:B:314:GLN:NE2	1.85	0.74
1:D:447:CYS:HB3	1:D:486:LEU:CD2	2.17	0.73
1:A:358:ILE:HD13	1:A:543:MET:HE2	1.69	0.73
1:D:358:ILE:HD13	1:D:543:MET:HE2	1.71	0.71
1:A:367:PHE:CZ	1:A:379:LEU:HD21	2.26	0.71
1:D:487:ILE:HD13	1:D:490:MET:CE	2.24	0.67
1:A:487:ILE:HD13	1:A:490:MET:CE	2.25	0.67
1:B:504:LEU:C	1:B:504:LEU:HD13	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:MET:HE3	1:A:418:VAL:HG23	1.79	0.63
1:B:465:THR:HG23	1:B:468:SER:HB2	1.81	0.63
1:A:534:VAL:CG2	1:A:535:PRO:HD2	2.28	0.63
1:A:342:MET:CE	1:A:418:VAL:HG23	2.31	0.61
1:D:447:CYS:CB	1:D:486:LEU:HD21	2.31	0.60
1:A:367:PHE:HZ	1:A:379:LEU:HD23	1.67	0.58
1:A:306:LEU:H	1:A:306:LEU:HD22	1.70	0.57
1:A:375:GLN:O	1:A:379:LEU:HD23	2.05	0.56
1:B:416:LYS:HA	1:B:422:VAL:HG22	1.86	0.56
1:C:424:ILE:HD13	1:C:427:MET:CE	2.36	0.55
1:A:396:MET:O	1:A:436:ARG:HD3	2.06	0.55
1:A:468:SER:O	1:A:472:LYS:HD3	2.06	0.55
1:D:525:LEU:HD21	1:D:534:VAL:CG2	2.36	0.55
1:D:534:VAL:HG13	1:D:535:PRO:HD2	1.88	0.54
1:A:487:ILE:HD13	1:A:490:MET:HE3	1.90	0.54
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.90	0.54
1:B:436:ARG:NH1	6:S:19:HOH:O	2.37	0.54
1:D:487:ILE:HD13	1:D:490:MET:HE3	1.90	0.53
1:C:396:MET:O	1:C:436:ARG:HD3	2.10	0.52
1:D:447:CYS:CB	1:D:486:LEU:CD2	2.87	0.52
1:D:346:LEU:HB3	2:D:601:LIG:C15	2.40	0.52
1:B:465:THR:CG2	1:B:468:SER:HB2	2.40	0.51
1:B:525:LEU:O	1:B:525:LEU:HD22	2.10	0.51
1:C:316:VAL:HG21	1:C:489:LEU:HD21	1.93	0.51
1:B:311:THR:N	1:B:314:GLN:HE21	2.02	0.51
1:A:413:ASN:N	1:A:413:ASN:HD22	2.08	0.51
1:A:459:TYR:CD2	1:B:513:HIS:HB2	2.45	0.51
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.93	0.51
1:A:323:GLU:OE1	1:A:449:LYS:NZ	2.30	0.50
1:D:525:LEU:HD22	2:D:601:LIG:C27	2.42	0.50
1:B:525:LEU:C	1:B:525:LEU:HD22	2.33	0.49
1:A:534:VAL:HG22	1:A:535:PRO:CD	2.40	0.49
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.95	0.49
1:D:307:ALA:HB1	1:D:365:PRO:HB3	1.95	0.49
1:B:411:ASP:H	1:B:414:GLN:NE2	2.11	0.48
1:A:307:ALA:HB1	1:A:365:PRO:HB3	1.95	0.48
1:A:311:THR:HG23	1:A:314:GLN:H	1.79	0.48
1:A:468:SER:O	1:A:472:LYS:CD	2.62	0.48
1:A:488:HIS:NE2	1:A:492:LYS:HD2	2.30	0.47
1:C:513:HIS:HB2	1:D:459:TYR:CD2	2.49	0.47
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:THR:HG23	1:D:314:GLN:H	1.80	0.47
1:D:355:VAL:HG22	1:D:543:MET:HE3	1.97	0.47
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.50	0.46
1:A:355:VAL:HG22	1:A:543:MET:HE3	1.98	0.46
1:A:401:LYS:CD	1:A:411:ASP:HB3	2.46	0.45
1:D:403:LEU:HD12	1:D:405:ALA:O	2.16	0.45
1:B:525:LEU:CD2	1:B:525:LEU:C	2.85	0.45
1:D:328:TYR:CE1	1:D:406:PRO:HB2	2.51	0.45
1:B:411:ASP:H	1:B:414:GLN:HE21	1.64	0.45
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.99	0.44
1:D:525:LEU:HD13	2:D:601:LIG:C28	2.47	0.44
1:A:341:SER:HB3	6:S:13:HOH:O	2.16	0.44
1:B:396:MET:O	1:B:436:ARG:NE	2.47	0.44
1:A:413:ASN:H	1:A:413:ASN:HD22	1.65	0.44
1:A:525:LEU:HG	2:A:601:LIG:C27	2.47	0.44
1:D:532:ASN:HA	1:D:532:ASN:HD22	1.63	0.44
1:A:350:ALA:O	1:A:354:LEU:HD13	2.18	0.43
1:C:513:HIS:HB2	1:D:459:TYR:CE2	2.53	0.43
1:D:370:LEU:O	1:D:375:GLN:NE2	2.51	0.43
1:A:370:LEU:O	1:A:375:GLN:NE2	2.51	0.42
1:B:465:THR:HG23	1:B:468:SER:H	1.85	0.42
1:D:468:SER:HA	1:D:471:GLU:HG3	2.02	0.42
1:A:353:GLU:OE2	2:A:601:LIG:O20	2.38	0.42
1:A:401:LYS:HE3	1:A:411:ASP:HB3	2.01	0.41
1:D:311:THR:HG22	1:D:314:GLN:CD	2.41	0.41
1:C:513:HIS:CD2	1:D:459:TYR:HB2	2.54	0.41
1:A:370:LEU:HD11	1:A:475:ILE:HD11	2.02	0.41
1:D:396:MET:O	1:D:436:ARG:NE	2.48	0.41
1:B:504:LEU:C	1:B:504:LEU:CD1	2.86	0.40
1:B:370:LEU:O	1:B:375:GLN:NE2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/257 (83%)	211 (99%)	2 (1%)	0	100	100
1	B	207/257 (80%)	204 (99%)	3 (1%)	0	100	100
1	C	188/257 (73%)	187 (100%)	1 (0%)	0	100	100
1	D	230/257 (90%)	224 (97%)	3 (1%)	3 (1%)	12	3
All	All	838/1028 (82%)	826 (99%)	9 (1%)	3 (0%)	34	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	304	ASN
1	D	468	SER
1	D	532	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/232 (85%)	186 (94%)	12 (6%)	18	5
1	B	188/232 (81%)	182 (97%)	6 (3%)	39	21
1	C	177/232 (76%)	172 (97%)	5 (3%)	43	26
1	D	211/232 (91%)	201 (95%)	10 (5%)	26	10
All	All	774/928 (83%)	741 (96%)	33 (4%)	29	12

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	341	SER
1	A	354	LEU
1	A	380	GLU
1	A	413	ASN

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Mol	Chain	Res	Type
1	A	421	MET
1	A	469	LEU
1	A	497	LEU
1	A	512	SER
1	A	520	LYS
1	A	533	VAL
1	A	539	LEU
1	B	304	ASN
1	B	329	SER
1	B	411	ASP
1	B	464	SER
1	B	512	SER
1	B	525	LEU
1	C	329	SER
1	C	412	ARG
1	C	469	LEU
1	C	512	SER
1	C	525	LEU
1	D	346	LEU
1	D	434	ARG
1	D	468	SER
1	D	469	LEU
1	D	472	LYS
1	D	512	SER
1	D	515	ARG
1	D	532	ASN
1	D	533	VAL
1	D	537	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	413	ASN
1	A	519	ASN
1	B	314	GLN
1	B	414	GLN
1	B	488	HIS
1	B	519	ASN
1	C	398	HIS
1	C	488	HIS
1	C	519	ASN

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Mol	Chain	Res	Type
1	D	519	ASN
1	D	532	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 4 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

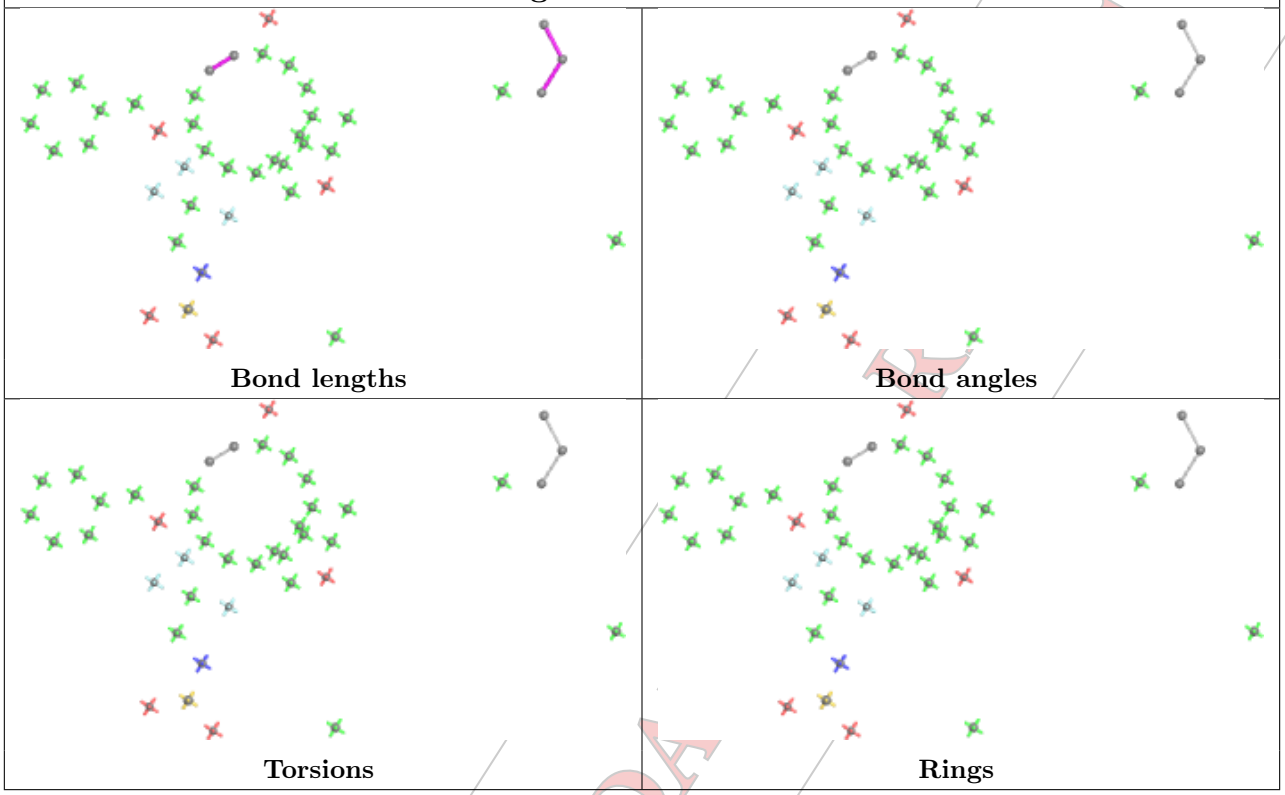
There are no torsion outliers.

There are no ring outliers.

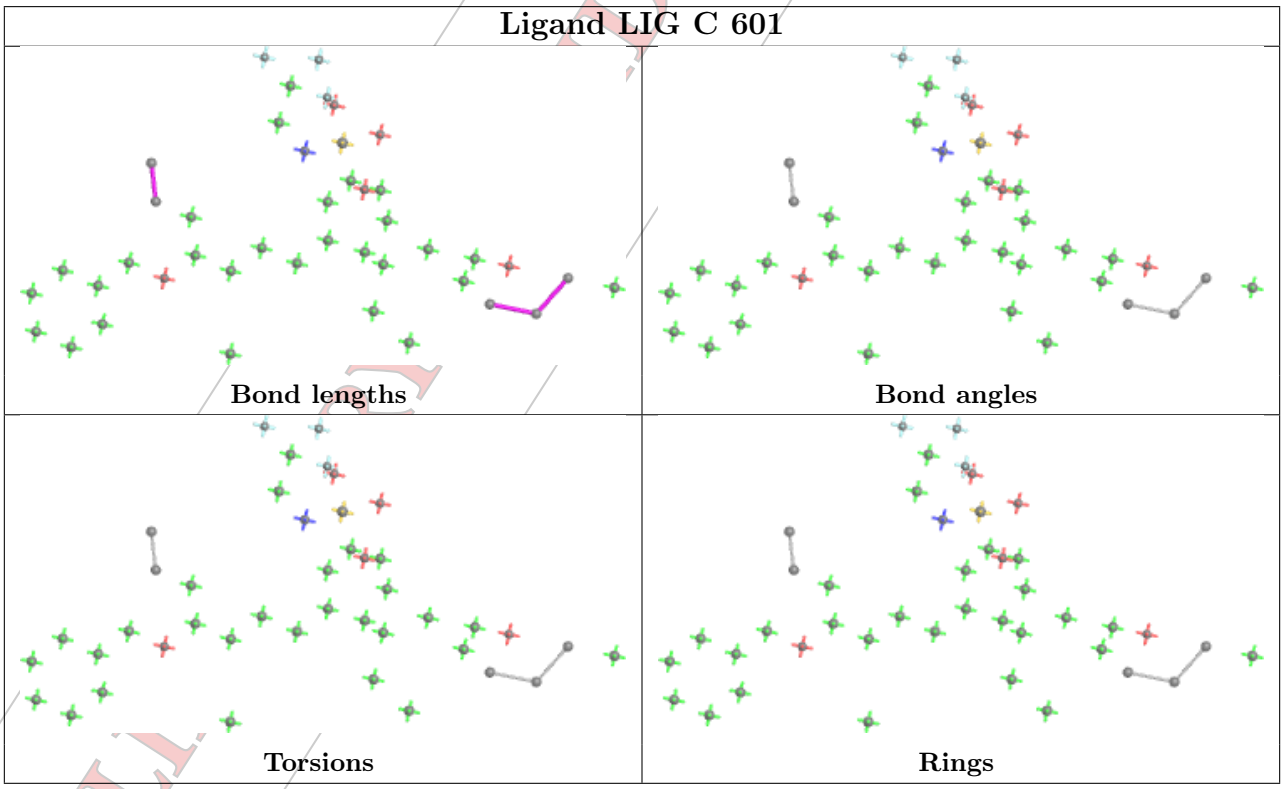
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

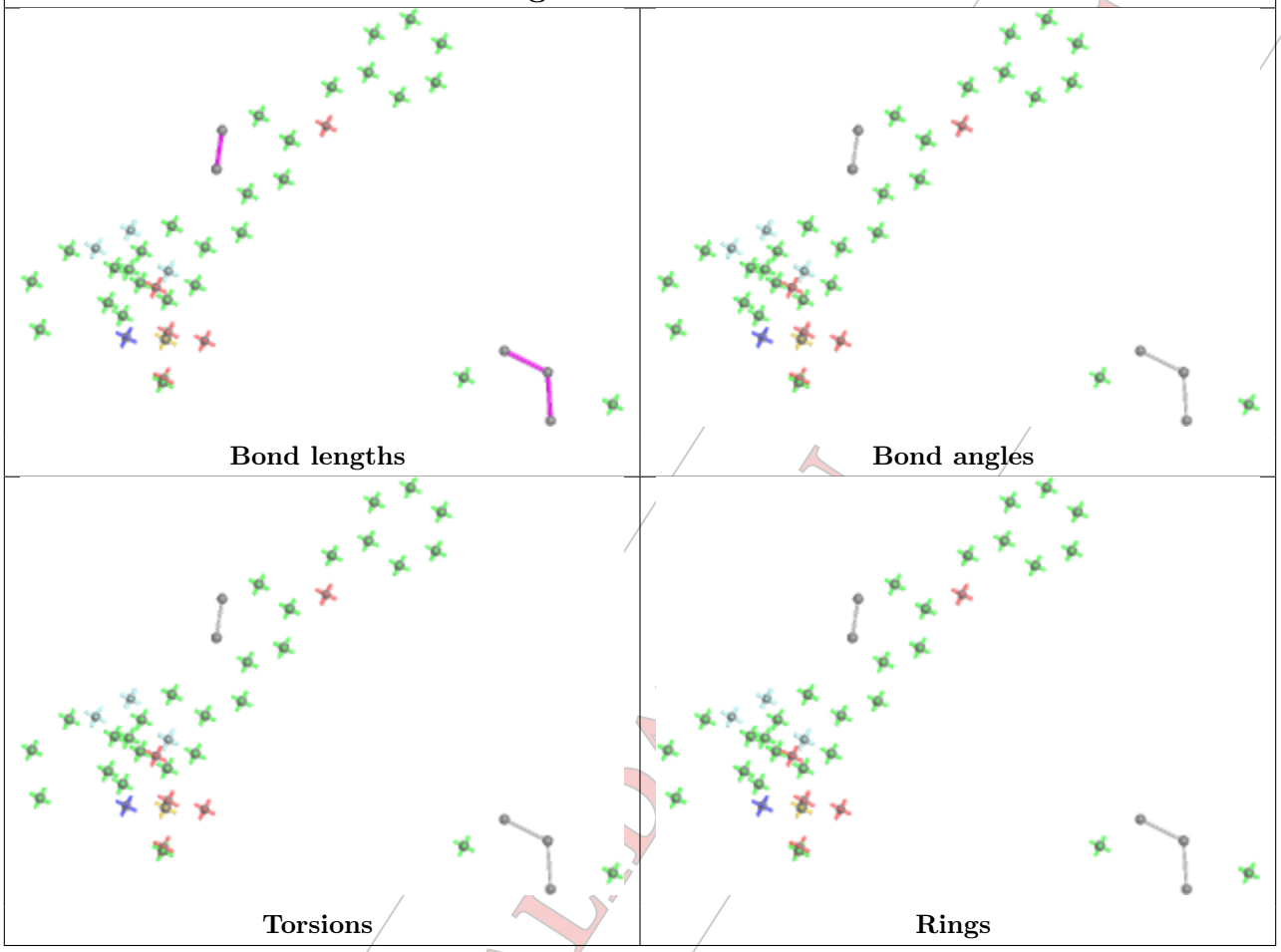
Ligand LIG A 601



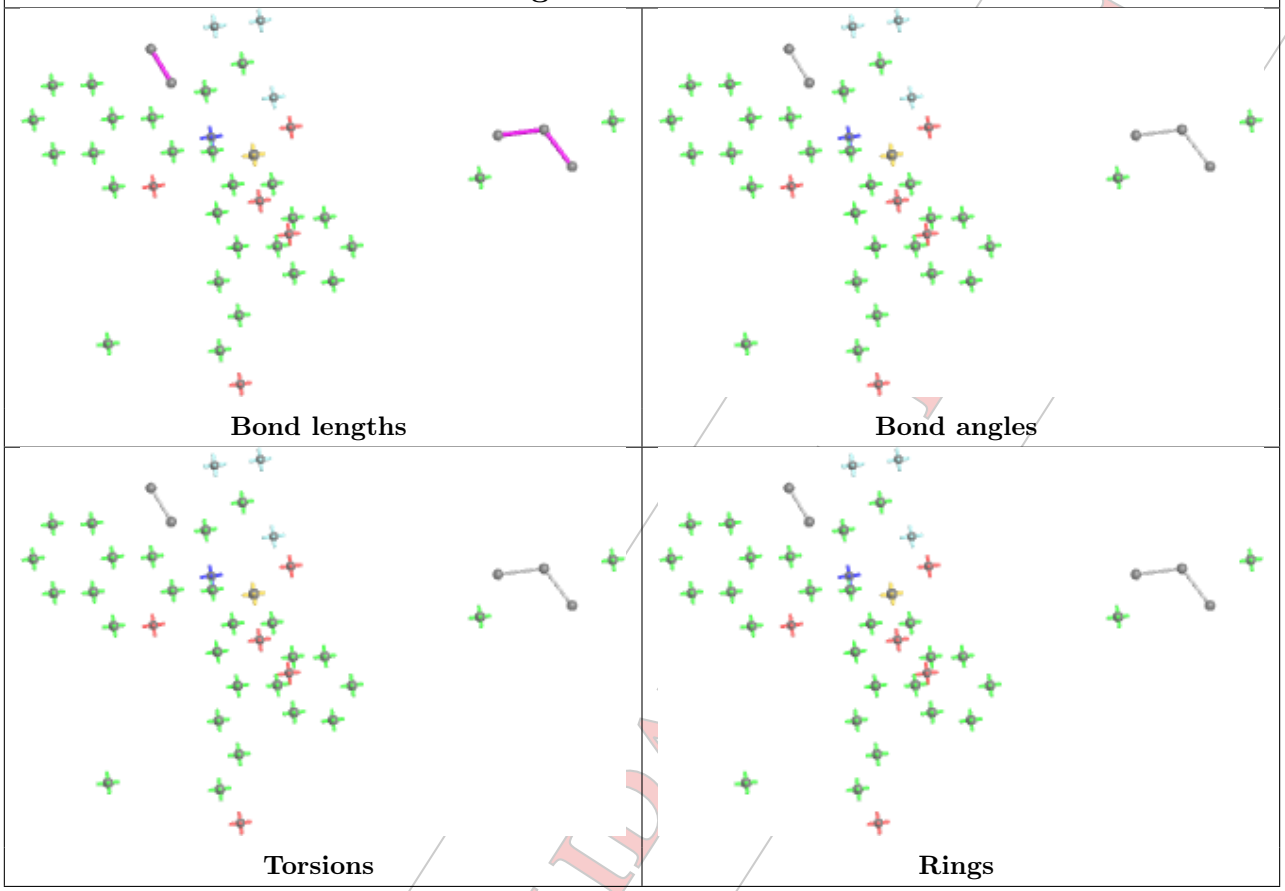
Ligand LIG C 601



Ligand LIG D 601



Ligand LIG B 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	222/257 (86%)	0.68	21 (9%) 8 7	19, 40, 88, 124	0
1	B	211/257 (82%)	0.44	12 (5%) 23 21	17, 36, 77, 102	0
1	C	197/257 (76%)	0.34	6 (3%) 50 47	17, 36, 74, 90	0
1	D	236/257 (91%)	0.77	24 (10%) 6 5	18, 41, 94, 135	0
All	All	866/1028 (84%)	0.57	63 (7%) 15 13	17, 38, 83, 135	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	459	TYR	13.2
1	A	459	TYR	12.3
1	D	305	SER	8.5
1	D	469	LEU	7.5
1	D	304	ASN	6.8
1	D	472	LYS	6.7
1	A	467	LYS	5.9
1	D	307	ALA	5.7
1	B	304	ASN	5.6
1	D	470	GLU	5.5
1	A	472	LYS	5.3
1	D	526	TYR	4.9
1	A	310	LEU	4.8
1	A	491	ALA	4.4
1	D	468	SER	4.4
1	A	308	LEU	4.3
1	B	305	SER	4.0
1	B	462	LEU	4.0
1	B	463	SER	3.9
1	A	458	VAL	3.9
1	D	458	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	467	LYS	3.8
1	C	373	HIS	3.8
1	D	473	ASP	3.7
1	D	497	LEU	3.7
1	A	306	LEU	3.5
1	D	310	LEU	3.5
1	C	461	PHE	3.5
1	A	305	SER	3.5
1	D	534	VAL	3.4
1	B	461	PHE	3.4
1	B	303	LYS	3.4
1	C	306	LEU	3.4
1	A	307	ALA	3.3
1	B	418	VAL	3.3
1	A	461	PHE	3.2
1	A	497	LEU	3.2
1	D	545	ASP	3.2
1	A	526	TYR	3.1
1	D	303	LYS	3.1
1	D	417	CYS	2.8
1	C	468	SER	2.7
1	A	473	ASP	2.6
1	A	545	ASP	2.6
1	D	358	ILE	2.6
1	C	341	SER	2.6
1	A	469	LEU	2.5
1	C	374	ASP	2.5
1	D	309	SER	2.4
1	A	494	GLY	2.4
1	B	306	LEU	2.3
1	D	471	GLU	2.3
1	A	537	TYR	2.3
1	A	541	LEU	2.3
1	A	468	SER	2.2
1	D	541	LEU	2.2
1	B	476	HIS	2.2
1	B	409	LEU	2.2
1	D	461	PHE	2.2
1	D	495	LEU	2.1
1	B	439	ASN	2.1
1	A	540	LEU	2.0
1	B	464	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

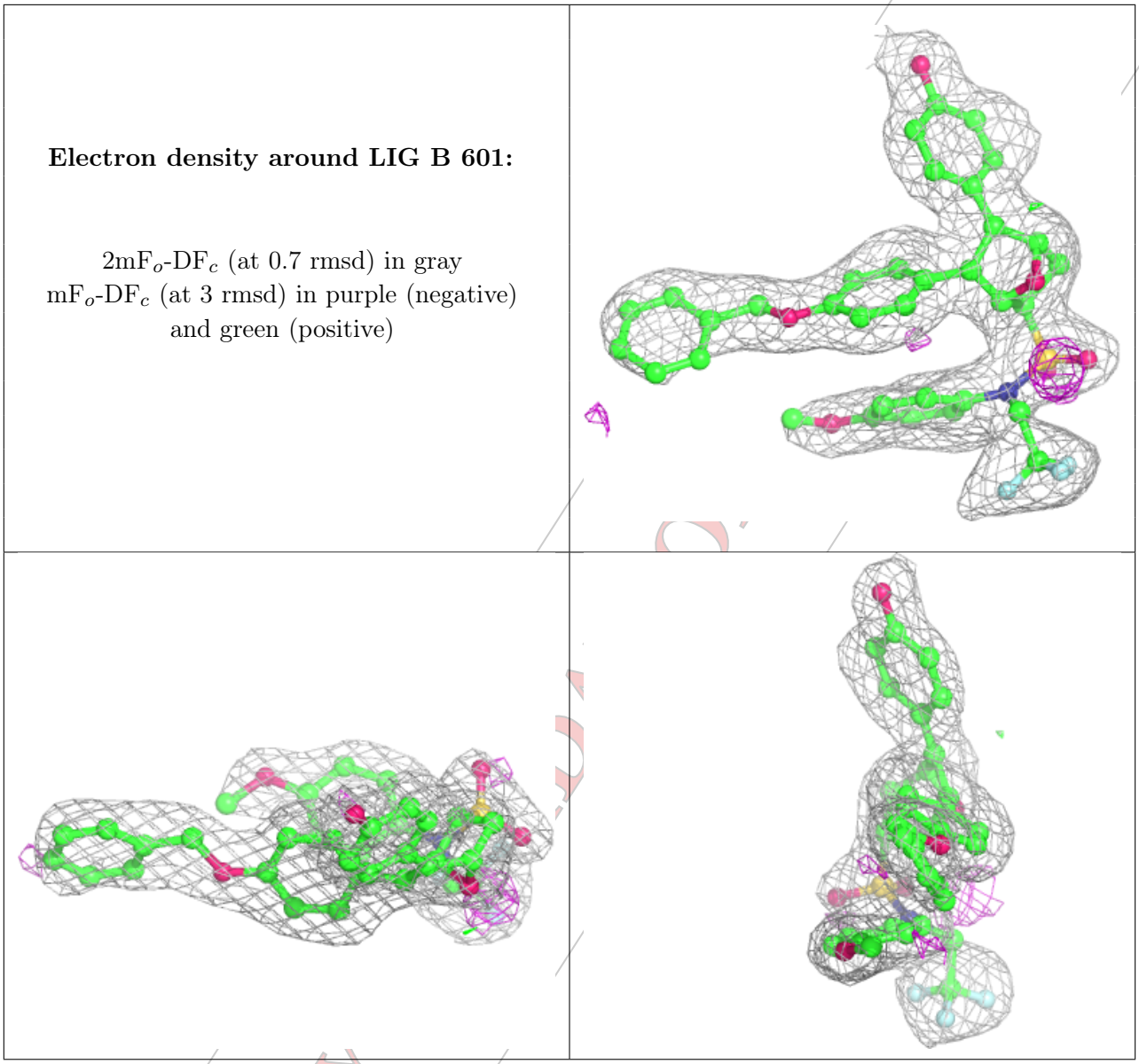
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TYR	B	526	5/?	0.74	0.19	30,30,30,30	0
3	TYR	C	526	5/?	0.78	0.22	30,30,30,30	0
4	SER	B	527	5/?	0.87	0.21	30,30,30,30	0
5	CYS	B	528	5/?	0.88	0.15	30,30,30,30	0
2	LIG	B	601	45/?	0.92	0.12	24,33,62,67	0
2	LIG	D	601	45/?	0.94	0.10	20,26,46,50	0
2	LIG	C	601	45/?	0.94	0.12	16,32,77,83	0
2	LIG	A	601	45/?	0.95	0.11	19,30,51,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

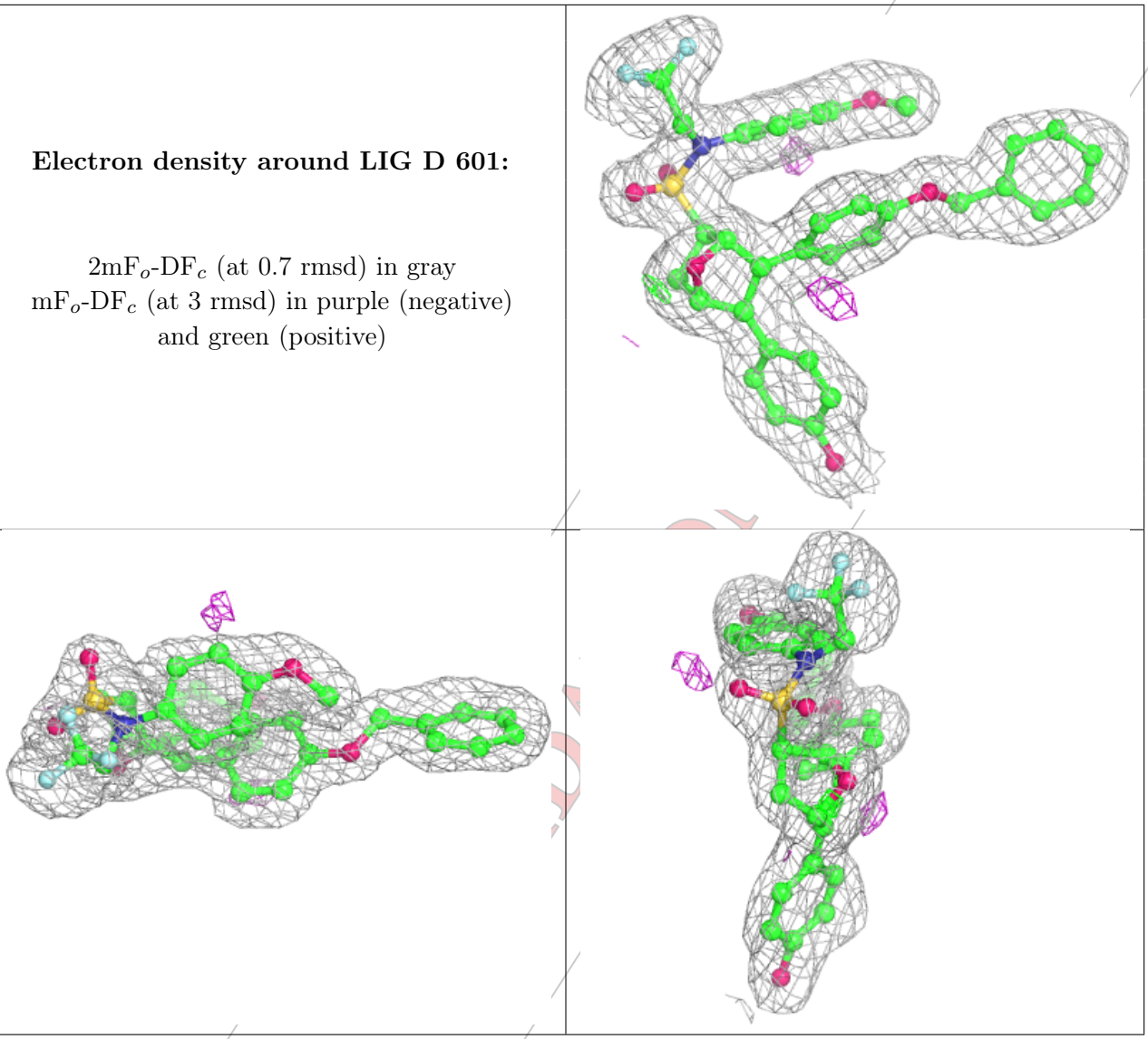
Electron density around LIG B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



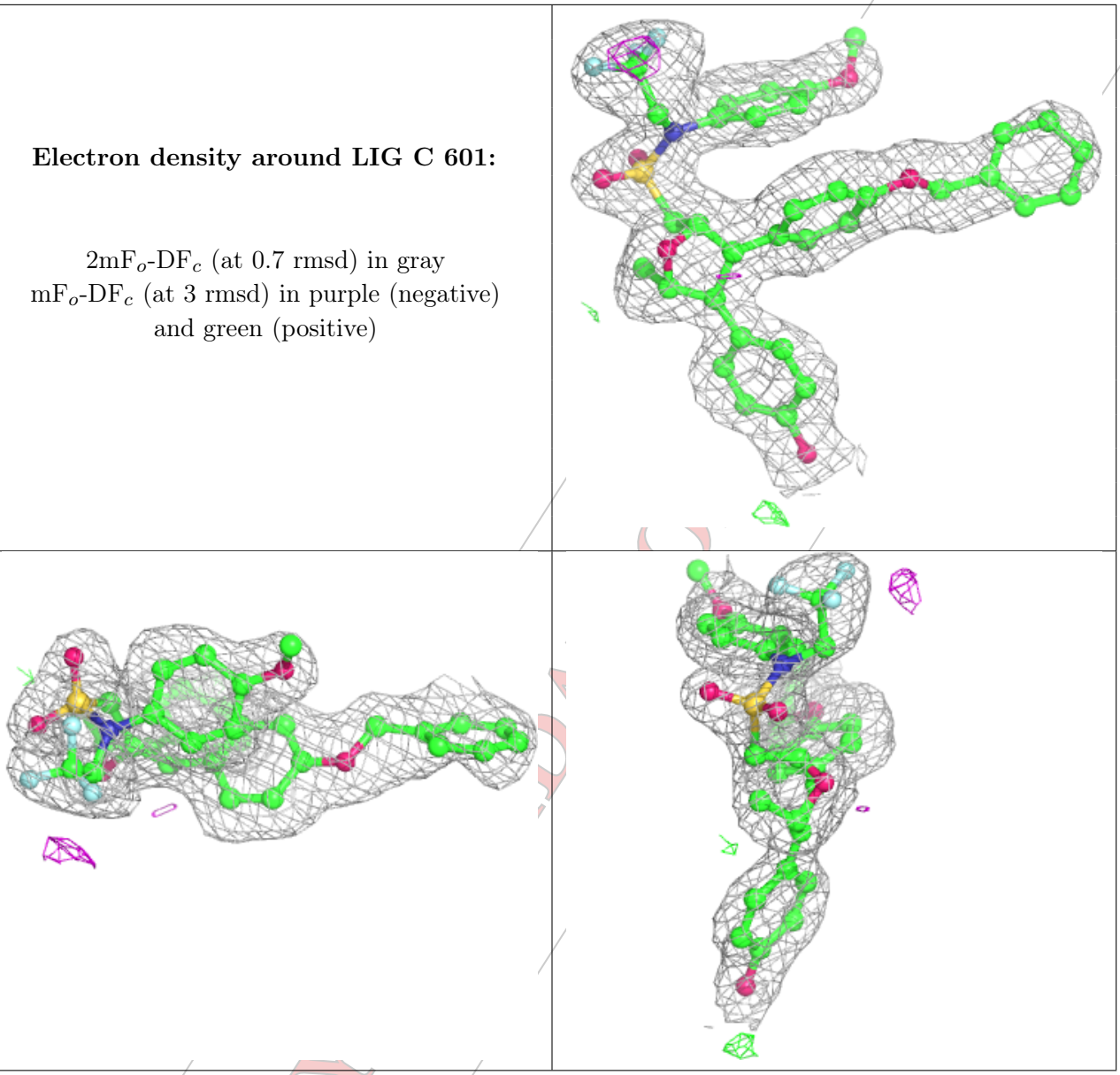
Electron density around LIG D 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



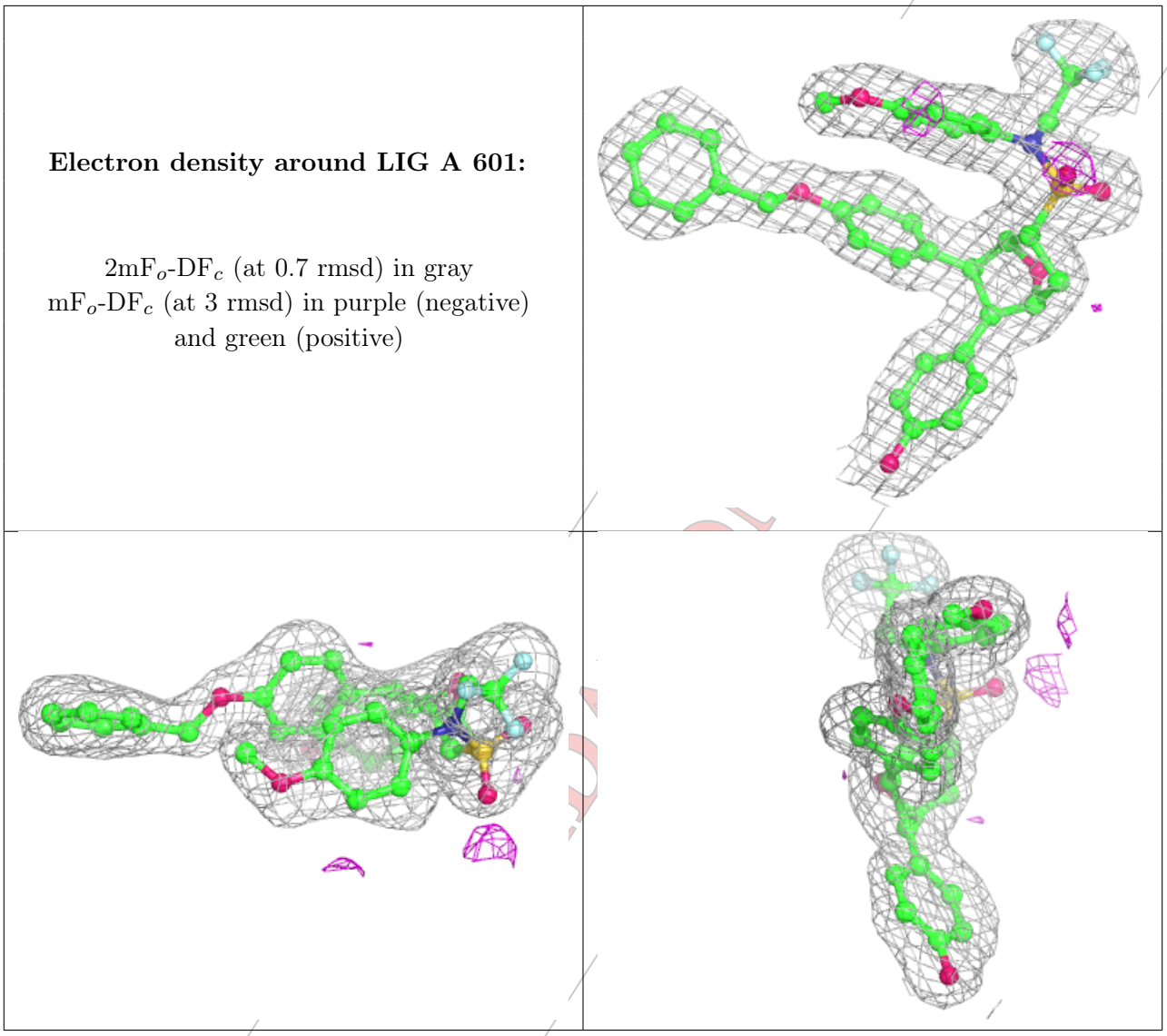
Electron density around LIG C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 11:03 PM EDT

Deposition ID : D_1000251222

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

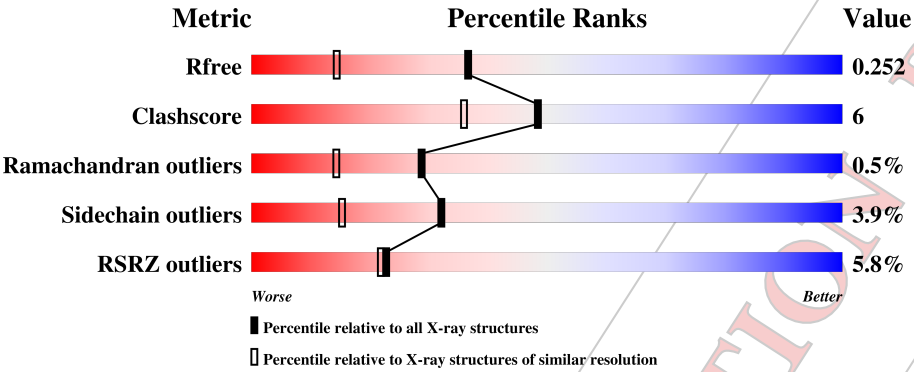
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	4% 84% 10% • 5%
1	B	257	7% 81% 13% • •
1	C	257	4% 83% 10% • 5%
1	D	257	7% 79% 15% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8147 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	1	0
			1956	1249	333	356	18			
1	B	246	Total	C	N	O	S	0	0	0
			1965	1254	337	355	19			
1	C	244	Total	C	N	O	S	0	0	0
			1944	1242	330	353	19			
1	D	243	Total	C	N	O	S	0	0	0
			1947	1245	336	347	19			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		

- Molecule 3 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total	C	Cl	F	N	O	0	0
			32	26	1	1	2	2		
3	E	1	Total	C	Cl	F	N	O	0	0
			32	26	1	1	2	2		
3	E	1	Total	C	Cl	F	N	O	0	0
			32	26	1	1	2	2		
3	E	1	Total	C	Cl	F	N	O	0	0
			32	26	1	1	2	2		

- Molecule 4 is water.

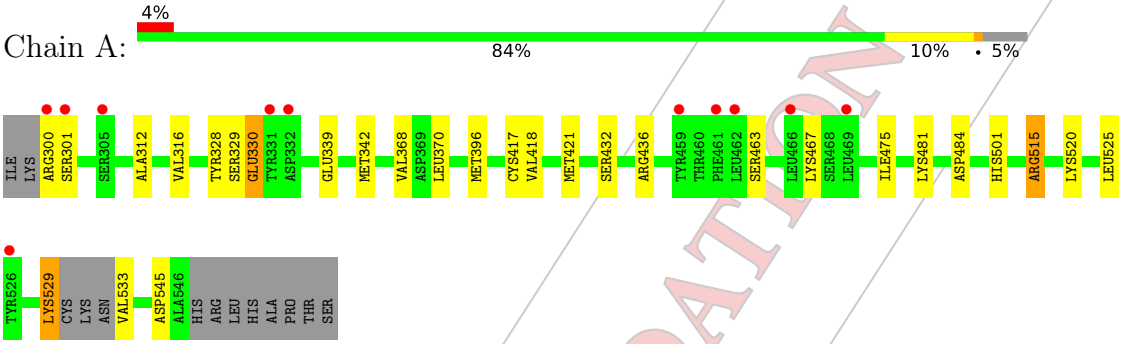
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	205	Total O 205 205	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

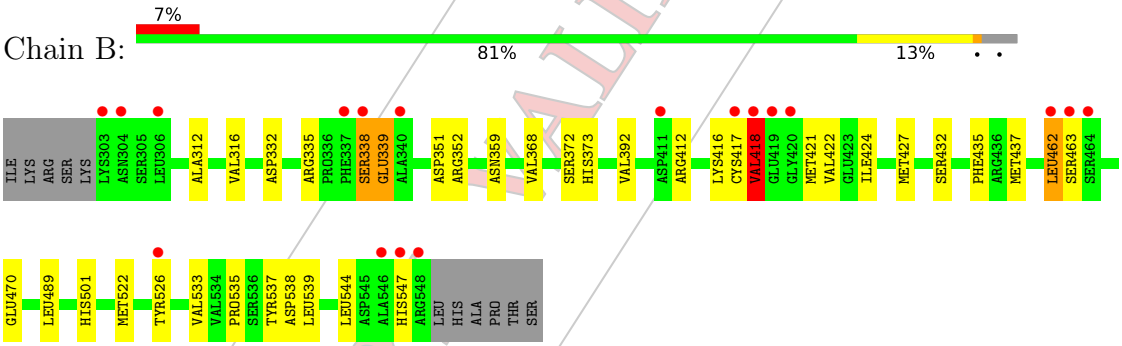
• Molecule 1: Estrogen Receptor

Chain A:



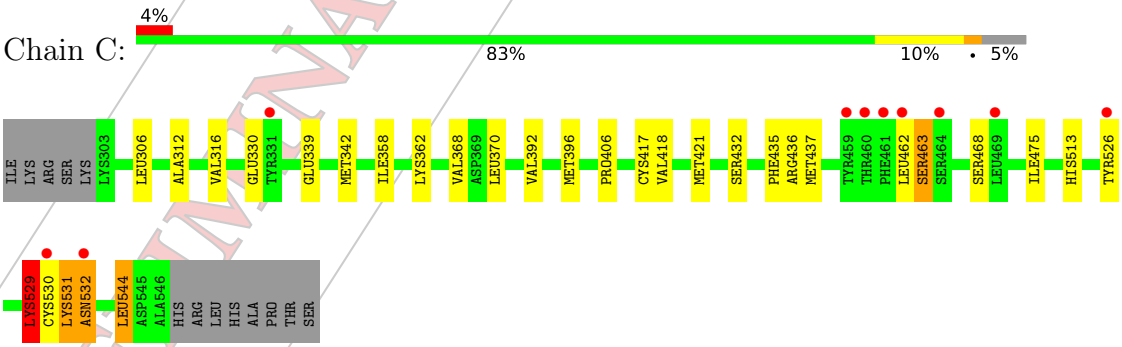
• Molecule 1: Estrogen Receptor

Chain B:



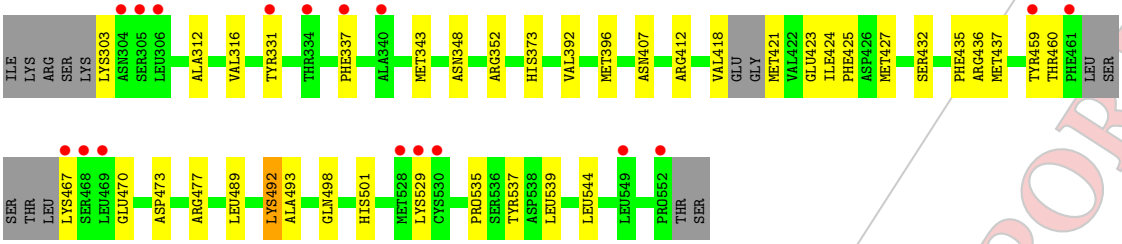
• Molecule 1: Estrogen Receptor

Chain C:



• Molecule 1: Estrogen Receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.09Å 58.82Å 93.71Å 86.88° 75.21° 63.40°	Depositor
Resolution (Å)	90.39 – 1.78 90.39 – 1.78	Depositor EDS
% Data completeness (in resolution range)	53.0 (90.39-1.78) 53.0 (90.39-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.251 0.205 , 0.252	Depositor DCC
R_{free} test set	2474 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.125 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8147	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LIG, YCM, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/1980	0.69	1/2671 (0.0%)
1	B	0.49	0/1991	0.71	0/2688
1	C	0.49	0/1969	0.71	0/2659
1	D	0.49	0/1973	0.68	0/2662
All	All	0.49	0/7913	0.70	1/10680 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	515	ARG	NE-CZ-NH1	5.56	123.08	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	338	SER	Peptide
1	C	529	LYS	Peptide
1	C	530	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1956	0	2002	18	2
1	B	1965	0	2011	29	2
1	C	1944	0	1991	28	0
1	D	1947	0	1991	27	0
2	F	2	0	0	1	0
3	E	128	0	4	2	0
4	S	205	0	0	14	0
All	All	8147	0	7999	95	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:HIS:HE1	4:S:11:HOH:O	1.50	0.94
1:D:343:MET:HG2	1:D:418:VAL:HG21	1.59	0.83
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.63	0.81
1:D:459:TYR:OH	4:S:120:HOH:O	1.99	0.80
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.65	0.78
1:A:525:LEU:HD13	1:A:533:VAL:HG11	1.65	0.78
1:B:417:CYS:O	1:B:418:VAL:HG13	1.85	0.77
1:C:342:MET:HE2	1:C:417:CYS:HB3	1.68	0.76
1:C:463:SER:OG	4:S:191:HOH:O	1.72	0.76
1:B:437:MET:HG3	4:S:207:HOH:O	1.85	0.75
1:C:463:SER:HB3	1:C:468:SER:HB2	1.70	0.73
1:B:338:SER:O	1:B:339:GLU:HG3	1.89	0.73
1:A:545:ASP:OD2	4:S:66:HOH:O	2.08	0.70
1:C:513:HIS:CD2	1:D:459:TYR:HD2	2.11	0.68
1:C:406:PRO:O	4:S:111:HOH:O	2.13	0.65
1:B:533:VAL:HG22	3:E:2:LIG:C21	2.28	0.64
1:A:501:HIS:CE1	4:S:11:HOH:O	2.35	0.64
1:C:532:ASN:CG	1:C:532:ASN:O	2.37	0.62
1:A:368:VAL:HG22	4:S:73:HOH:O	2.00	0.61
1:B:359:ASN:OD1	1:B:547:HIS:CE1	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:MET:O	1:A:436:ARG:HD3	2.01	0.60
1:C:396:MET:O	1:C:436:ARG:HD3	2.02	0.60
1:A:484:ASP:OD1	1:B:501:HIS:HE1	1.84	0.60
1:D:396:MET:O	1:D:436:ARG:HD3	2.02	0.60
1:D:489:LEU:O	1:D:492:LYS:HE3	2.03	0.59
1:A:418:VAL:CG1	1:A:421:MET:HE3	2.34	0.58
1:A:418:VAL:HG11	1:A:421:MET:HE3	1.84	0.57
1:C:531:LYS:HG3	1:C:532:ASN:H	1.68	0.57
1:B:501:HIS:HD2	4:S:11:HOH:O	1.87	0.56
1:B:338:SER:O	1:B:339:GLU:CG	2.53	0.56
1:B:332:ASP:HB3	1:B:335:ARG:HG2	1.88	0.55
1:D:535:PRO:HA	1:D:539:LEU:HD23	1.90	0.54
1:D:348:ASN:ND2	1:D:352:ARG:HH21	2.05	0.53
1:B:462:LEU:O	1:B:462:LEU:HD13	2.08	0.53
1:C:418:VAL:HG22	1:C:421:MET:HB2	1.91	0.53
1:B:338:SER:O	1:B:339:GLU:CB	2.57	0.53
1:A:418:VAL:HG22	1:A:421:MET:HB2	1.92	0.52
1:A:342:MET:CE	1:A:417:CYS:HB3	2.39	0.52
1:B:535:PRO:HA	1:B:539:LEU:HD23	1.91	0.52
1:C:513:HIS:CD2	1:D:459:TYR:CD2	2.96	0.52
1:C:532:ASN:ND2	1:C:532:ASN:O	2.43	0.52
1:D:492:LYS:C	1:D:492:LYS:HD2	2.30	0.52
1:A:342:MET:HE2	1:A:417:CYS:HB3	1.91	0.51
1:C:513:HIS:CE1	1:D:459:TYR:CE2	2.99	0.51
1:B:417:CYS:O	1:B:418:VAL:CG1	2.58	0.51
1:C:342:MET:CE	1:C:417:CYS:HB3	2.39	0.51
1:C:531:LYS:HG3	1:C:532:ASN:N	2.25	0.51
1:D:467:LYS:HB2	4:S:175:HOH:O	2.12	0.50
1:D:418:VAL:HB	1:D:421:MET:SD	2.52	0.50
1:D:423:GLU:HG3	1:D:424:ILE:N	2.25	0.50
1:B:418:VAL:HG22	1:B:421:MET:HB2	1.94	0.50
1:C:362:LYS:HD3	1:C:544:LEU:HD12	1.94	0.50
1:D:373:HIS:CD2	1:D:537:TYR:OH	2.65	0.50
1:B:373:HIS:CD2	1:B:537:TYR:OH	2.65	0.49
1:D:424:ILE:HD13	1:D:427:MET:CE	2.43	0.49
1:C:342:MET:HE3	1:C:418:VAL:HG13	1.95	0.49
1:C:368:VAL:HG22	4:S:156:HOH:O	2.13	0.49
1:C:339:GLU:HG3	1:C:418:VAL:HB	1.94	0.48
1:B:424:ILE:HD13	1:B:427:MET:CE	2.43	0.48
1:C:342:MET:HE3	1:C:418:VAL:CG1	2.44	0.48
1:B:416:LYS:CG	1:B:422:VAL:HG11	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:HIS:CG	1:D:459:TYR:HD2	2.33	0.47
1:C:513:HIS:CE1	1:D:459:TYR:CD2	3.02	0.47
1:C:513:HIS:NE2	1:D:459:TYR:CD2	2.83	0.47
1:A:339:GLU:HG3	1:A:418:VAL:HB	1.96	0.47
1:B:462:LEU:HD22	1:B:462:LEU:C	2.36	0.46
1:B:533:VAL:HG22	3:E:2:LIG:C22	2.46	0.46
1:B:352:ARG:HD2	2:F:2:CL:CL	2.53	0.46
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.51	0.46
1:C:358:ILE:HG23	1:C:544:LEU:HD13	1.99	0.45
1:D:473:ASP:OD2	1:D:477:ARG:NH1	2.50	0.45
1:A:312:ALA:O	1:A:316:VAL:HG23	2.16	0.44
1:C:312:ALA:O	1:C:316:VAL:HG23	2.17	0.44
1:D:492:LYS:HD2	1:D:493:ALA:N	2.32	0.44
1:B:501:HIS:CD2	4:S:11:HOH:O	2.67	0.44
1:B:416:LYS:HG3	1:B:422:VAL:HG11	2.00	0.43
1:B:417:CYS:C	1:B:418:VAL:CG1	2.87	0.43
1:C:463:SER:CB	1:C:468:SER:HB2	2.45	0.43
1:A:529:LYS:HD3	1:A:529:LYS:N	2.35	0.42
1:B:522:MET:HG3	1:B:526:TYR:CE1	2.53	0.42
1:D:392:VAL:HG12	1:D:435:PHE:CD2	2.55	0.42
1:B:312:ALA:O	1:B:316:VAL:HG23	2.19	0.42
1:C:526:TYR:O	1:C:529:LYS:O	2.37	0.42
1:B:351:ASP:HB2	1:B:533:VAL:HG11	2.00	0.42
1:B:392:VAL:HG12	1:B:435:PHE:CD2	2.55	0.41
1:A:342:MET:HE3	1:A:418:VAL:HG13	2.02	0.41
1:D:489:LEU:O	1:D:492:LYS:HG3	2.20	0.41
1:B:368:VAL:HG22	4:S:37:HOH:O	2.21	0.41
1:D:316:VAL:HG21	1:D:489:LEU:HD21	2.01	0.41
1:D:312:ALA:O	1:D:316:VAL:HG23	2.20	0.41
1:D:331:TYR:OH	1:D:407:ASN:O	2.31	0.41
1:C:392:VAL:HG12	1:C:435:PHE:CD2	2.55	0.41
1:D:460:THR:HG23	4:S:181:HOH:O	2.22	0.40
1:A:329:SER:O	1:A:330:GLU:C	2.60	0.40
1:B:316:VAL:HG21	1:B:489:LEU:HD21	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:OH	1:B:359:ASN:ND2[1_645]	2.05	0.15
1:A:481:LYS:NZ	1:B:538:ASP:OD2[1_655]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	240/257 (93%)	237 (99%)	2 (1%)	1 (0%)	34 19
1	B	243/257 (95%)	237 (98%)	4 (2%)	2 (1%)	19 7
1	C	241/257 (94%)	236 (98%)	3 (1%)	2 (1%)	19 7
1	D	236/257 (92%)	233 (99%)	3 (1%)	0	100 100
All	All	960/1028 (93%)	943 (98%)	12 (1%)	5 (0%)	29 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	GLU
1	C	531	LYS
1	A	330	GLU
1	B	418	VAL
1	C	330	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	220/232 (95%)	212 (96%)	8 (4%)	35 18
1	B	221/232 (95%)	213 (96%)	8 (4%)	35 18
1	C	219/232 (94%)	211 (96%)	8 (4%)	34 17
1	D	218/232 (94%)	208 (95%)	10 (5%)	27 11
All	All	878/928 (95%)	844 (96%)	34 (4%)	32 15

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	ARG
1	A	301	SER
1	A	432	SER
1	A	463	SER
1	A	467	LYS
1	A	515	ARG
1	A	520	LYS
1	A	529	LYS
1	B	372	SER
1	B	412	ARG
1	B	418	VAL
1	B	432	SER
1	B	462	LEU
1	B	463	SER
1	B	470	GLU
1	B	544	LEU
1	C	306	LEU
1	C	432	SER
1	C	437	MET
1	C	462	LEU
1	C	463	SER
1	C	529	LYS
1	C	532	ASN
1	C	544	LEU
1	D	303	LYS
1	D	337	PHE
1	D	412	ARG
1	D	425	PHE
1	D	432	SER
1	D	437	MET
1	D	470	GLU
1	D	492	LYS
1	D	529	LYS
1	D	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	488	HIS
1	A	501	HIS

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Mol	Chain	Res	Type
1	B	373	HIS
1	B	398	HIS
1	B	501	HIS
1	B	547	HIS
1	C	398	HIS
1	C	413	ASN
1	C	513	HIS
1	C	532	ASN
1	D	348	ASN
1	D	373	HIS
1	D	398	HIS
1	D	439	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

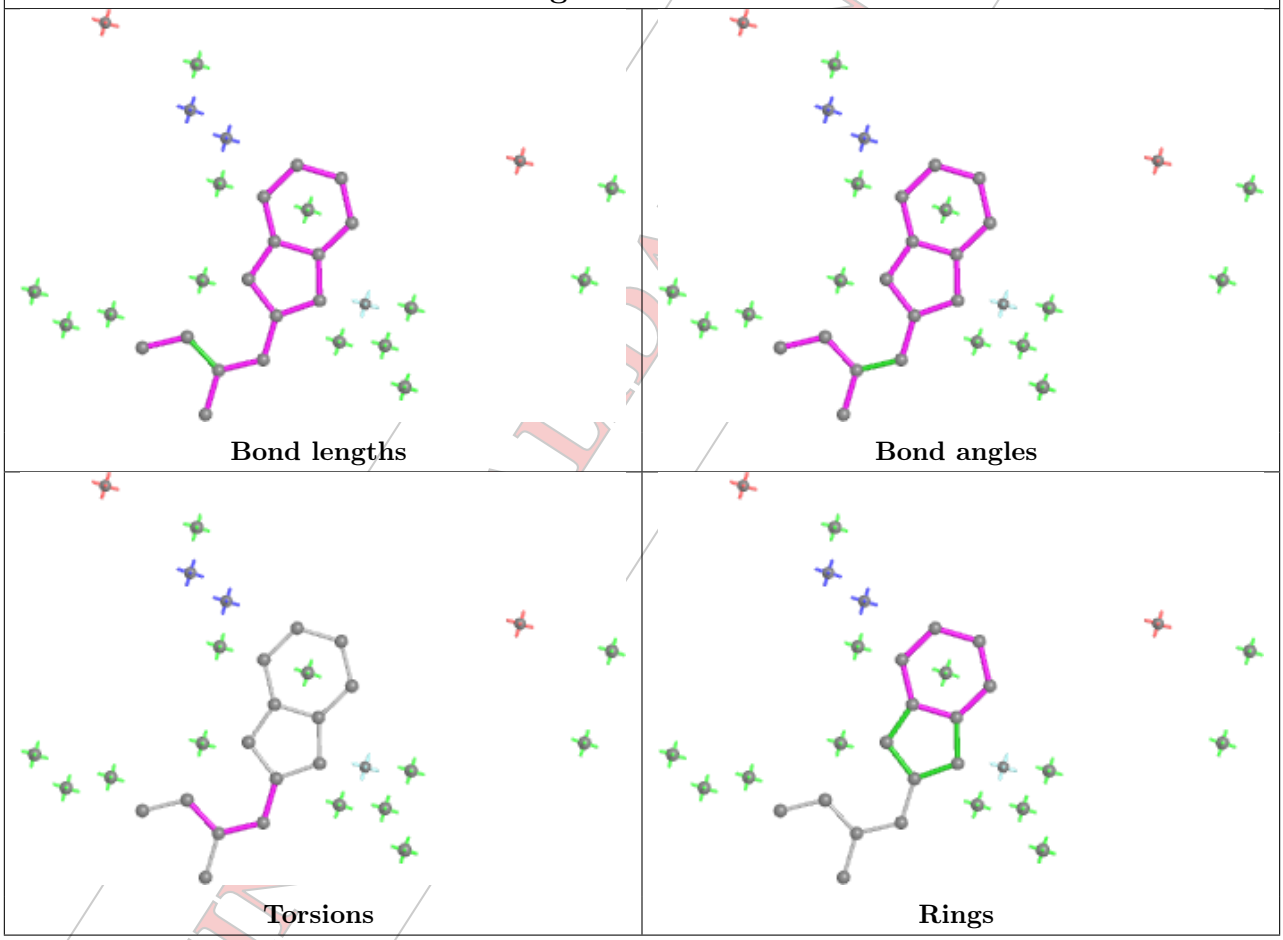
There are no torsion outliers.

There are no ring outliers.

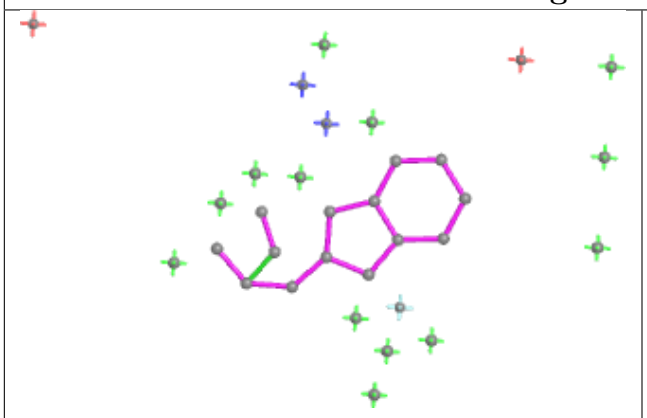
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

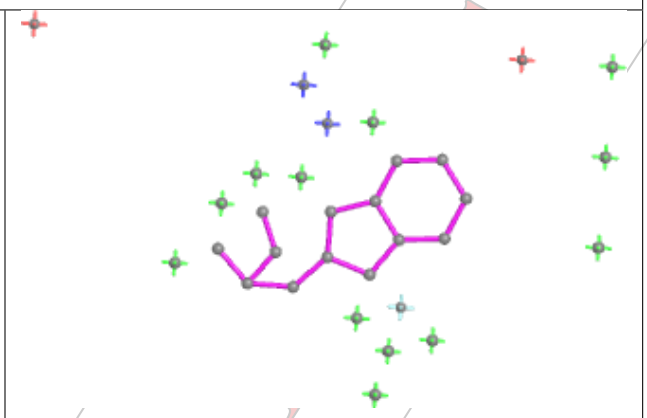
Ligand LIG E 3



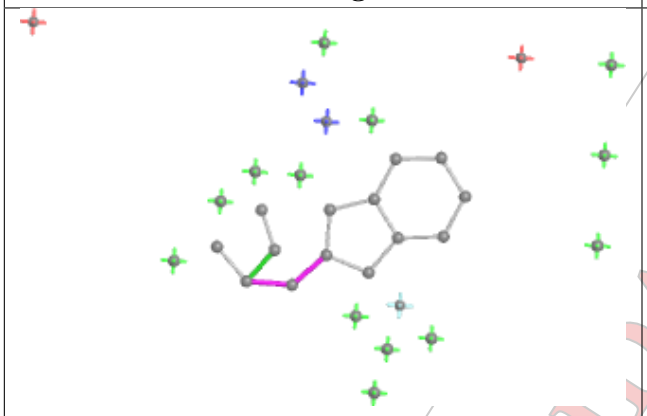
Ligand LIG E 4



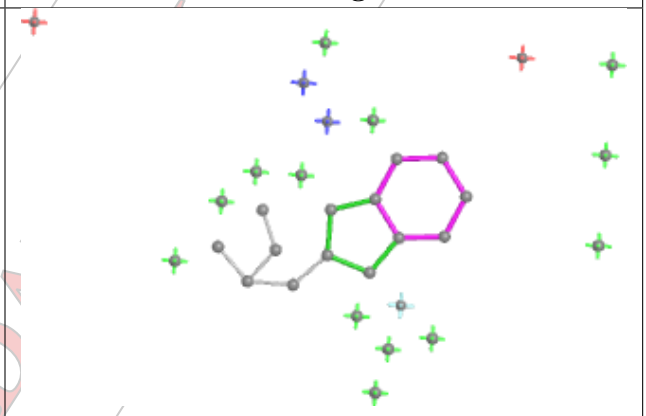
Bond lengths



Bond angles

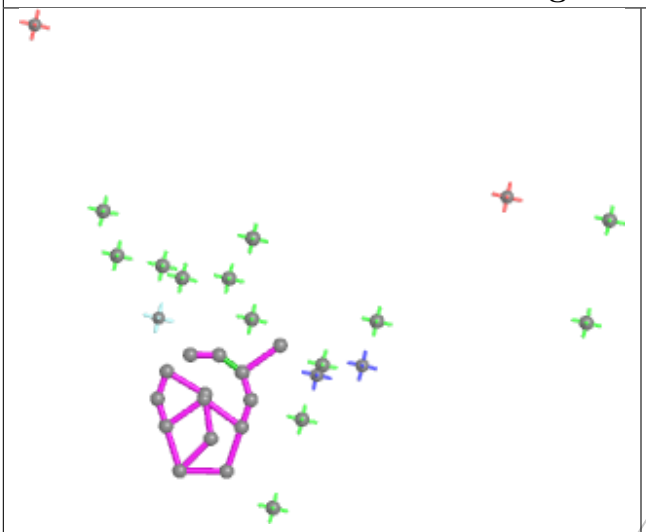


Torsions

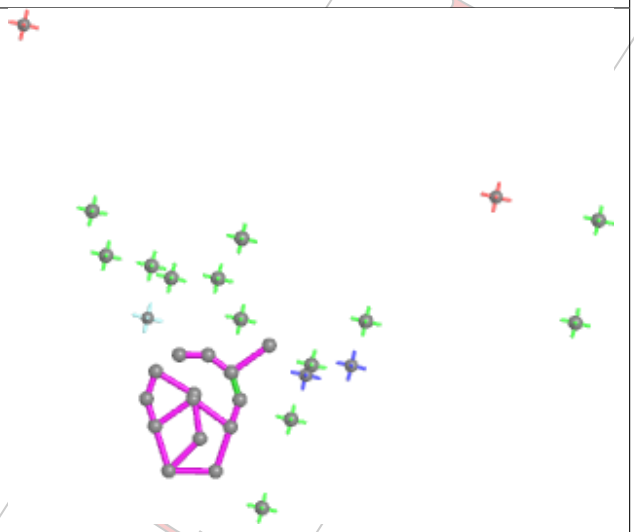


Rings

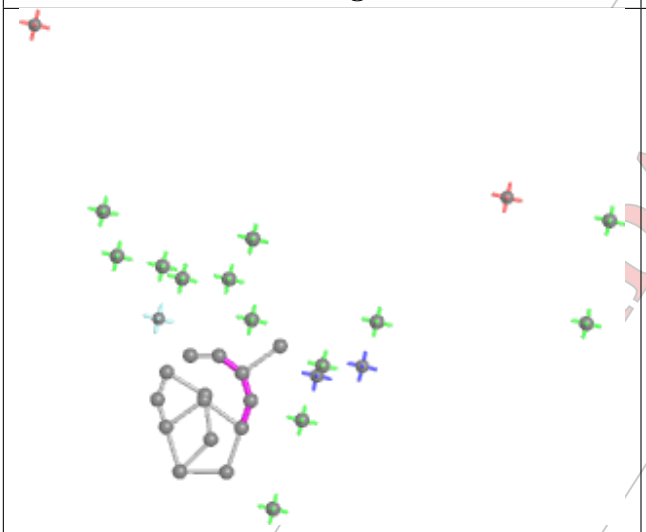
Ligand LIG E 2



Bond lengths



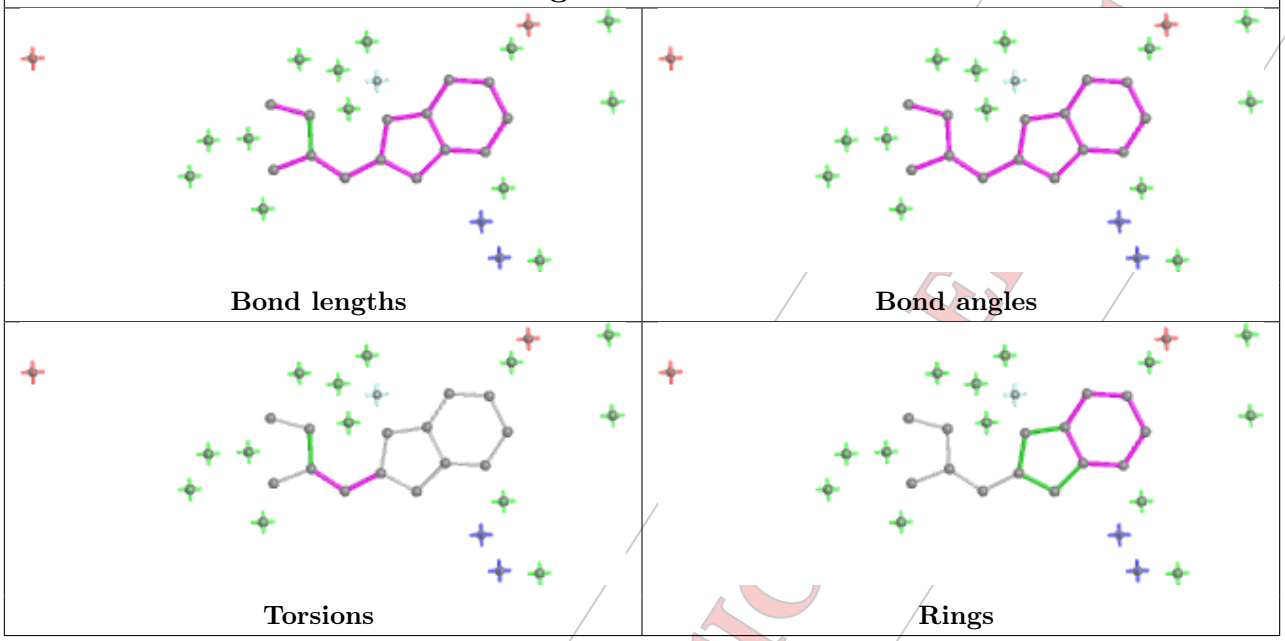
Bond angles



Torsions

Rings

Ligand LIG E 1



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	243/257 (94%)	0.23	11 (4%)	33	31	18, 31, 60, 96	0
1	B	245/257 (95%)	0.40	18 (7%)	15	14	16, 31, 68, 108	0
1	C	243/257 (94%)	0.17	10 (4%)	37	35	17, 30, 61, 108	0
1	D	242/257 (94%)	0.46	17 (7%)	16	16	17, 32, 76, 123	0
All	All	973/1028 (94%)	0.31	56 (5%)	23	22	16, 31, 69, 123	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	468	SER	9.2
1	D	304	ASN	8.1
1	D	467	LYS	8.1
1	C	462	LEU	7.5
1	A	462	LEU	7.5
1	D	469	LEU	7.3
1	B	304	ASN	7.1
1	D	337	PHE	7.0
1	B	337	PHE	5.8
1	B	418	VAL	5.8
1	B	420	GLY	5.7
1	B	419	GLU	5.6
1	C	530	CYS	5.4
1	B	462	LEU	5.3
1	B	526	TYR	4.3
1	B	464	SER	4.3
1	C	532	ASN	4.3
1	D	340	ALA	4.3
1	A	300	ARG	4.3
1	C	526	TYR	4.2
1	B	463	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	526	TYR	4.0
1	A	461	PHE	4.0
1	B	546	ALA	3.9
1	C	460	THR	3.9
1	B	417	CYS	3.6
1	D	306	LEU	3.4
1	A	331	TYR	3.3
1	B	338	SER	3.3
1	B	547	HIS	3.3
1	B	340	ALA	3.2
1	A	332	ASP	3.1
1	B	303	LYS	3.1
1	D	459	TYR	3.1
1	D	305	SER	3.0
1	D	530	CYS	3.0
1	A	469	LEU	3.0
1	D	552	PRO	2.9
1	A	305	SER	2.9
1	A	301	SER	2.9
1	D	461	PHE	2.8
1	D	334	THR	2.8
1	C	331	TYR	2.8
1	D	331	TYR	2.5
1	B	306	LEU	2.5
1	B	548	ARG	2.4
1	D	529	LYS	2.3
1	D	549	LEU	2.3
1	C	464	SER	2.2
1	A	459	TYR	2.1
1	C	461	PHE	2.1
1	A	466	LEU	2.1
1	D	528	MET	2.1
1	C	469	LEU	2.1
1	C	459	TYR	2.1
1	B	411	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

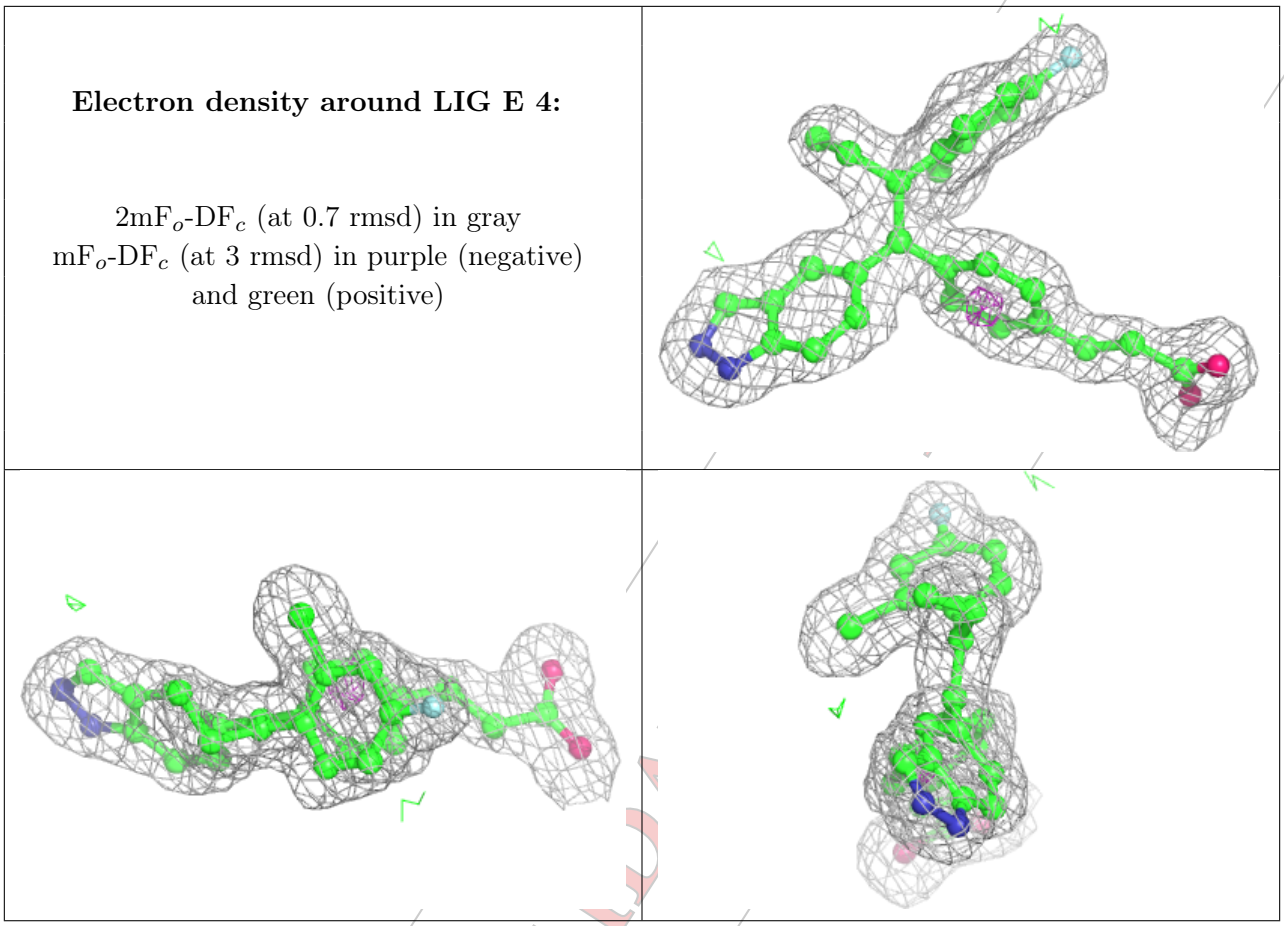
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LIG	E	4	32/?	0.95	0.09	18,26,36,40	0
3	LIG	E	3	32/?	0.96	0.09	16,20,26,30	0
3	LIG	E	2	32/?	0.96	0.09	16,25,33,35	0
3	LIG	E	1	32/?	0.96	0.07	16,19,27,29	0
2	CL	F	1	1/?	0.99	0.09	34,34,34,34	0
2	CL	F	2	1/?	0.99	0.06	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

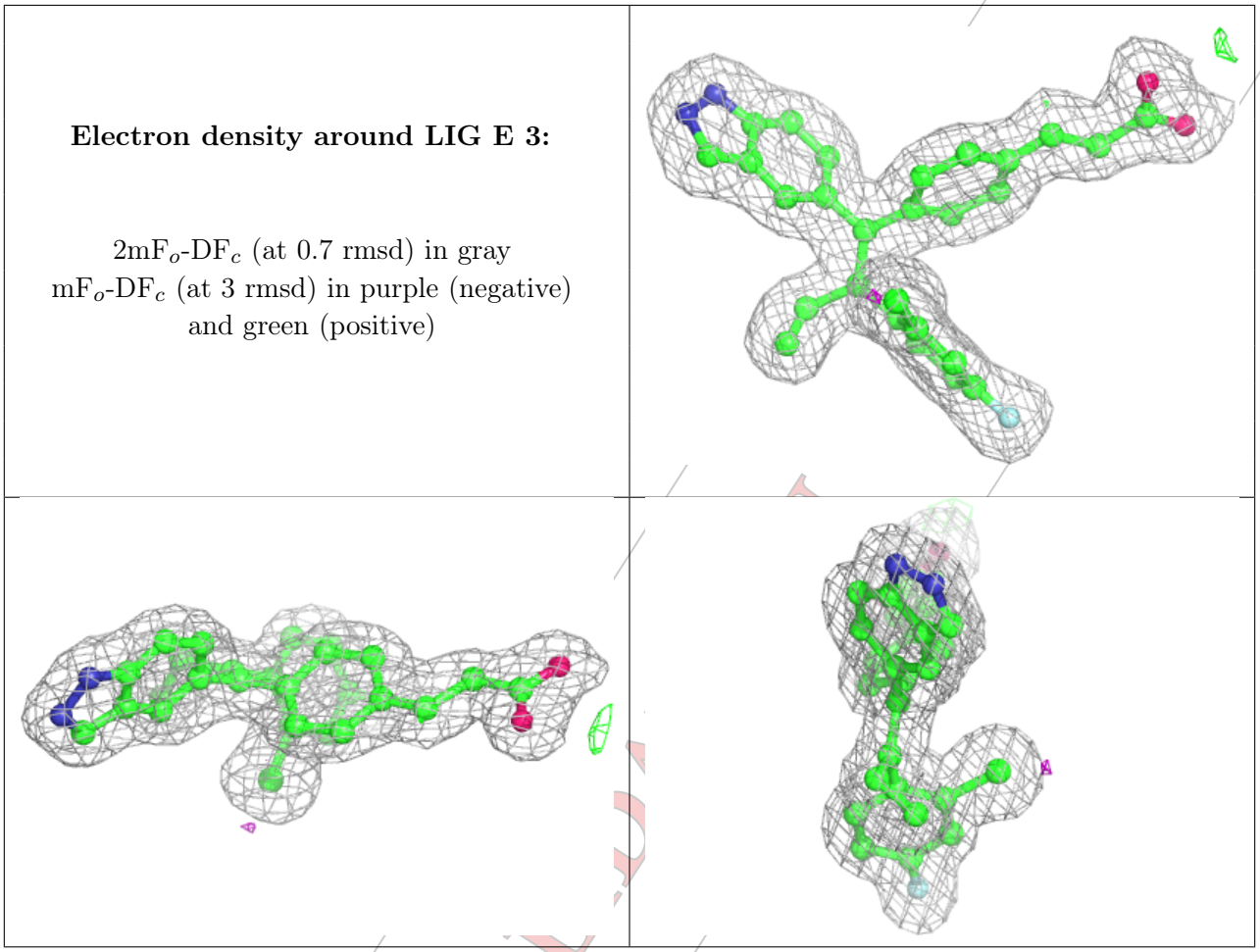
Electron density around LIG E 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



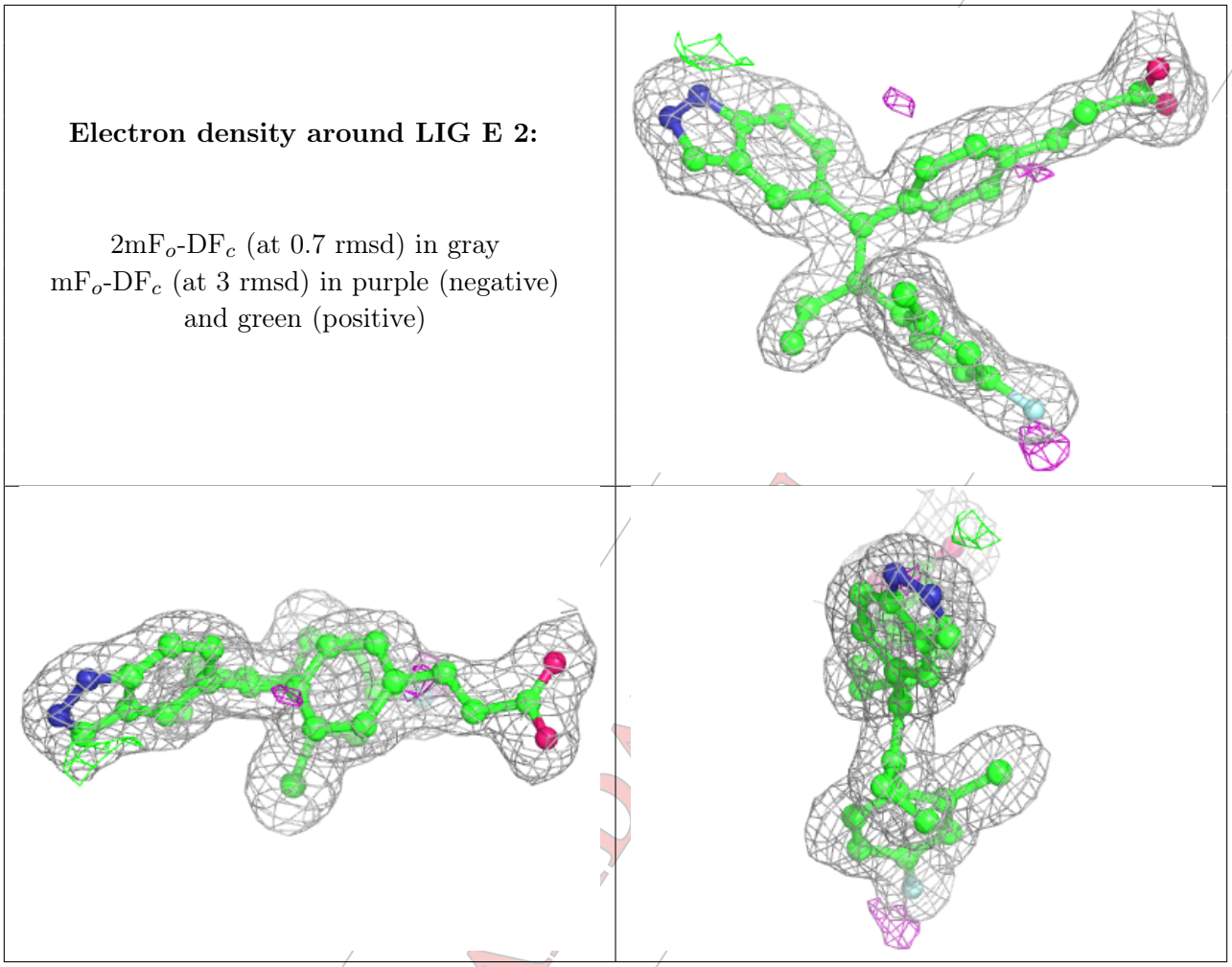
Electron density around LIG E 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



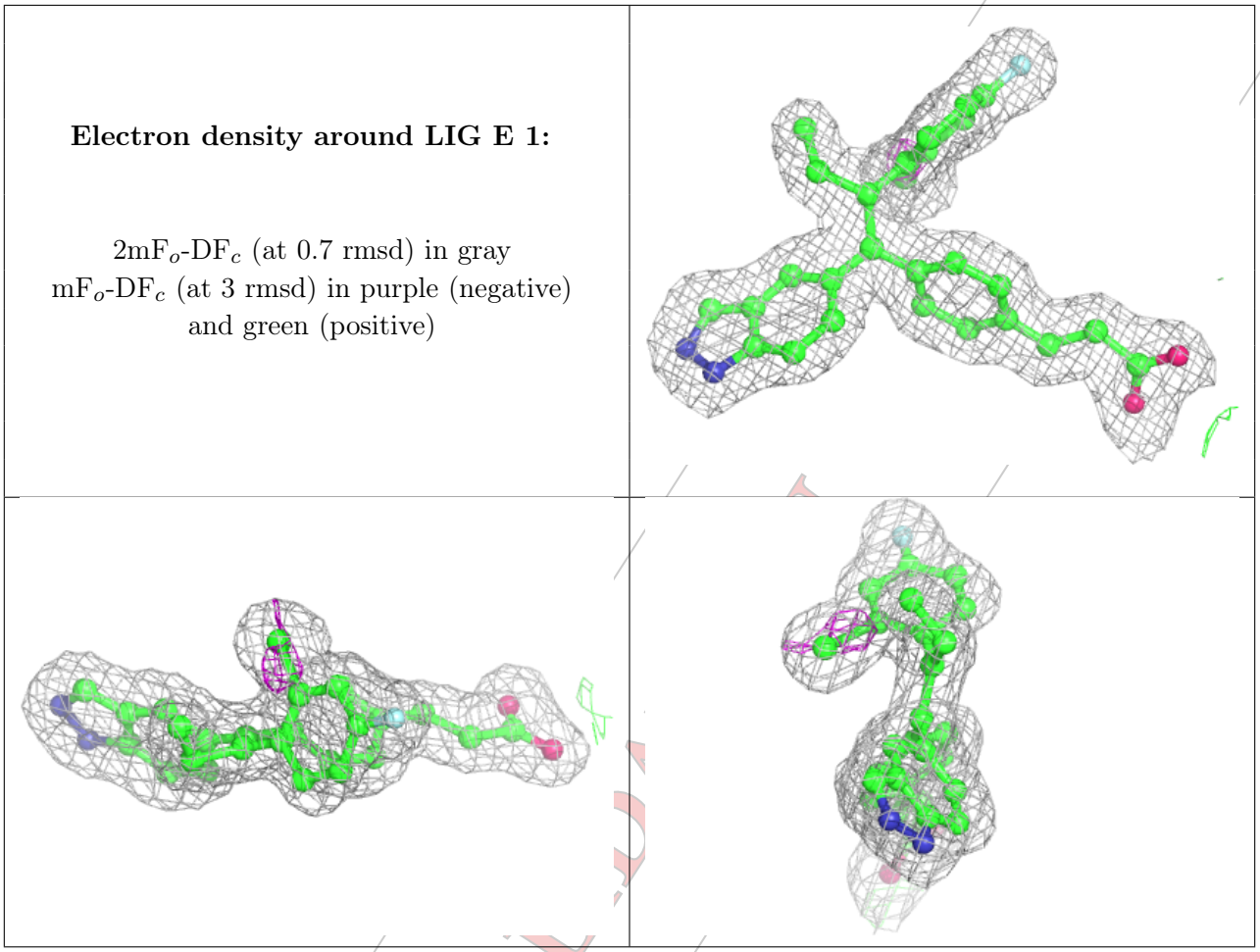
Electron density around LIG E 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LIG E 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.