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

Feb 5, 2021 – 09:46 AM GMT

Deposition ID : D_1292113836

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:

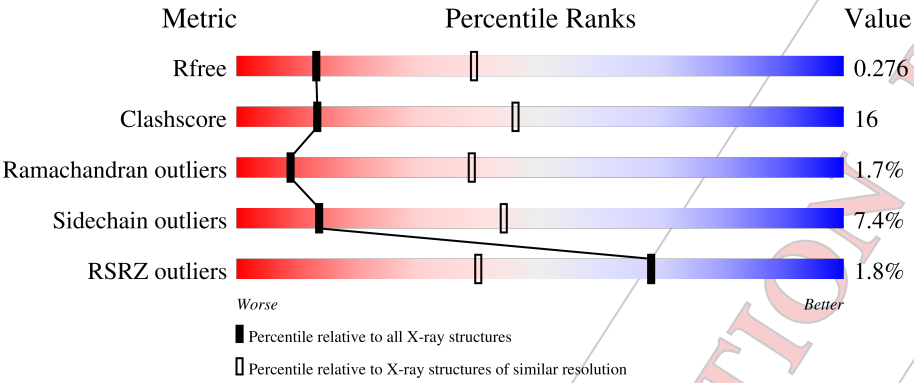
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

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

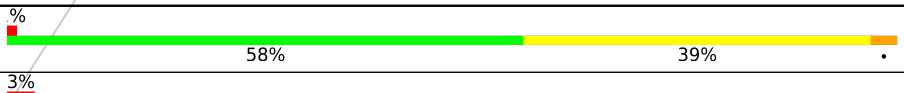
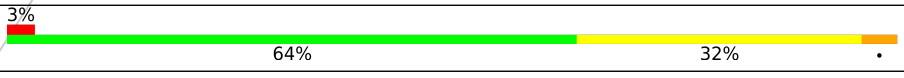
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of 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	200	
2	B	238	

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
3	DMS	C	2	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3640 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.

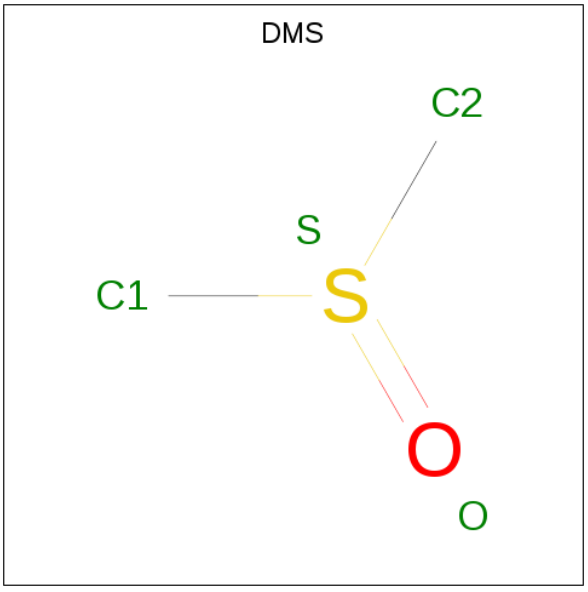
- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1630	1044	288	288	10	0	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	238	1950	1246	331	361	12	0	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	C	1	4	2	1	1	0	0

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			33	25	6	2		

- Molecule 5 is water.

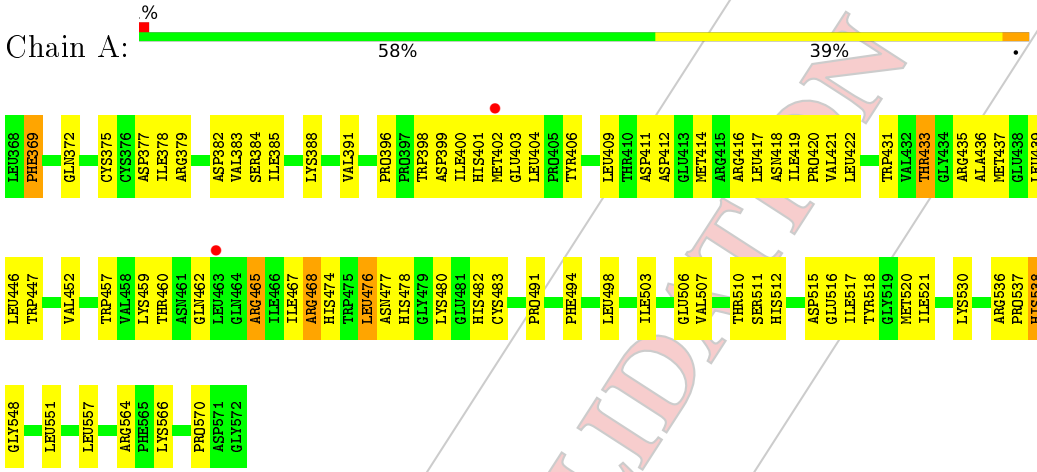
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	23	Total	O	0	0
			23	23		

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.

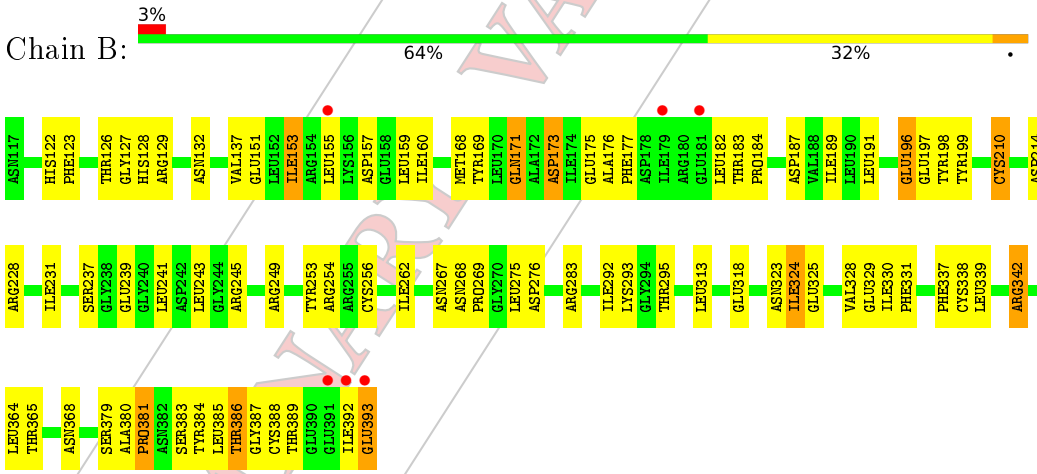
- Molecule 1:

Chain A:



- Molecule 2:

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.09Å 64.09Å 225.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.80 – 3.00 49.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-3.00) 100.0 (49.79-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.186 , 0.263 0.194 , 0.276	Depositor DCC
R_{free} test set	508 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3640	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: DMS, UNL

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	0.74	0/1674	0.75	0/2275
2	B	0.76	0/1997	0.75	0/2703
All	All	0.75	0/3671	0.75	0/4978

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	1630	0	1602	58	0
2	B	1950	0	1896	59	0
3	C	4	0	6	5	0
4	C	33	0	0	0	0
5	E	23	0	0	0	0
All	All	3640	0	3504	115	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 16.

All (115) 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:B:256:CYS:SG	2:B:292:ILE:HD11	1.63	1.38
2:B:256:CYS:SG	2:B:292:ILE:CD1	2.49	1.00
2:B:249:ARG:HH11	3:C:2:DMS:H23	1.41	0.86
1:A:507:VAL:HG12	1:A:507:VAL:O	1.81	0.79
2:B:393:GLU:OE2	2:B:393:GLU:N	2.16	0.78
1:A:383:VAL:HG23	1:A:421:VAL:HG11	1.67	0.76
2:B:128:HIS:CE1	2:B:269:PRO:HG3	2.26	0.70
1:A:512:HIS:ND1	1:A:538:HIS:HE1	1.90	0.69
1:A:372:GLN:OE1	1:A:557:LEU:N	2.25	0.68
2:B:169:TYR:HA	2:B:359:THR:O	1.94	0.67
2:B:267:ASN:O	2:B:268:ASN:ND2	2.28	0.66
1:A:468:ARG:HG3	1:A:477:ASN:OD1	1.97	0.65
2:B:153:ILE:O	2:B:153:ILE:HG22	1.97	0.64
2:B:254:ARG:HA	3:C:2:DMS:O	1.98	0.63
1:A:452:VAL:O	2:B:283:ARG:NH2	2.32	0.62
1:A:512:HIS:CE1	1:A:538:HIS:HE1	2.18	0.61
1:A:468:ARG:HD2	1:A:468:ARG:N	2.14	0.61
2:B:151:GLU:HG2	2:B:151:GLU:O	2.01	0.61
2:B:157:ASP:HA	2:B:160:ILE:HD12	1.82	0.60
1:A:396:PRO:HG2	1:A:398:TRP:CE2	2.37	0.60
2:B:171:GLN:HG3	2:B:364:LEU:O	2.00	0.60
1:A:375:CYS:HA	1:A:548:GLY:O	2.02	0.60
2:B:175:GLU:HG2	2:B:176:ALA:N	2.16	0.60
2:B:228:ARG:HH12	2:B:295:THR:C	2.05	0.60
1:A:378:ILE:HG22	1:A:378:ILE:O	2.03	0.59
2:B:128:HIS:NE2	2:B:269:PRO:HG3	2.18	0.58
1:A:396:PRO:HG2	1:A:398:TRP:NE1	2.20	0.57
2:B:249:ARG:HG3	3:C:2:DMS:H21	1.88	0.56
1:A:442:GLU:O	1:A:446:LEU:HG	2.07	0.55
1:A:512:HIS:CE1	1:A:538:HIS:CE1	2.94	0.55
1:A:385:ILE:O	1:A:564:ARG:HD2	2.05	0.55
1:A:460:THR:O	1:A:506:GLU:HA	2.07	0.55
2:B:160:ILE:HA	2:B:387:GLY:O	2.07	0.55
2:B:249:ARG:NH1	3:C:2:DMS:H23	2.15	0.54
2:B:323:ASN:OD1	2:B:325:GLU:HG3	2.08	0.54
1:A:457:TRP:O	1:A:480:LYS:HA	2.08	0.54
1:A:411:ASP:OD1	1:A:435:ARG:NH2	2.41	0.53
1:A:510:THR:HG23	1:A:511:SER:N	2.23	0.53
2:B:338:CYS:O	2:B:386:THR:HG22	2.08	0.53
2:B:187:ASP:OD2	2:B:342:ARG:HB2	2.08	0.53
1:A:388:LYS:HA	1:A:422:LEU:O	2.11	0.51
2:B:228:ARG:HA	2:B:293:LYS:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ASP:OD2	2:B:365:THR:HG23	2.10	0.51
2:B:168:MET:HA	2:B:368:ASN:HD21	1.76	0.51
1:A:402:MET:HG2	1:A:402:MET:O	2.10	0.51
2:B:275:LEU:HD12	2:B:275:LEU:O	2.11	0.50
1:A:419:ILE:N	1:A:420:PRO:CD	2.75	0.50
1:A:566:LYS:O	1:A:570:PRO:HA	2.11	0.50
2:B:228:ARG:HH12	2:B:295:THR:N	2.09	0.50
1:A:507:VAL:O	1:A:507:VAL:CG1	2.51	0.50
1:A:431:TRP:CE3	1:A:483:CYS:HB2	2.46	0.50
1:A:512:HIS:CG	1:A:538:HIS:CE1	2.99	0.50
1:A:536:ARG:HB3	1:A:537:PRO:CD	2.42	0.50
1:A:383:VAL:CG2	1:A:421:VAL:HG11	2.39	0.50
2:B:182:LEU:O	2:B:183:THR:HG23	2.11	0.50
1:A:491:PRO:HB2	1:A:494:PHE:CE1	2.46	0.49
1:A:439:LEU:O	1:A:442:GLU:HB3	2.12	0.49
1:A:382:ASP:OD1	1:A:384:SER:OG	2.31	0.49
2:B:159:LEU:HB3	2:B:388:CYS:O	2.13	0.49
2:B:267:ASN:C	2:B:268:ASN:HD22	2.15	0.48
1:A:414:MET:O	1:A:417:LEU:HB2	2.14	0.47
1:A:377:ASP:OD1	1:A:379:ARG:HB2	2.13	0.47
2:B:129:ARG:O	2:B:132:ASN:HB2	2.13	0.47
1:A:518:TYR:CD1	1:A:541:GLN:HG3	2.50	0.47
1:A:399:ASP:HB2	1:A:409:LEU:O	2.14	0.47
1:A:512:HIS:ND1	1:A:538:HIS:CE1	2.79	0.47
1:A:418:ASN:O	1:A:421:VAL:HG12	2.15	0.47
2:B:169:TYR:HB2	2:B:364:LEU:HD23	1.96	0.47
2:B:173:ASP:O	2:B:177:PHE:HB2	2.15	0.46
1:A:467:ILE:HG22	1:A:468:ARG:H	1.79	0.46
2:B:249:ARG:NH1	3:C:2:DMS:C2	2.78	0.46
2:B:231:ILE:HG22	2:B:253:TYR:CD2	2.50	0.46
2:B:183:THR:HA	2:B:184:PRO:C	2.36	0.46
1:A:412:ASP:HB3	1:A:416:ARG:NH1	2.31	0.46
1:A:391:VAL:HB	1:A:530:LYS:HG2	1.98	0.46
1:A:375:CYS:HB2	1:A:551:LEU:O	2.17	0.45
1:A:460:THR:HA	1:A:465:ARG:O	2.16	0.45
1:A:437:MET:HE2	1:A:482:HIS:CG	2.52	0.45
1:A:369:PHE:O	1:A:542:PRO:HA	2.16	0.45
2:B:241:LEU:O	2:B:245:ARG:HD2	2.17	0.45
2:B:126:THR:OG1	2:B:127:GLY:N	2.48	0.45
2:B:330:ILE:HG23	2:B:331:PHE:N	2.31	0.45
1:A:412:ASP:OD1	1:A:412:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ASP:O	1:A:385:ILE:HG12	2.16	0.44
1:A:503:ILE:HD11	1:A:520:MET:SD	2.58	0.44
2:B:198:TYR:HB3	2:B:324:ILE:HD11	2.00	0.44
2:B:189:ILE:O	2:B:231:ILE:HA	2.18	0.44
2:B:324:ILE:HG23	2:B:324:ILE:O	2.17	0.44
1:A:510:THR:HG23	1:A:511:SER:H	1.82	0.43
2:B:128:HIS:NE2	2:B:269:PRO:CG	2.81	0.43
1:A:378:ILE:CG2	1:A:378:ILE:O	2.65	0.43
1:A:474:HIS:HB3	1:A:478:HIS:NE2	2.33	0.43
2:B:169:TYR:HB2	2:B:364:LEU:CD2	2.49	0.43
1:A:404:LEU:HD22	1:A:406:TYR:CZ	2.53	0.43
1:A:459:LYS:HB3	1:A:507:VAL:HG23	2.01	0.43
1:A:512:HIS:CE1	1:A:536:ARG:CZ	3.02	0.42
2:B:214:ASP:O	2:B:218:LYS:HG2	2.19	0.42
1:A:517:ILE:O	1:A:521:ILE:HG13	2.19	0.42
2:B:239:GLU:HB2	2:B:243:LEU:HD12	2.01	0.42
2:B:197:GLU:O	2:B:199:TYR:N	2.53	0.42
1:A:433:THR:O	1:A:436:ALA:HB3	2.19	0.42
1:A:443:CYS:O	1:A:447:TRP:CG	2.73	0.42
2:B:262:ILE:HD12	2:B:313:LEU:HD22	2.01	0.42
2:B:122:HIS:CE1	2:B:126:THR:HG21	2.55	0.41
2:B:330:ILE:HA	2:B:330:ILE:HD12	1.85	0.41
2:B:228:ARG:NH1	2:B:295:THR:N	2.67	0.41
2:B:151:GLU:O	2:B:151:GLU:CG	2.66	0.41
2:B:123:PHE:O	2:B:127:GLY:N	2.53	0.41
2:B:196:GLU:OE2	2:B:210:CYS:HB3	2.21	0.41
1:A:476:LEU:HD13	2:B:337:PHE:CZ	2.56	0.41
1:A:462:GLN:NE2	1:A:462:GLN:HA	2.36	0.41
2:B:330:ILE:CG2	2:B:331:PHE:N	2.84	0.40
2:B:380:ALA:HA	2:B:381:PRO:HA	1.83	0.40
2:B:337:PHE:HB3	2:B:339:LEU:HD21	2.04	0.40
2:B:328:VAL:O	2:B:331:PHE:N	2.53	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	196/200 (98%)	174 (89%)	20 (10%)	2 (1%)	15 53
2	B	228/238 (96%)	208 (91%)	15 (7%)	5 (2%)	6 31
All	All	424/438 (97%)	382 (90%)	35 (8%)	7 (2%)	9 39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	385	LEU
1	A	515	ASP
2	B	196	GLU
1	A	400	ILE
2	B	329	GLU
2	B	153	ILE
2	B	381	PRO

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	178/178 (100%)	168 (94%)	10 (6%)	21 56
2	B	214/214 (100%)	195 (91%)	19 (9%)	9 35
All	All	392/392 (100%)	363 (93%)	29 (7%)	13 44

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	PHE
1	A	401	HIS
1	A	403	GLU
1	A	433	THR
1	A	465	ARG

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Mol	Chain	Res	Type
1	A	468	ARG
1	A	476	LEU
1	A	498	LEU
1	A	516	GLU
1	A	538	HIS
2	B	137	VAL
2	B	155	LEU
2	B	171	GLN
2	B	173	ASP
2	B	191	LEU
2	B	210	CYS
2	B	217	MET
2	B	237	SER
2	B	276	ASP
2	B	318	GLU
2	B	324	ILE
2	B	342	ARG
2	B	379	SER
2	B	383	SER
2	B	384	TYR
2	B	386	THR
2	B	389	THR
2	B	392	ILE
2	B	393	GLU

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

Mol	Chain	Res	Type
1	A	462	GLN
1	A	464	GLN
1	A	512	HIS
1	A	538	HIS
1	A	550	GLN
1	A	555	HIS
2	B	122	HIS
2	B	268	ASN
2	B	366	ASN

5.3.3 RNA

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 2 ligands modelled in this entry, 1 is unknown - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DMS	C	2	-	3,3,3	0.36	0	3,3,3	0.17	0

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.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	DMS	5	0

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
2	B	4
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	295:THR	C	310:ASP	N	19.99
1	B	137:VAL	C	151:GLU	N	16.76
1	B	200:ARG	C	209:LYS	N	14.81
1	A	468:ARG	C	474:HIS	N	12.96
1	B	270:GLY	C	275:LEU	N	10.74

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	200/200 (100%)	-0.21	2 (1%) 82 59	40, 60, 102, 137	0
2	B	238/238 (100%)	-0.22	6 (2%) 57 29	38, 57, 104, 135	0
All	All	438/438 (100%)	-0.21	8 (1%) 68 40	38, 59, 103, 137	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	392	ILE	3.9
2	B	393	GLU	3.1
2	B	391	GLU	2.6
2	B	179	ILE	2.5
2	B	155	LEU	2.3
2	B	181	GLU	2.2
1	A	463	LEU	2.1
1	A	402	MET	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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,

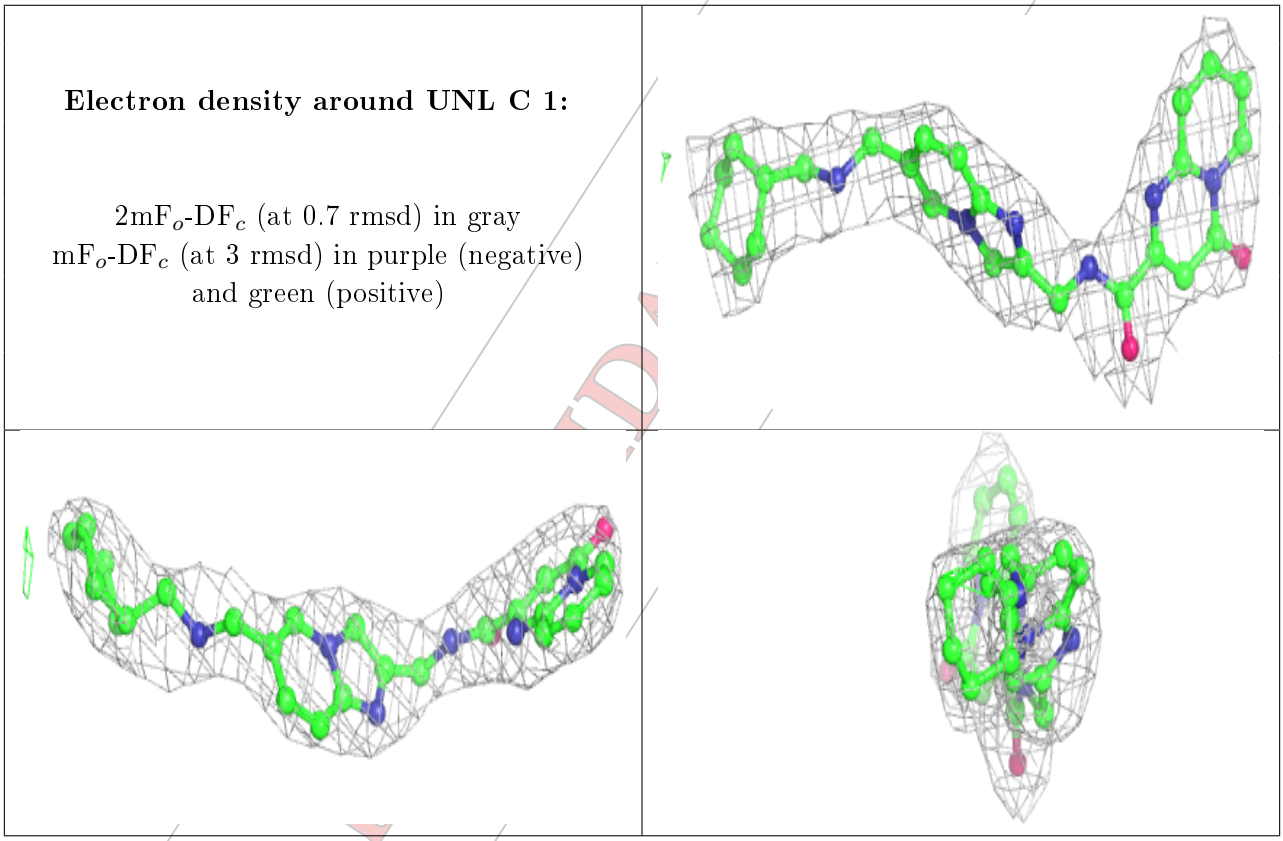
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DMS	C	2	4/?	0.90	0.23	80,81,85,87	0
4	UNL	C	1	33/-	0.92	0.23	44,54,67,69	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 UNL C 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.