Full wwPDB X-ray Structure Validation Report (i)

May 12, 2023 – 02:01 PM EDT

PDB ID	:	8STP
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (Y181C) varient in Complex with 8-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)indolizine-2-carbonitrile (JLJ555), a non-nucleoside inhibitor
Deposited on	:	2023-05-11
Resolution	:	3.09 Å(reported)

This wwPDB validation report is for manuscript review

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

This report is produced by the wwPDB biocuration pipeline after 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

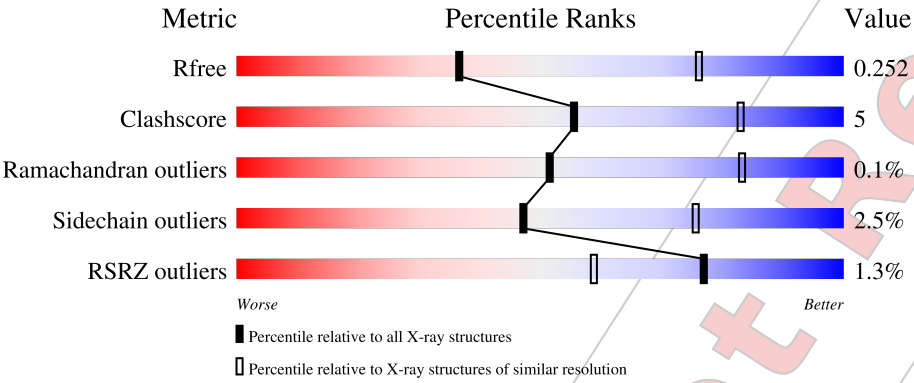
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	557	% 82% 15% .
2	B	428	% 83% 13% . .

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7607 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4286	2768	709	801	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	conflict	UNP P03366
A	173	ALA	LYS	conflict	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

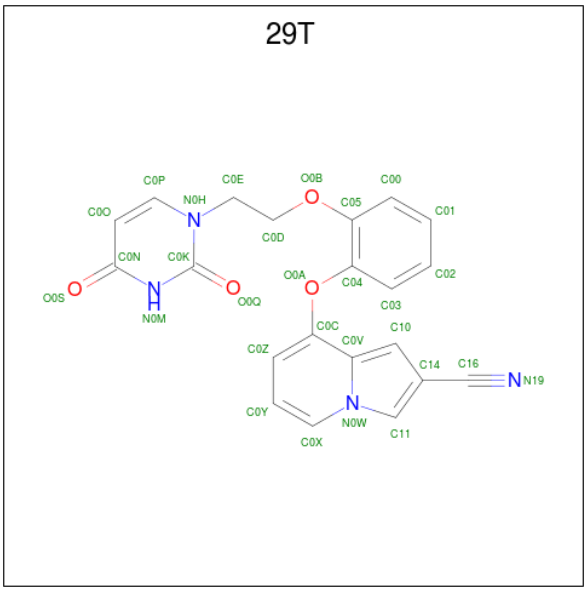
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	415	3292	2142	535	610	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 8-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}indolizine-2-carbonitrile (three-letter code: 29T) (formula: $C_{21}H_{16}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



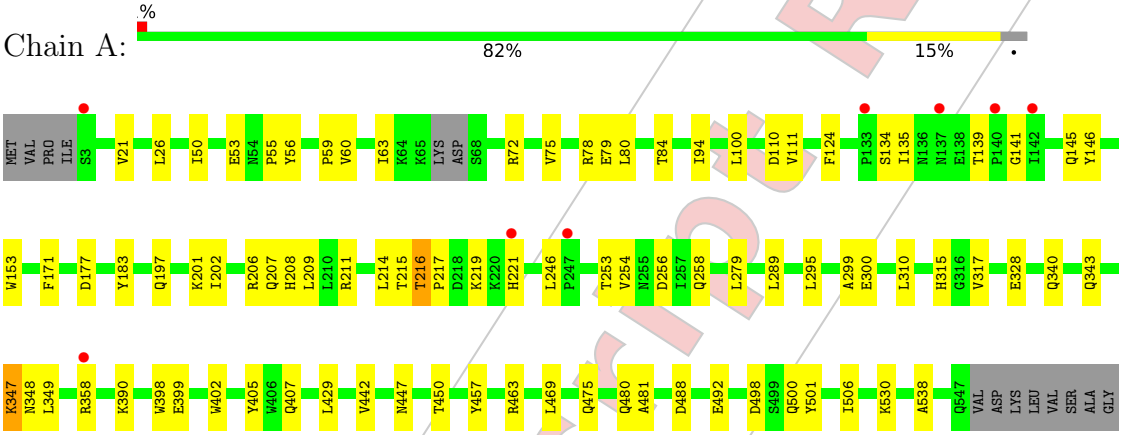
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	29	21	4	4	0	0

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.

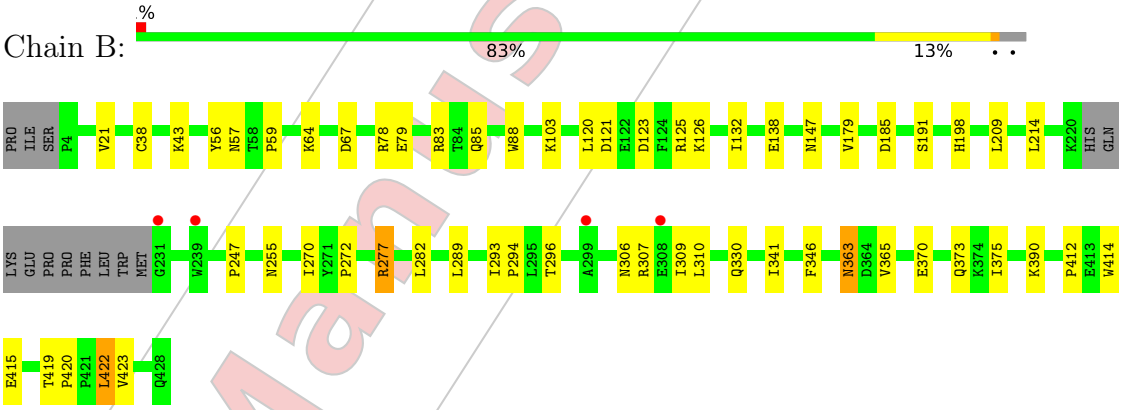
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



• Molecule 2: p51 RT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.73Å 68.80Å 105.21Å 90.00° 105.66° 90.00°	Depositor
Resolution (Å)	35.90 – 3.09 35.90 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.90-3.09) 99.2 (35.90-3.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.215 , 0.252 0.218 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (7.04%)	wwPDB-VP
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: 29T

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	0.23	0/4398	0.43	0/5999
2	B	0.24	0/3388	0.43	0/4631
All	All	0.23	0/7786	0.43	0/10630

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	4286	0	4204	47	0
2	B	3292	0	3181	30	0
3	A	29	0	16	1	0
All	All	7607	0	7401	77	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 (77) 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:343:GLN:HG3	1:A:349:LEU:HD11	1.72	0.70
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.59	0.66
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.61	0.66
1:A:134:SER:HB3	1:A:139:THR:HG23	1.82	0.62
2:B:64:LYS:HB3	2:B:67:ASP:HA	1.83	0.60
1:A:100:LEU:HB3	3:A:601:29T:H11	1.83	0.60
1:A:253:THR:HG23	1:A:256:ASP:H	1.67	0.58
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.86	0.58
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.86	0.57
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.38	0.57
1:A:60:VAL:HG22	1:A:75:VAL:HG22	1.86	0.56
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.87	0.56
2:B:422:LEU:HG	2:B:423:VAL:HG23	1.86	0.56
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.42	0.53
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.44	0.52
1:A:139:THR:HG22	1:A:141:GLY:H	1.75	0.51
2:B:293:ILE:HD12	2:B:294:PRO:HD2	1.92	0.51
1:A:197:GLN:O	1:A:201:LYS:HG2	2.11	0.51
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.93	0.50
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.46	0.50
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.46	0.50
2:B:282:LEU:HD13	2:B:296:THR:HG23	1.92	0.50
2:B:270:ILE:O	2:B:272:PRO:HD3	2.12	0.49
1:A:317:VAL:HG11	1:A:347:LYS:HE3	1.94	0.49
1:A:254:VAL:HB	1:A:289:LEU:HA	1.95	0.49
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.78	0.48
1:A:80:LEU:O	1:A:84:THR:HG23	2.14	0.48
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.49	0.48
1:A:207:GLN:O	1:A:211:ARG:HG3	2.13	0.48
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.48	0.48
2:B:363:ASN:HD21	2:B:365:VAL:HB	1.79	0.48
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.96	0.47
2:B:79:GLU:HG3	2:B:83:ARG:HD2	1.95	0.47
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.96	0.47
2:B:270:ILE:HG13	2:B:346:PHE:HB3	1.96	0.47
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.97	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.47
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.55	0.47
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.29	0.47
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.96	0.46
2:B:277:ARG:N	2:B:277:ARG:HD3	2.31	0.46
1:A:50:ILE:HG21	1:A:145:GLN:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.97	0.46
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.32	0.45
1:A:216:THR:HG22	1:A:217:PRO:HD2	1.97	0.45
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.98	0.45
1:A:139:THR:HG22	1:A:141:GLY:N	2.32	0.44
1:A:94:ILE:HG22	1:A:183:TYR:HE2	1.81	0.44
1:A:78:ARG:HG3	1:A:79:GLU:N	2.31	0.43
1:A:463:ARG:NH1	1:A:488:ASP:O	2.51	0.43
2:B:191:SER:OG	2:B:198:HIS:ND1	2.36	0.43
1:A:111:VAL:HA	1:A:215:THR:O	2.18	0.43
2:B:78:ARG:NH1	2:B:412:PRO:O	2.51	0.43
1:A:279:LEU:HD23	1:A:299:ALA:HB1	2.01	0.43
2:B:125:ARG:HD3	2:B:147:ASN:HA	2.01	0.43
2:B:341:ILE:HD11	2:B:375:ILE:HG23	2.01	0.42
1:A:398:TRP:CD1	1:A:402:TRP:HD1	2.36	0.42
2:B:21:VAL:O	2:B:57:ASN:ND2	2.40	0.42
2:B:121:ASP:O	2:B:125:ARG:HG3	2.19	0.42
1:A:254:VAL:O	1:A:258:GLN:HG3	2.20	0.42
1:A:177:ASP:N	1:A:177:ASP:OD1	2.52	0.42
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.42
2:B:209:LEU:HD22	2:B:214:LEU:HD12	2.01	0.42
2:B:43:LYS:HE3	2:B:43:LYS:HB2	1.77	0.42
2:B:306:ASN:O	2:B:310:LEU:HB2	2.20	0.42
1:A:340:GLN:HB3	1:A:348:ASN:ND2	2.35	0.41
2:B:247:PRO:O	2:B:307:ARG:NH2	2.49	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.02	0.41
1:A:469:LEU:HD11	1:A:480:GLN:HG2	2.02	0.41
1:A:63:ILE:O	1:A:72:ARG:N	2.46	0.41
1:A:358:ARG:HA	1:A:358:ARG:HD3	1.73	0.41
2:B:370:GLU:HA	2:B:373:GLN:HE21	1.85	0.41
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.03	0.41
1:A:202:ILE:O	1:A:206:ARG:HG3	2.21	0.40
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.03	0.40
1:A:295:LEU:HD23	1:A:300:GLU:HG2	2.03	0.40
2:B:419:THR:HA	2:B:420:PRO:HD3	1.93	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	539/557 (97%)	523 (97%)	15 (3%)	1 (0%)	47 79
2	B	411/428 (96%)	401 (98%)	10 (2%)	0	100 100
All	All	950/985 (96%)	924 (97%)	25 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	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	453/495 (92%)	441 (97%)	12 (3%)	46 74
2	B	345/390 (88%)	337 (98%)	8 (2%)	50 77
All	All	798/885 (90%)	778 (98%)	20 (2%)	47 75

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	53	GLU
1	A	56	TYR
1	A	110	ASP
1	A	135	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	146	TYR
1	A	216	THR
1	A	219	LYS
1	A	221	HIS
1	A	315	HIS
1	A	347	LYS
1	A	500	GLN
2	B	123	ASP
2	B	138	GLU
2	B	185	ASP
2	B	277	ARG
2	B	330	GLN
2	B	363	ASN
2	B	414	TRP
2	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	464	GLN

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)

1 ligand is modelled in this entry.

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	29T	A	601	-	30,32,32	1.32	3 (10%)	35,44,44	1.84	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	29T	A	601	-	-	0/10/12/12	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	29T	C0P-N0H	3.90	1.42	1.37
3	A	601	29T	C0Y-C0Z	2.95	1.45	1.38
3	A	601	29T	C0Z-C0C	2.24	1.43	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	29T	C0E-N0H-C0K	7.30	126.23	118.54
3	A	601	29T	C0E-N0H-C0P	-4.01	113.63	119.75
3	A	601	29T	C0C-C0V-N0W	-2.67	115.68	121.31
3	A	601	29T	O0Q-C0K-N0H	2.48	125.03	122.85
3	A	601	29T	C0D-C0E-N0H	2.35	116.50	111.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

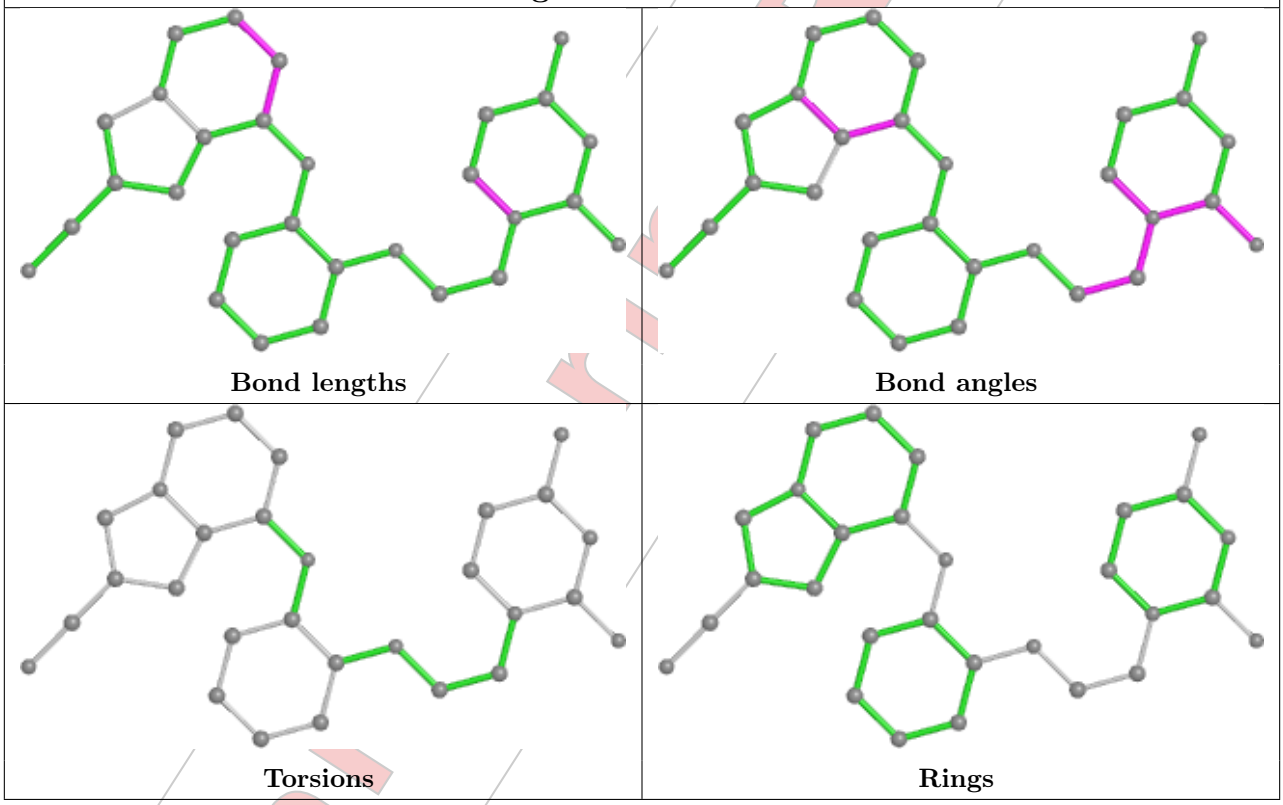
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	29T	1	0

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 29T A 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	543/557 (97%)	-0.19	8 (1%) 73 54	64, 109, 159, 206	0
2	B	415/428 (96%)	-0.18	4 (0%) 82 67	68, 98, 161, 207	0
All	All	958/985 (97%)	-0.18	12 (1%) 77 59	64, 105, 161, 207	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	4.9
1	A	221	HIS	2.9
1	A	358	ARG	2.7
2	B	231	GLY	2.4
2	B	239	TRP	2.3
1	A	140	PRO	2.3
2	B	308	GLU	2.3
1	A	247	PRO	2.3
1	A	3	SER	2.3
1	A	137	ASN	2.3
1	A	142	ILE	2.1
2	B	299	ALA	2.0

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

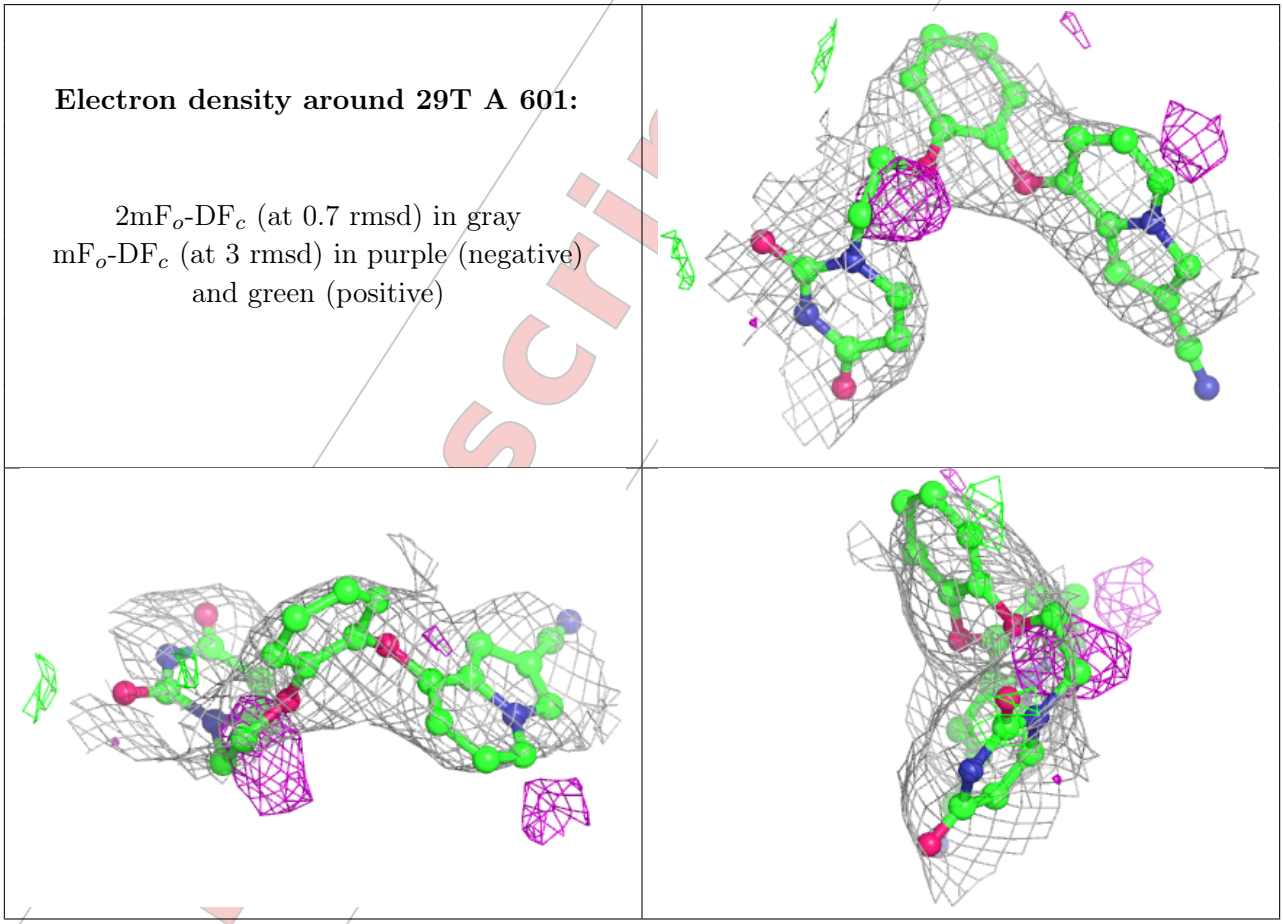
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	29T	A	601	29/29	0.93	0.30	73,89,103,124	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 29T 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.

Full wwPDB X-ray Structure Validation Report (i)

May 12, 2023 – 03:51 PM EDT

PDB ID	:	8STQ
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (Y181C) varient in Complex with 5-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)-2-naphthonitrile (JLJ600), a non-nucleoside inhibitor
Deposited on	:	2023-05-11
Resolution	:	2.96 Å(reported)

This wwPDB validation report is for manuscript review

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

This report is produced by the wwPDB biocuration pipeline after 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

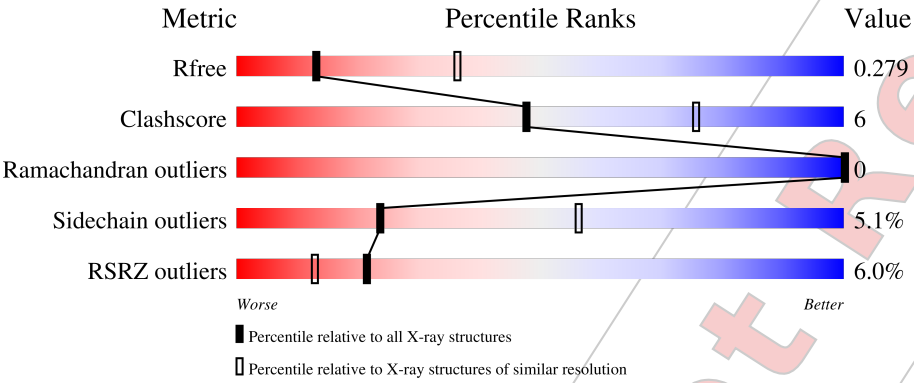
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	557	6% 78% 18%
2	B	428	5% 75% 15% 8%

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7593 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	541	4336	2805	713	809	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	conflict	UNP P03366
A	173	ALA	LYS	conflict	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

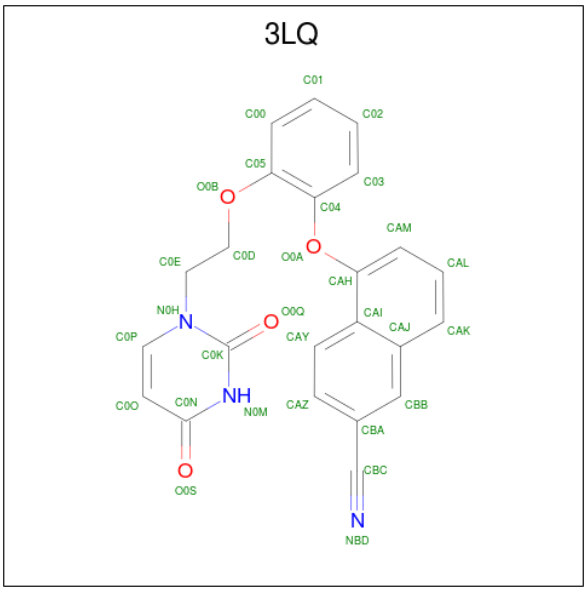
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	395	3225	2098	531	590	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 5-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}naphthalene-2-carbonitrile (three-letter code: 3LQ) (formula: $C_{23}H_{17}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 30 23 3 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

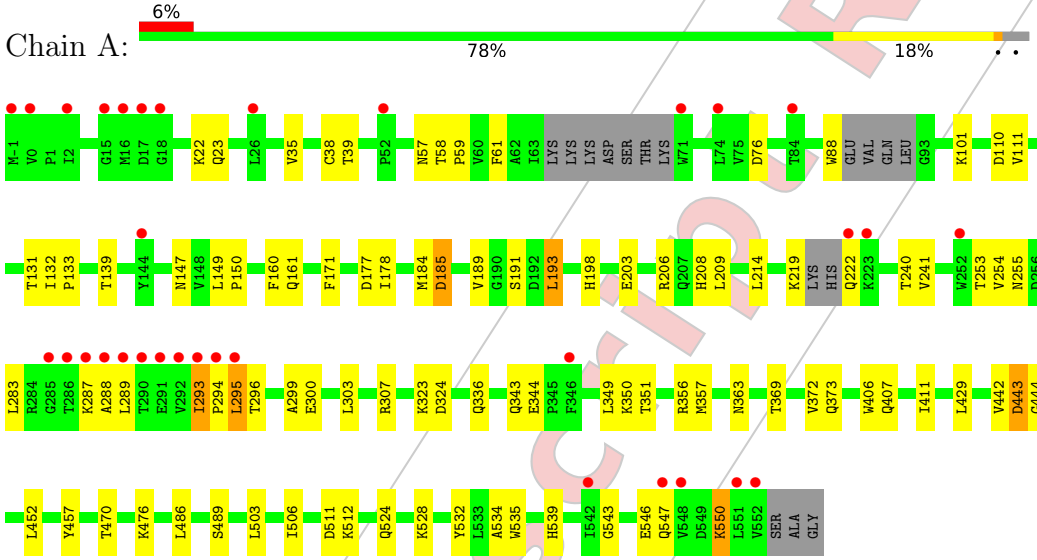
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0

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.

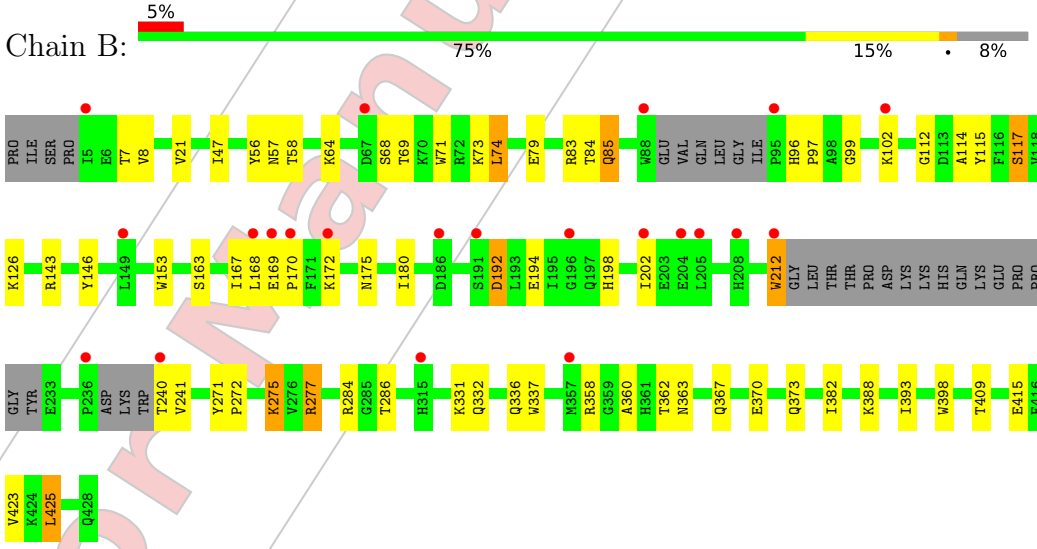
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



• Molecule 2: p51 RT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.28Å 73.84Å 107.26Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	35.24 – 2.96 35.24 – 2.96	Depositor EDS
% Data completeness (in resolution range)	97.4 (35.24-2.96) 97.4 (35.24-2.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.226 , 0.278 0.230 , 0.279	Depositor DCC
R_{free} test set	2000 reflections (7.81%)	wwPDB-VP
Wilson B-factor (Å^2)	86.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7593	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: MG, 3LQ

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	0.23	0/4449	0.41	0/6065
2	B	0.23	0/3315	0.42	0/4509
All	All	0.23	0/7764	0.41	0/10574

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	4336	0	4297	57	0
2	B	3225	0	3208	37	0
3	A	30	0	17	0	0
4	A	2	0	0	0	0
All	All	7593	0	7522	92	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 (92) 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:191:SER:HG	1:A:198:HIS:HD1	1.31	0.75
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.68	0.73
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.53	0.73
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.70	0.71
1:A:447:ASN:OD1	1:A:448:ARG:NH1	2.26	0.68
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.78	0.66
1:A:323:LYS:NZ	1:A:344:GLU:OE2	2.29	0.65
1:A:448:ARG:HD3	1:A:448:ARG:H	1.61	0.65
1:A:219:LYS:HB2	1:A:222:GLN:HB3	1.78	0.64
2:B:388:LYS:HE3	2:B:415:GLU:HG3	1.79	0.64
2:B:56:TYR:O	2:B:143:ARG:NH2	2.31	0.62
2:B:74:LEU:HD21	2:B:409:THR:HA	1.82	0.62
1:A:178:ILE:HG13	1:A:191:SER:HB3	1.82	0.62
1:A:185:ASP:N	1:A:185:ASP:OD1	2.33	0.62
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.83	0.61
2:B:332:GLN:HB2	2:B:336:GLN:HB2	1.82	0.61
1:A:539:HIS:H	1:A:547:GLN:HE22	1.49	0.59
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.84	0.59
2:B:212:TRP:HA	2:B:212:TRP:CE3	2.37	0.59
1:A:324:ASP:O	1:A:343:GLN:NE2	2.35	0.58
2:B:212:TRP:HA	2:B:212:TRP:HE3	1.69	0.57
2:B:360:ALA:HB1	2:B:367:GLN:HG2	1.86	0.57
1:A:539:HIS:N	1:A:547:GLN:HE22	2.03	0.56
1:A:356:ARG:NH1	1:A:357:MET:O	2.39	0.56
1:A:489:SER:O	1:A:528:LYS:NZ	2.39	0.56
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.88	0.55
1:A:296:THR:HG23	1:A:299:ALA:H	1.71	0.55
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.89	0.54
2:B:172:LYS:HG2	2:B:180:ILE:HD13	1.88	0.54
1:A:369:THR:O	1:A:373:GLN:HG2	2.08	0.54
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.89	0.53
2:B:163:SER:O	2:B:167:ILE:HG12	2.09	0.53
1:A:115:TYR:HB3	1:A:149:LEU:HB2	1.90	0.53
1:A:254:VAL:HG13	1:A:283:LEU:HD22	1.89	0.53
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.42	0.52
2:B:275:LYS:HD2	2:B:277:ARG:HG2	1.90	0.52
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.45	0.51
2:B:112:GLY:HA2	2:B:115:TYR:HD2	1.75	0.51
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.74	0.51
1:A:240:THR:OG1	1:A:241:VAL:N	2.45	0.50
2:B:421:PRO:HB2	2:B:423:VAL:HG22	1.94	0.50
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.44	0.49
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.48	0.49
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.95	0.49
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.95	0.48
2:B:123:ASP:O	2:B:126:LYS:NZ	2.37	0.48
1:A:253:THR:O	1:A:257:ILE:HG12	2.14	0.48
1:A:546:GLU:OE1	1:A:546:GLU:N	2.44	0.47
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.96	0.46
1:A:443:ASP:HB3	1:A:550:LYS:HG2	1.98	0.46
1:A:443:ASP:OD1	1:A:550:LYS:NZ	2.40	0.46
1:A:111:VAL:HG21	1:A:160:PHE:HZ	1.80	0.46
2:B:194:GLU:O	2:B:198:HIS:N	2.39	0.45
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.97	0.45
1:A:293:ILE:HG22	1:A:294:PRO:HD2	1.98	0.45
1:A:295:LEU:HD13	1:A:300:GLU:HB2	1.98	0.45
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.57	0.45
1:A:111:VAL:HG22	1:A:185:ASP:O	2.17	0.44
1:A:539:HIS:H	1:A:547:GLN:NE2	2.15	0.44
2:B:21:VAL:O	2:B:57:ASN:ND2	2.43	0.44
2:B:425:LEU:HD23	2:B:425:LEU:H	1.83	0.44
1:A:350:LYS:NZ	1:A:351:THR:O	2.46	0.44
2:B:363:ASN:O	2:B:367:GLN:HG3	2.18	0.44
1:A:452:LEU:HD23	1:A:470:THR:HA	2.00	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.53	0.43
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.53	0.43
1:A:444:GLY:O	1:A:550:LYS:NZ	2.51	0.43
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.99	0.43
2:B:192:ASP:OD2	2:B:192:ASP:N	2.52	0.43
1:A:277:ARG:HB2	1:A:336:GLN:OE1	2.18	0.43
1:A:406:TRP:CZ2	1:A:407:GLN:HG3	2.54	0.43
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.88	0.42
1:A:303:LEU:O	1:A:307:ARG:HG3	2.19	0.42
1:A:23:GLN:HG3	1:A:133:PRO:HG3	2.02	0.42
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.36	0.42
2:B:85:GLN:H	2:B:85:GLN:HG3	1.69	0.42
2:B:114:ALA:O	2:B:117:SER:OG	2.38	0.42
1:A:254:VAL:HB	1:A:288:ALA:O	2.19	0.42
1:A:255:ASN:HB2	1:A:289:LEU:HD22	2.01	0.41
2:B:47:ILE:HG22	2:B:146:TYR:HA	2.02	0.41
2:B:96:HIS:HE1	2:B:382:ILE:O	2.03	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:HE3	1:A:476:LYS:HB2	1.86	0.41
2:B:198:HIS:O	2:B:202:ILE:HG12	2.21	0.41
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.03	0.41
1:A:191:SER:HB2	1:A:193:LEU:HD22	2.03	0.41
1:A:35:VAL:O	1:A:39:THR:OG1	2.29	0.41
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.73	0.40
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.56	0.40
2:B:370:GLU:HA	2:B:373:GLN:HE21	1.86	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.84	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	533/557 (96%)	518 (97%)	15 (3%)	0	100	100
2	B	387/428 (90%)	379 (98%)	8 (2%)	0	100	100
All	All	920/985 (93%)	897 (98%)	23 (2%)	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	468/495 (94%)	446 (95%)	22 (5%)	26	59
2	B	350/390 (90%)	330 (94%)	20 (6%)	20	52
All	All	818/885 (92%)	776 (95%)	42 (5%)	24	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	58	THR
1	A	61	PHE
1	A	101	LYS
1	A	110	ASP
1	A	126	LYS
1	A	139	THR
1	A	161	GLN
1	A	177	ASP
1	A	184	MET
1	A	185	ASP
1	A	189	VAL
1	A	193	LEU
1	A	287	LYS
1	A	293	ILE
1	A	295	LEU
1	A	349	LEU
1	A	443	ASP
1	A	448	ARG
1	A	449	GLU
1	A	512	LYS
1	A	550	LYS
2	B	7	THR
2	B	8	VAL
2	B	58	THR
2	B	68	SER
2	B	69	THR
2	B	74	LEU
2	B	85	GLN
2	B	117	SER
2	B	175	ASN
2	B	192	ASP
2	B	212	TRP
2	B	240	THR
2	B	241	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	275	LYS
2	B	277	ARG
2	B	286	THR
2	B	358	ARG
2	B	362	THR
2	B	417	VAL
2	B	425	LEU

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	208	HIS
1	A	255	ASN
1	A	258	GLN
1	A	340	GLN
1	A	373	GLN
1	A	464	GLN
1	A	471	ASN
1	A	487	GLN
1	A	547	GLN
2	B	85	GLN
2	B	96	HIS
2	B	147	ASN
2	B	208	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 (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - 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	3LQ	A	601	-	33,33,33	1.33	3 (9%)	44,45,45	1.10	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3LQ	A	601	-	-	1/12/12/12	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	3LQ	C0P-N0H	3.53	1.42	1.37
3	A	601	3LQ	CAY-CAZ	2.89	1.42	1.36
3	A	601	3LQ	CAL-CAK	2.48	1.42	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	3LQ	C0E-N0H-C0K	3.70	122.44	118.54
3	A	601	3LQ	CBB-CBA-CBC	2.55	121.86	119.65
3	A	601	3LQ	C0O-C0P-N0H	-2.48	120.12	122.44
3	A	601	3LQ	C0E-N0H-C0P	-2.42	116.06	119.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

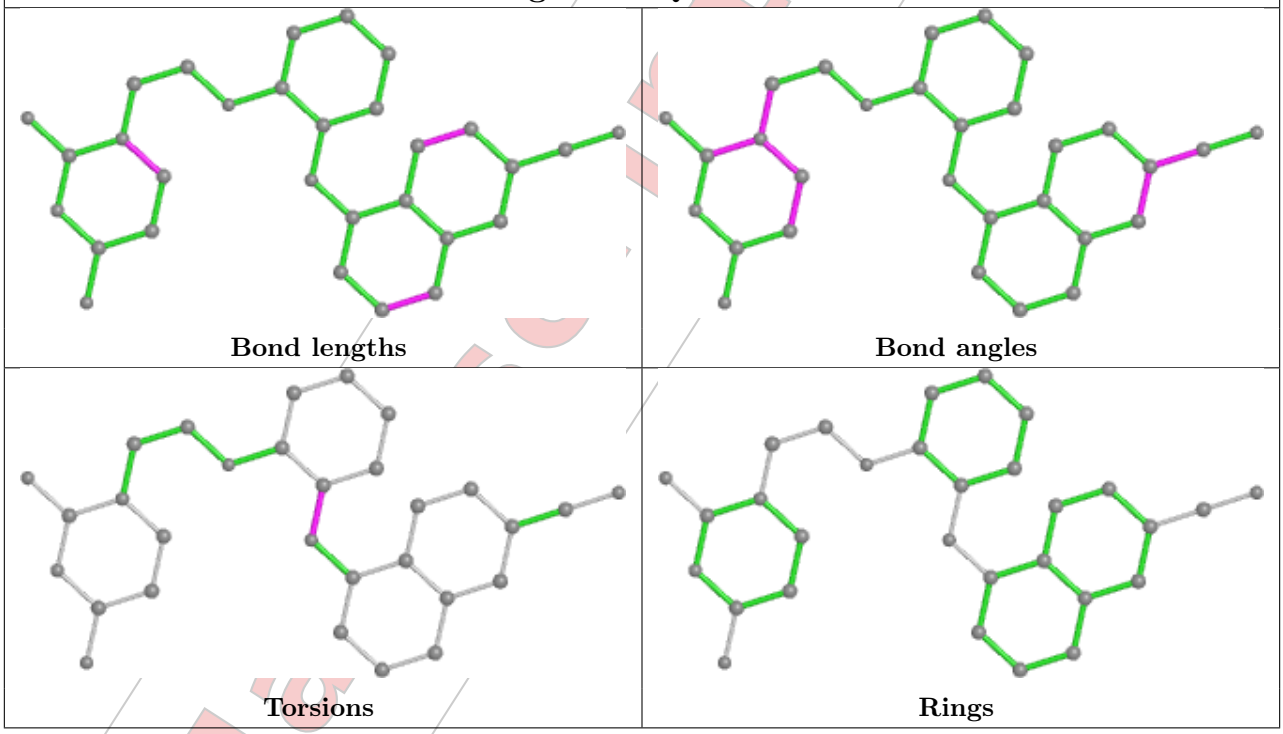
Mol	Chain	Res	Type	Atoms
3	A	601	3LQ	C05-C04-O0A-CAH

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 3LQ A 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	541/557 (97%)	0.20	33 (6%)	21	12	50, 92, 145, 165	0
2	B	395/428 (92%)	0.23	23 (5%)	23	14	56, 88, 141, 152	0
All	All	936/985 (95%)	0.21	56 (5%)	21	13	50, 89, 143, 165	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	GLY	4.7
1	A	286	THR	4.4
2	B	170	PRO	4.2
1	A	16	MET	4.0
2	B	236	PRO	3.9
1	A	-1	MET	3.8
1	A	222	GLN	3.7
2	B	5	ILE	3.7
1	A	0	VAL	3.6
2	B	168	LEU	3.5
1	A	542	ILE	3.4
2	B	95	PRO	3.4
2	B	88	TRP	3.3
2	B	357	MET	3.3
2	B	191	SER	3.2
2	B	240	THR	3.2
2	B	149	LEU	3.0
1	A	252	TRP	3.0
1	A	287	LYS	2.9
1	A	285	GLY	2.9
2	B	169	GLU	2.8
1	A	144	TYR	2.8
1	A	295	LEU	2.8
1	A	292	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	212	TRP	2.6
2	B	102	LYS	2.6
2	B	205	LEU	2.6
1	A	291	GLU	2.5
1	A	552	VAL	2.5
1	A	288	ALA	2.5
1	A	548	VAL	2.5
2	B	202	ILE	2.4
2	B	196	GLY	2.4
1	A	52	PRO	2.4
1	A	547	GLN	2.4
1	A	290	THR	2.3
1	A	346	PHE	2.3
1	A	71	TRP	2.3
1	A	293	ILE	2.3
1	A	551	LEU	2.3
2	B	208	HIS	2.3
1	A	74	LEU	2.2
1	A	289	LEU	2.2
1	A	223	LYS	2.2
1	A	18	GLY	2.2
1	A	17	ASP	2.2
1	A	294	PRO	2.2
2	B	186	ASP	2.1
1	A	2	ILE	2.1
2	B	204	GLU	2.1
1	A	26	LEU	2.0
2	B	119	PRO	2.0
2	B	315	HIS	2.0
2	B	172	LYS	2.0
2	B	67	ASP	2.0
1	A	84	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

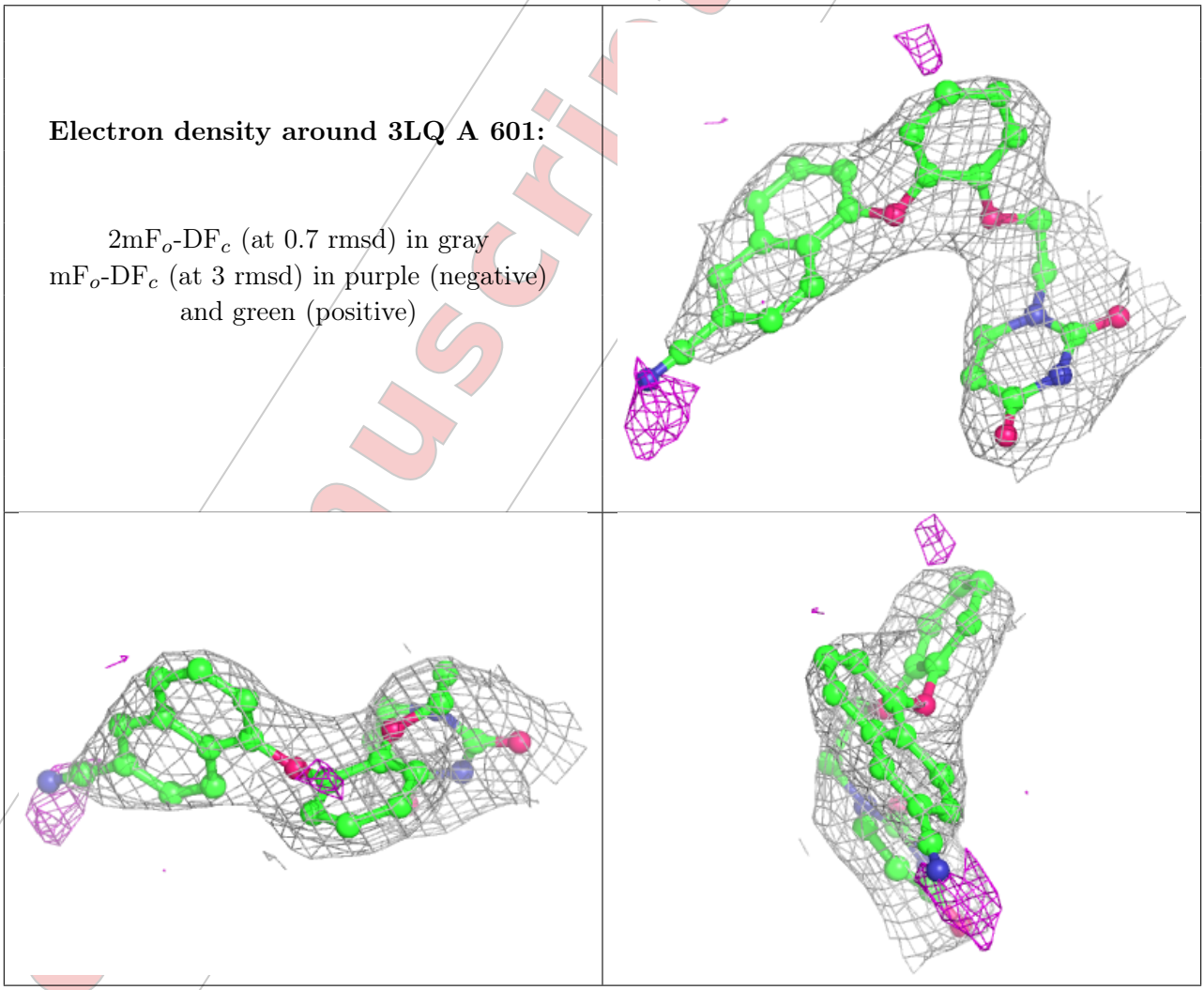
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	MG	A	602	1/1	0.91	0.30	72,72,72,72	0
3	3LQ	A	601	30/30	0.94	0.25	60,74,81,87	0
4	MG	A	603	1/1	0.95	0.21	93,93,93,93	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 3LQ 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 (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report (i)

May 12, 2023 – 04:00 PM EDT

PDB ID	:	8STR
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (Y181C) varient in Complex with 5-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)-4-fluorophenoxy)-7-fluoro-2-naphthonitrile (JLJ636), a non-nucleoside inhibitor
Deposited on	:	2023-05-11
Resolution	:	2.77 Å(reported)

This wwPDB validation report is for manuscript review

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

This report is produced by the wwPDB biocuration pipeline after 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

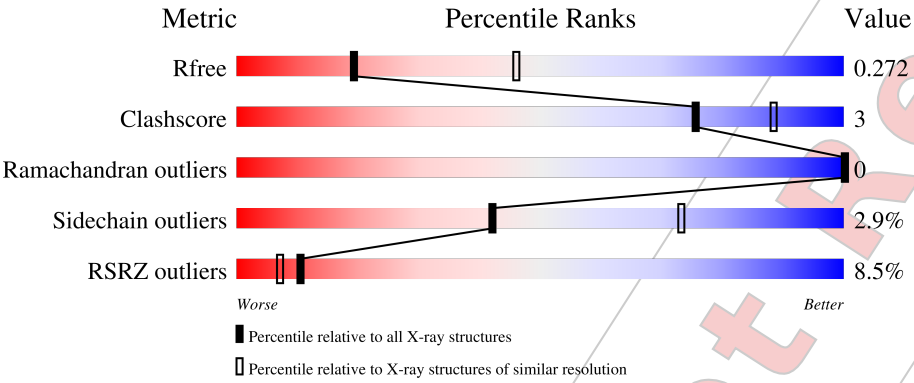
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 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	557	10% 87% 9% .
2	B	428	6% 82% 10% 7%

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7484 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	534	4236	2733	705	789	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	conflict	UNP P03366
A	173	ALA	LYS	conflict	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

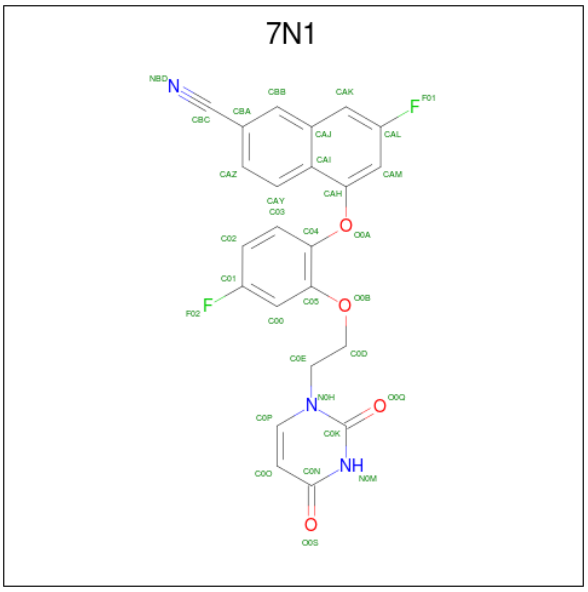
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	396	3194	2079	522	587	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 5-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]-4-fluorophenoxy}-7-fluoronaphthalene-2-carbonitrile (three-letter code: 7N1) (formula: $C_{23}H_{15}F_2N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O 32 23 2 3 4	0	0

- Molecule 4 is water.

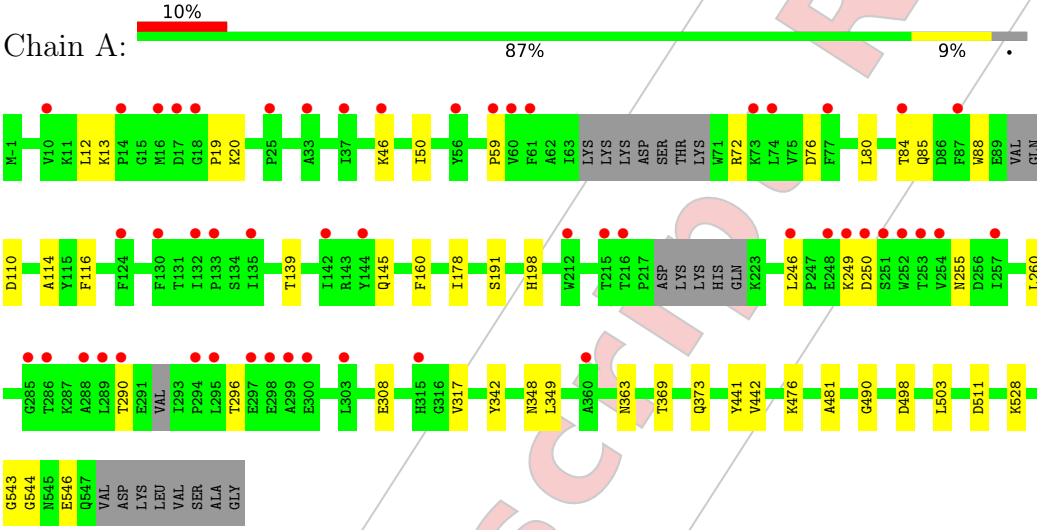
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	5	Total O 5 5	0	0

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.

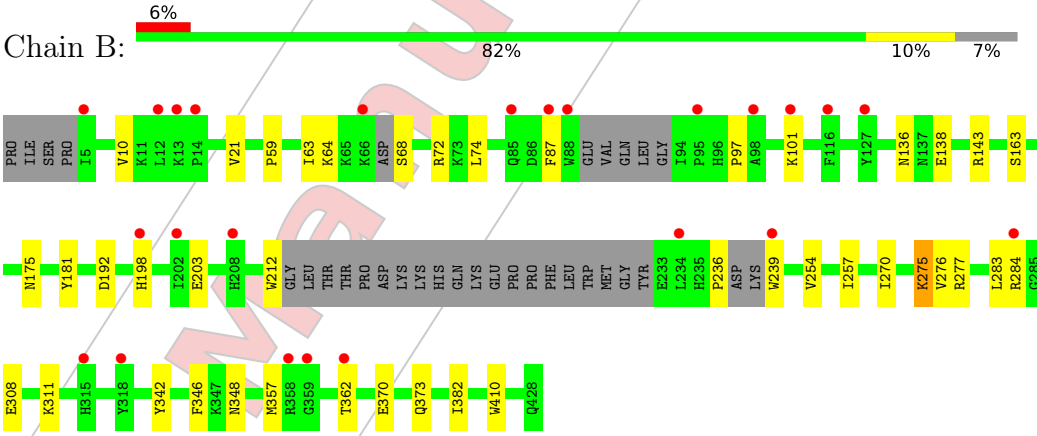
- Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



- Molecule 2: p51 RT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.73Å 74.04Å 107.83Å 90.00° 99.09° 90.00°	Depositor
Resolution (Å)	39.92 – 2.77 41.38 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.92-2.77) 99.6 (41.38-2.77)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.240 , 0.268 0.242 , 0.272	Depositor DCC
R_{free} test set	1609 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7484	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: 7N1

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	0.24	0/4346	0.43	0/5921
2	B	0.24	0/3285	0.42	0/4477
All	All	0.24	0/7631	0.43	0/10398

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	4236	0	4152	25	0
2	B	3194	0	3118	24	0
3	A	32	0	0	0	0
4	A	17	0	0	1	0
4	B	5	0	0	0	0
All	All	7484	0	7270	45	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 (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:A:191:SER:OG	1:A:198:HIS:ND1	2.28	0.62
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.85	0.58
2:B:10:VAL:HG13	2:B:87:PHE:HZ	1.69	0.57
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.89	0.55
2:B:275:LYS:HD3	2:B:276:VAL:H	1.72	0.54
1:A:50:ILE:HG21	1:A:145:GLN:HB3	1.89	0.53
1:A:544:GLY:HA2	2:B:286:THR:HG23	1.91	0.53
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.91	0.53
2:B:308:GLU:HA	2:B:311:LYS:HE2	1.91	0.52
1:A:369:THR:O	1:A:373:GLN:HG2	2.09	0.52
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.46	0.51
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.94	0.50
2:B:10:VAL:HG13	2:B:87:PHE:CZ	2.46	0.50
1:A:490:GLY:O	1:A:528:LYS:NZ	2.31	0.49
1:A:46:LYS:HZ3	1:A:116:PHE:HD2	1.60	0.49
1:A:178:ILE:HG22	1:A:191:SER:HB3	1.95	0.49
1:A:13:LYS:HG2	1:A:85:GLN:HA	1.95	0.48
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.95	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
1:A:441:TYR:CD1	2:B:286:THR:HG22	2.49	0.47
2:B:212:TRP:N	2:B:212:TRP:CD1	2.83	0.47
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.97	0.46
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.97	0.46
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.97	0.46
2:B:275:LYS:HD2	2:B:277:ARG:HG2	1.98	0.46
2:B:275:LYS:HD3	2:B:276:VAL:N	2.30	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.45
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.99	0.45
1:A:476:LYS:NZ	4:A:702:HOH:O	2.49	0.44
1:A:80:LEU:O	1:A:84:THR:OG1	2.31	0.44
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.53	0.44
2:B:101:LYS:HD3	2:B:382:ILE:HG23	1.99	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.18	0.43
2:B:236:PRO:HA	2:B:239:TRP:HD1	1.83	0.43
1:A:498:ASP:HB2	1:A:538:ALA:HB2	2.01	0.43
1:A:342:TYR:HB3	1:A:348:ASN:HA	2.01	0.43
2:B:370:GLU:HA	2:B:373:GLN:HE21	1.84	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.00	0.42
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.02	0.42
2:B:136:ASN:HB3	2:B:138:GLU:HG3	2.01	0.42
1:A:72:ARG:HD3	1:A:72:ARG:HA	1.95	0.41
1:A:12:LEU:HD23	1:A:84:THR:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.21	0.40
2:B:342:TYR:HB3	2:B:348:ASN:HA	2.02	0.40
2:B:97:PRO:HG3	2:B:181:TYR:HB2	2.03	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	524/557 (94%)	511 (98%)	13 (2%)	0	100	100
2	B	386/428 (90%)	374 (97%)	12 (3%)	0	100	100
All	All	910/985 (92%)	885 (97%)	25 (3%)	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	448/495 (90%)	437 (98%)	11 (2%)	47	77
2	B	340/390 (87%)	328 (96%)	12 (4%)	36	67
All	All	788/885 (89%)	765 (97%)	23 (3%)	42	73

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	101	LYS
1	A	110	ASP
1	A	139	THR
1	A	249	LYS
1	A	250	ASP
1	A	255	ASN
1	A	290	THR
1	A	296	THR
1	A	308	GLU
1	A	546	GLU
2	B	64	LYS
2	B	68	SER
2	B	72	ARG
2	B	175	ASN
2	B	192	ASP
2	B	198	HIS
2	B	203	GLU
2	B	275	LYS
2	B	286	THR
2	B	357	MET
2	B	362	THR
2	B	410	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is modelled in this entry.

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	7N1	A	601	-	35,35,35	2.22	7 (20%)	48,49,49	1.72	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7N1	A	601	-	-	1/12/12/12	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	7N1	C0P-N0H	7.97	1.48	1.37
3	A	601	7N1	C0K-N0H	5.56	1.45	1.37
3	A	601	7N1	C0O-C0N	4.24	1.53	1.43
3	A	601	7N1	CBA-CBC	3.96	1.53	1.44
3	A	601	7N1	O0S-C0N	-2.81	1.19	1.24
3	A	601	7N1	C0K-N0M	2.26	1.42	1.38
3	A	601	7N1	O0Q-C0K	-2.17	1.19	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	7N1	N0M-C0K-N0H	5.25	119.67	114.86
3	A	601	7N1	C0N-N0M-C0K	-4.66	120.44	126.58
3	A	601	7N1	O0Q-C0K-N0H	-3.63	119.67	122.85
3	A	601	7N1	C0O-C0N-N0M	3.33	119.82	114.84
3	A	601	7N1	O0S-C0N-C0O	-3.24	119.46	125.16
3	A	601	7N1	CBB-CBA-CBC	2.67	121.96	119.65
3	A	601	7N1	C0O-C0P-N0H	-2.22	120.36	122.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	7N1	C02-C01-C00	-2.14	120.51	123.29
3	A	601	7N1	C03-C02-C01	2.14	120.57	118.36
3	A	601	7N1	CAH-CAI-CAJ	2.13	120.68	118.01
3	A	601	7N1	CAK-CAL-CAM	-2.07	122.45	124.09
3	A	601	7N1	O0A-CAH-CAM	2.04	124.11	119.36

There are no chirality outliers.

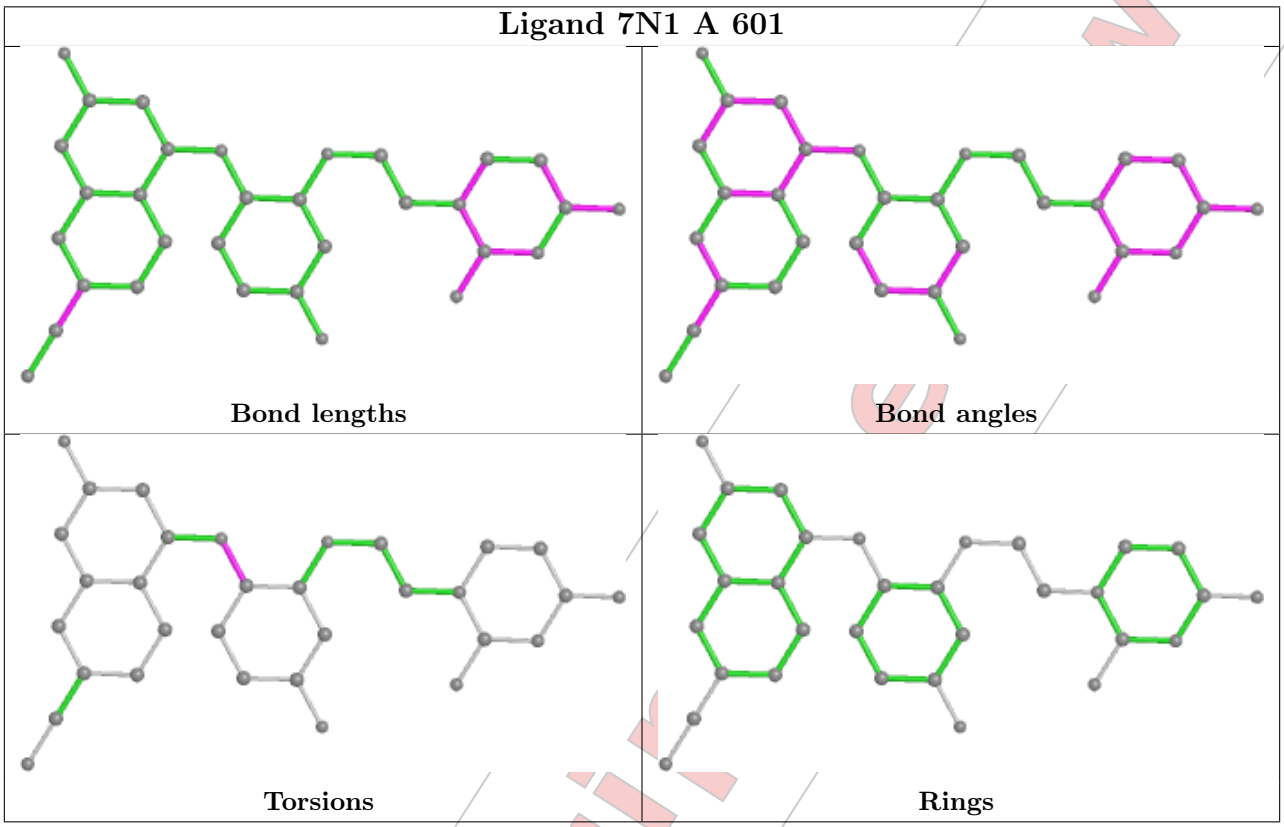
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	7N1	C05-C04-O0A-CAH

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.



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	534/557 (95%)	0.52	53 (9%) 7 5	38, 79, 122, 143	0
2	B	396/428 (92%)	0.47	26 (6%) 18 13	44, 74, 120, 130	0
All	All	930/985 (94%)	0.50	79 (8%) 10 7	38, 77, 122, 143	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	TRP	5.2
2	B	66	LYS	4.5
1	A	286	THR	4.4
1	A	254	VAL	4.3
2	B	239	TRP	4.3
1	A	289	LEU	4.1
1	A	279	LEU	4.0
1	A	300	GLU	3.9
2	B	198	HIS	3.9
2	B	116	PHE	3.8
2	B	88	TRP	3.7
1	A	16	MET	3.7
1	A	299	ALA	3.7
1	A	251	SER	3.7
1	A	294	PRO	3.7
2	B	12	LEU	3.7
2	B	95	PRO	3.6
1	A	74	LEU	3.6
2	B	14	PRO	3.6
1	A	61	PHE	3.5
1	A	133	PRO	3.5
2	B	168	LEU	3.5
1	A	295	LEU	3.5
2	B	85	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	PHE	3.3
1	A	288	ALA	3.3
2	B	358	ARG	3.3
1	A	249	LYS	3.3
2	B	87	PHE	3.2
1	A	282	LEU	3.1
1	A	215	THR	3.1
1	A	253	THR	3.1
1	A	18	GLY	3.0
1	A	14	PRO	3.0
1	A	360	ALA	3.0
1	A	135	ILE	3.0
2	B	5	ILE	2.9
1	A	73	LYS	2.9
1	A	248	GLU	2.9
2	B	127	TYR	2.9
2	B	13	LYS	2.8
1	A	303	LEU	2.8
1	A	10	VAL	2.7
1	A	144	TYR	2.7
2	B	202	ILE	2.7
1	A	17	ASP	2.7
2	B	284	ARG	2.6
1	A	290	THR	2.6
2	B	234	LEU	2.6
1	A	246	LEU	2.5
1	A	298	GLU	2.5
1	A	250	ASP	2.5
2	B	359	GLY	2.5
2	B	318	TYR	2.5
1	A	124	PHE	2.4
1	A	216	THR	2.4
2	B	362	THR	2.4
1	A	59	PRO	2.4
1	A	46	LYS	2.3
2	B	171	PHE	2.3
1	A	33	ALA	2.3
1	A	142	ILE	2.3
1	A	56	TYR	2.2
1	A	297	GLU	2.2
2	B	315	HIS	2.2
1	A	84	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	208	HIS	2.2
1	A	132	ILE	2.1
1	A	257	ILE	2.1
1	A	285	GLY	2.1
1	A	315	HIS	2.1
1	A	37	ILE	2.1
1	A	212	TRP	2.1
1	A	77	PHE	2.1
2	B	98	ALA	2.1
1	A	87	PHE	2.1
1	A	60	VAL	2.1
1	A	25	PRO	2.1
2	B	101	LYS	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)

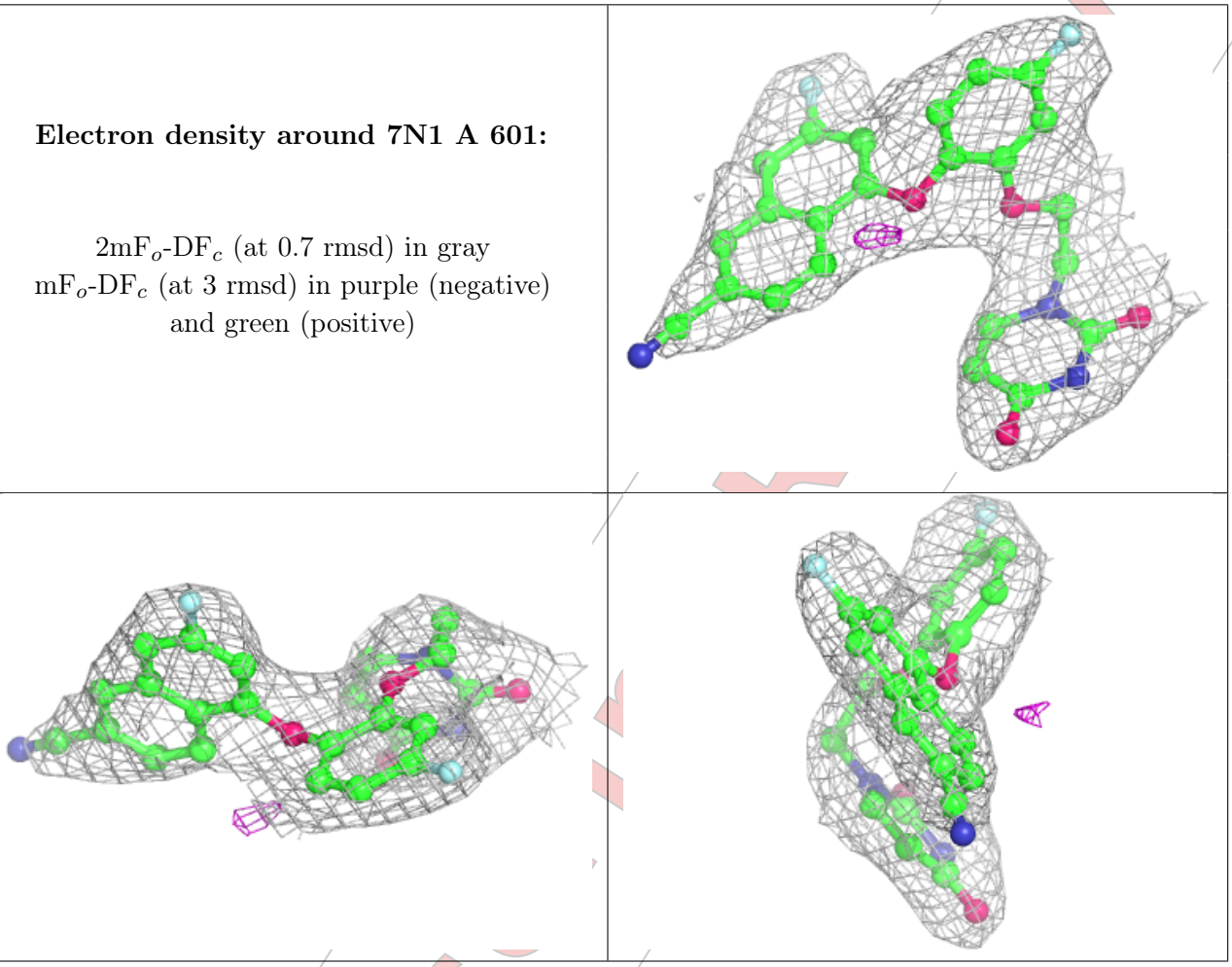
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	7N1	A	601	32/32	0.94	0.20	50,66,72,76	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 7N1 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.

Full wwPDB X-ray Structure Validation Report (i)

May 23, 2023 – 12:26 PM EDT

PDB ID	:	8STT
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (Y181C, V106A) varient in Complex with 8-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)indolizine-2-carbonitrile (JLJ555), a non-nucleoside inhibitor
Deposited on	:	2023-05-11
Resolution	:	2.62 Å(reported)

This wwPDB validation report is for manuscript review

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

This report is produced by the wwPDB biocuration pipeline after 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

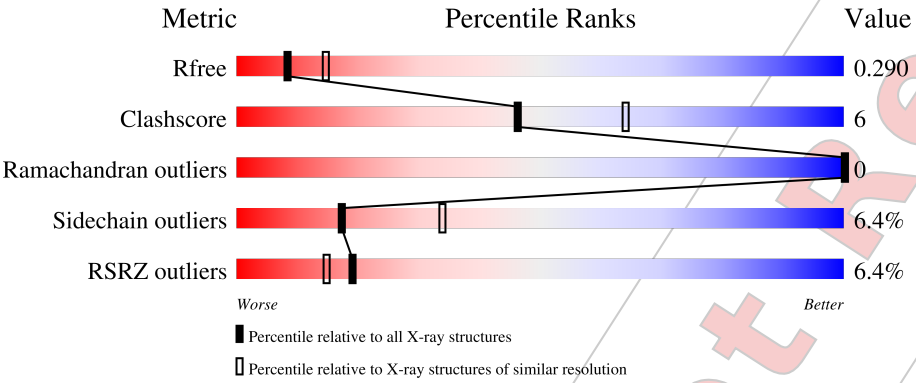
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

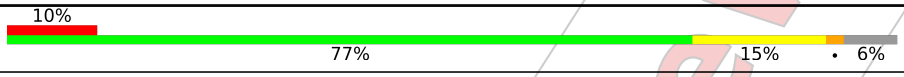
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	558	4% 81% 16%
1	C	558	8% 77% 19%
2	B	428	2% 75% 18% 5%

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	428	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14881 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	1	0
			4184	2692	686	799	7			
1	C	544	Total	C	N	O	S	0	3	0
			4225	2706	704	808	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	106	ALA	VAL	engineered mutation	UNP P03366
A	172	ALA	LYS	conflict	UNP P03366
A	173	ALA	LYS	conflict	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	106	ALA	VAL	engineered mutation	UNP P03366
C	172	ALA	LYS	conflict	UNP P03366
C	173	ALA	LYS	conflict	UNP P03366
C	181	CYS	TYR	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	23	2	0
			3270	2123	532	609	6			
2	D	401	Total	C	N	O	S	14	1	0
			3078	1989	508	577	4			

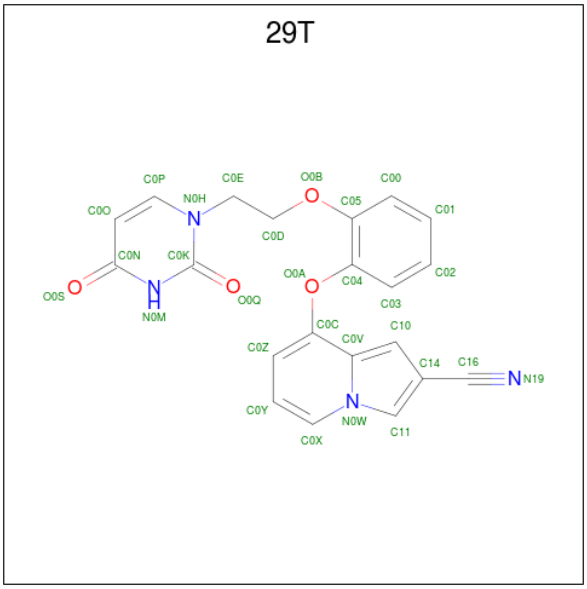
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 8-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}indolizine-2-carbonitrile (three-letter code: 29T) (formula: $C_{21}H_{16}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 29 21 4 4	0	0
4	C	1	Total C N O 29 21 4 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	26	Total O 26 26	0	0

Continued on next page...

Continued from previous page...

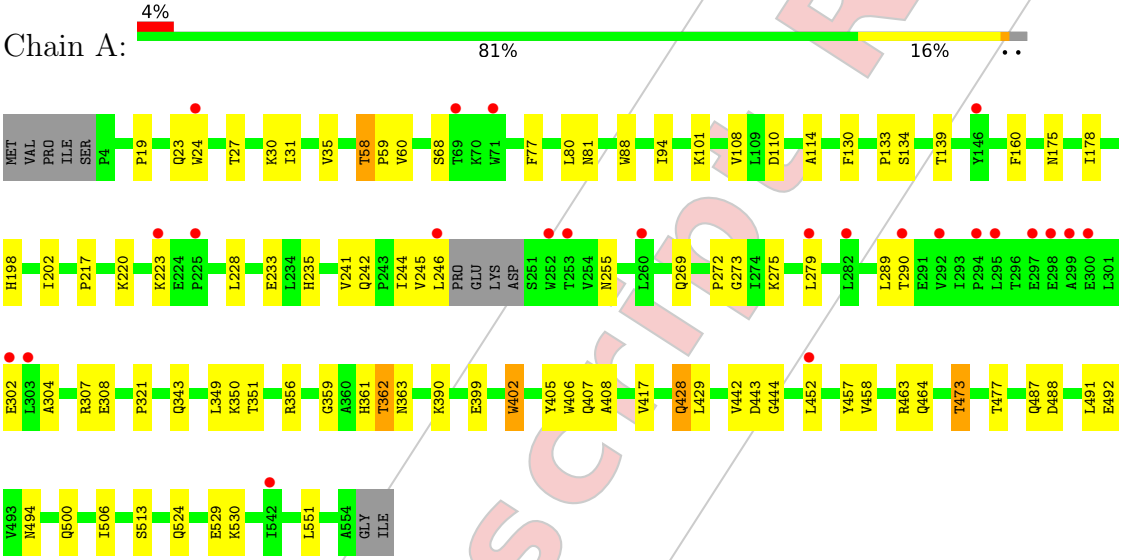
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	27	Total O 27 27	0	0
5	C	10	Total O 10 10	0	0
5	D	1	Total O 1 1	0	0

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.

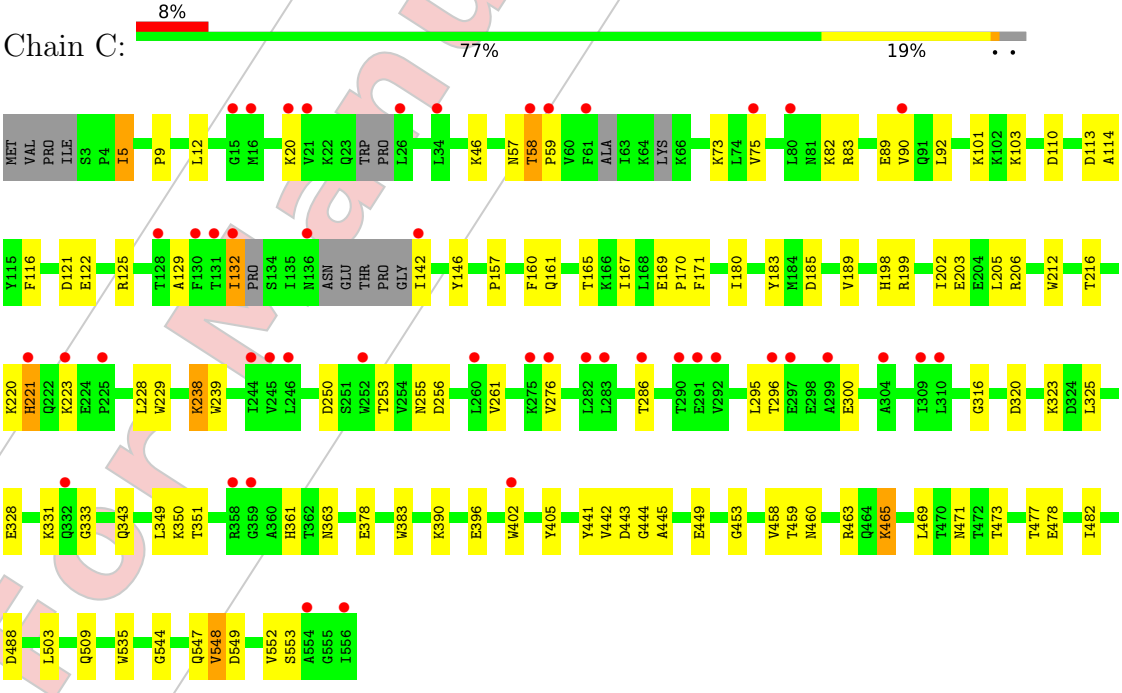
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



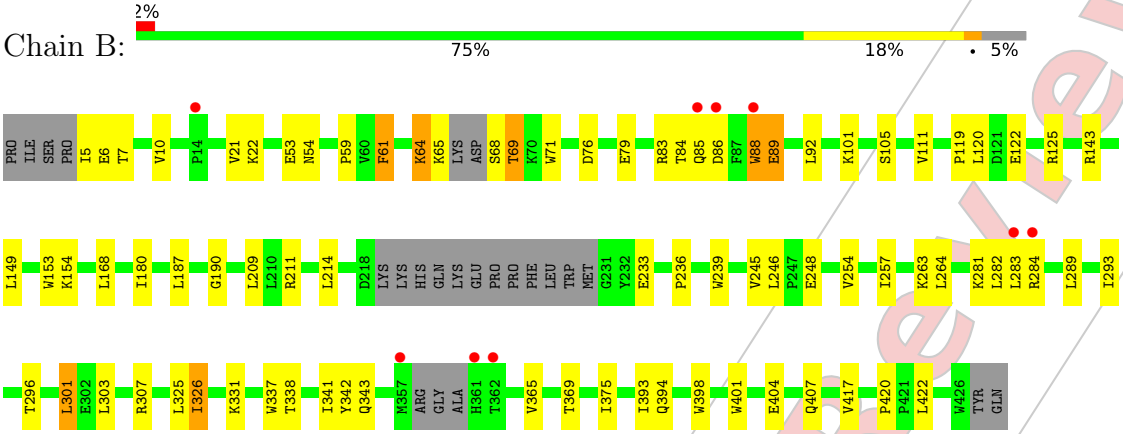
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain C:



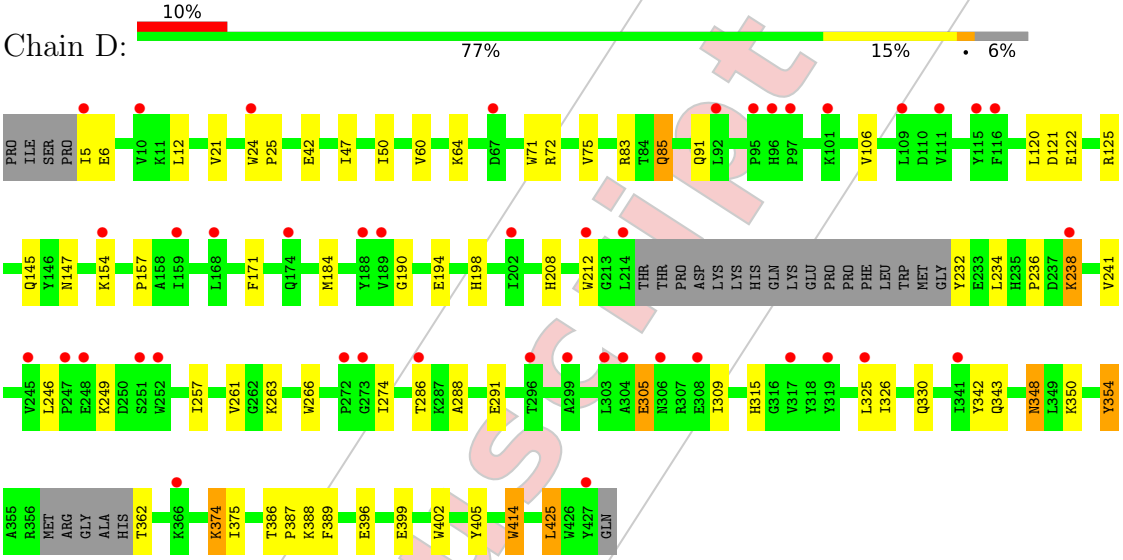
• Molecule 2: p51 RT

Chain B:



• Molecule 2: p51 RT

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.69Å 73.01Å 170.47Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	54.79 – 2.62 54.79 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.79-2.62) 99.1 (54.79-2.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.263 , 0.291 0.262 , 0.290	Depositor DCC
R_{free} test set	4011 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14881	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: 29T, MG

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	0/4296	0.49	0/5880
1	C	0.29	0/4328	0.47	0/5894
2	B	0.32	0/3366	0.51	0/4592
2	D	0.27	0/3169	0.45	0/4343
All	All	0.30	0/15159	0.48	0/20709

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	4184	0	3930	51	0
1	C	4225	0	4032	46	0
2	B	3270	0	3199	52	0
2	D	3078	0	2821	40	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	29	0	16	0	0
4	C	29	0	16	1	0
5	A	26	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	27	0	0	2	0
5	C	10	0	0	0	0
5	D	1	0	0	0	0
All	All	14881	0	14014	180	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 (180) 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:328:GLU:HG2	1:C:390:LYS:HB2	1.76	0.68
1:C:132:ILE:HB	1:C:142:ILE:HD12	1.76	0.67
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.77	0.66
1:C:460:ASN:HD22	2:D:288:ALA:HB2	1.63	0.64
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.64	0.63
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.80	0.63
1:C:90:VAL:HG21	1:C:157:PRO:HB2	1.83	0.60
2:D:157:PRO:HG2	2:D:184:MET:HA	1.83	0.60
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.36	0.60
2:B:85:GLN:O	2:B:89:GLU:N	2.34	0.60
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.83	0.60
2:B:64:LYS:HD2	2:B:69:THR:O	2.01	0.60
2:D:348:ASN:N	2:D:348:ASN:OD1	2.34	0.60
1:A:356:ARG:NH1	1:A:359:GLY:O	2.34	0.59
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.37	0.59
1:C:253:THR:HG23	1:C:256:ASP:H	1.67	0.59
2:D:194:GLU:O	2:D:198:HIS:N	2.32	0.59
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.86	0.57
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.87	0.57
1:C:444:GLY:HA2	1:C:552:VAL:HG21	1.86	0.56
1:C:331:LYS:NZ	1:C:333:GLY:O	2.38	0.56
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.87	0.56
1:C:89:GLU:HG2	1:C:92:LEU:HG	1.87	0.56
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.87	0.56
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.89	0.56
2:B:65:LYS:HA	2:B:407:GLN:OE1	2.06	0.55
1:A:23:GLN:HE22	1:A:133:PRO:HD3	1.70	0.55
1:C:445:ALA:HB3	1:C:553:SER:HB3	1.89	0.55
2:B:64:LYS:HD3	2:B:71:TRP:CE2	2.43	0.54
1:A:402:TRP:C	1:A:402:TRP:CD1	2.81	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.89	0.53
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.44	0.53
1:A:241:VAL:HG12	1:A:242:GLN:O	2.09	0.53
1:C:343:GLN:HG3	1:C:349:LEU:HD21	1.91	0.52
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.91	0.52
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.45	0.52
2:D:325:LEU:HD23	2:D:343:GLN:HG3	1.90	0.52
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.90	0.52
2:D:12:LEU:HD22	2:D:83:ARG:HB2	1.92	0.52
2:D:125:ARG:HD3	2:D:147:ASN:HA	1.91	0.52
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.90	0.51
2:D:60:VAL:HG12	2:D:75:VAL:HG22	1.92	0.51
2:B:54:ASN:O	2:B:143:ARG:NH2	2.44	0.51
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.93	0.51
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.92	0.50
1:C:46:LYS:HD2	1:C:116:PHE:HB3	1.94	0.50
1:C:58:THR:HG22	1:C:59:PRO:HD2	1.93	0.50
1:A:110:ASP:O	1:A:217:PRO:HD3	2.12	0.49
2:D:375:ILE:HB	2:D:389:PHE:HZ	1.76	0.49
2:D:24[B]:TRP:HZ3	2:D:402:TRP:HE1	1.60	0.49
1:A:443:ASP:OD1	1:A:444:GLY:N	2.46	0.49
2:B:5:ILE:HD12	2:B:6:GLU:HG3	1.95	0.49
2:B:233:GLU:HG3	5:B:527:HOH:O	2.12	0.49
1:C:453:GLY:HA3	1:C:469:LEU:HB2	1.94	0.49
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.78	0.49
2:B:245:VAL:O	2:B:263:LYS:NZ	2.38	0.49
1:A:500:GLN:HG3	2:B:422:LEU:HD13	1.94	0.48
2:D:388:LYS:O	2:D:414:TRP:HA	2.14	0.48
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.48	0.47
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.95	0.47
1:C:180:ILE:HG23	1:C:189:VAL:HG22	1.95	0.47
1:A:491:LEU:HD13	1:A:529:GLU:OE2	2.14	0.47
1:A:31:ILE:O	1:A:35:VAL:HG23	2.15	0.47
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.72	0.47
2:B:365:VAL:O	2:B:369:THR:HG23	2.15	0.47
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.50	0.47
1:C:167:ILE:O	1:C:170:PRO:HD2	2.15	0.47
1:C:458:VAL:HG23	1:C:548:VAL:HG13	1.96	0.47
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.45	0.47
2:B:120:LEU:HD13	2:B:149:LEU:HD23	1.97	0.47
2:D:64:LYS:HE2	2:D:71:TRP:CZ2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:PRO:HD2	2:D:389:PHE:HE2	1.80	0.46
2:B:79:GLU:OE1	2:B:83:ARG:NH1	2.48	0.46
2:B:211:ARG:HB3	1:C:212:TRP:CZ2	2.51	0.46
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.51	0.46
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.80	0.46
2:B:303:LEU:O	2:B:307:ARG:HG3	2.15	0.46
2:B:325:LEU:HD23	2:B:343:GLN:HG3	1.97	0.46
2:D:50:ILE:HG21	2:D:145:GLN:HB3	1.96	0.46
2:D:238:LYS:HA	2:D:238:LYS:HD2	1.59	0.46
2:D:396:GLU:OE1	2:D:396:GLU:N	2.45	0.46
2:B:84:THR:HG21	2:B:153:TRP:CZ2	2.48	0.46
1:C:203:GLU:OE2	1:C:206:ARG:NH1	2.47	0.46
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.98	0.46
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.97	0.46
1:C:9:PRO:HA	1:C:121:ASP:OD2	2.15	0.46
2:D:171:PHE:HB2	2:D:208:HIS:ND1	2.31	0.46
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.81	0.45
2:B:394:GLN:NE2	5:B:507:HOH:O	2.49	0.45
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.46	0.45
1:A:473:THR:O	1:A:477:THR:HG23	2.16	0.45
2:D:305:GLU:O	2:D:309:ILE:HG12	2.16	0.45
1:A:134:SER:HB2	1:A:139:THR:HB	1.97	0.45
1:C:465:LYS:HE3	1:C:488:ASP:OD2	2.17	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.51	0.45
1:A:27:THR:O	1:A:31:ILE:HG13	2.17	0.45
1:A:273:GLY:O	1:A:275:LYS:NZ	2.44	0.45
1:A:487:GLN:HG2	1:A:524:GLN:NE2	2.32	0.45
1:C:296:THR:O	1:C:300:GLU:HG2	2.17	0.44
2:D:266:TRP:CG	2:D:425:LEU:HD13	2.52	0.44
2:D:24[A]:TRP:CD2	2:D:25:PRO:HD2	2.52	0.44
1:C:12:LEU:HD22	1:C:83:ARG:HB3	1.99	0.44
2:D:326:ILE:HG22	2:D:388:LYS:HB3	2.00	0.44
1:C:171:PHE:CZ	1:C:205:LEU:HB2	2.52	0.44
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.99	0.44
2:D:274:ILE:HD12	2:D:274:ILE:HA	1.90	0.44
1:A:272:PRO:HA	1:A:351:THR:HG21	1.98	0.44
1:A:406:TRP:CD1	2:B:420:PRO:HB3	2.53	0.43
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.00	0.43
1:C:320:ASP:OD2	1:C:323:LYS:NZ	2.51	0.43
2:D:326:ILE:HG12	2:D:342:TYR:O	2.18	0.43
1:A:23:GLN:NE2	1:A:60:VAL:HB	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.99	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.00	0.43
1:C:59:PRO:O	1:C:75:VAL:HG13	2.17	0.43
2:B:101:LYS:O	2:B:236:PRO:HB2	2.18	0.43
1:C:325:LEU:HD21	1:C:383:TRP:CE3	2.54	0.43
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.99	0.43
1:C:82:LYS:HB2	1:C:82:LYS:HE3	1.81	0.43
2:B:248:GLU:HB2	2:B:307:ARG:HH22	1.84	0.43
1:A:233:GLU:HB3	1:A:235:HIS:CE1	2.54	0.43
2:B:281:LYS:HA	2:B:284:ARG:HG3	2.01	0.43
2:B:341:ILE:HD11	2:B:375:ILE:HG23	2.01	0.43
1:C:473:THR:O	1:C:477:THR:HG23	2.18	0.43
2:B:64:LYS:HG3	2:B:71:TRP:HA	2.01	0.43
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.19	0.42
2:D:234:LEU:O	2:D:236:PRO:HD3	2.19	0.42
1:C:221:HIS:CD2	1:C:221:HIS:H	2.35	0.42
2:D:24[A]:TRP:CG	2:D:25:PRO:HD2	2.53	0.42
1:A:88:TRP:CE2	2:B:143:ARG:HD3	2.53	0.42
1:A:408:ALA:O	2:B:393:ILE:HG13	2.19	0.42
2:B:248:GLU:HB2	2:B:307:ARG:NH2	2.35	0.42
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.35	0.42
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.01	0.42
2:D:354:TYR:HB2	2:D:374:LYS:HE3	2.00	0.42
1:C:229:TRP:CD2	4:C:602:29T:H2	2.55	0.42
1:C:239:TRP:NE1	1:C:316:GLY:HA3	2.34	0.42
2:B:282:LEU:HD12	2:B:293:ILE:CG2	2.49	0.42
1:C:471:ASN:O	1:C:471:ASN:ND2	2.52	0.42
2:B:401:TRP:HD1	2:B:404[A]:GLU:HG3	1.84	0.42
2:D:122:GLU:HA	2:D:125:ARG:NE	2.35	0.42
2:D:375:ILE:HB	2:D:389:PHE:CZ	2.54	0.42
2:B:122:GLU:HA	2:B:125:ARG:HG3	2.02	0.42
2:B:326:ILE:HG12	2:B:342:TYR:CE2	2.55	0.42
1:C:90:VAL:HG13	1:C:161:GLN:HG3	2.02	0.42
1:C:165:THR:O	1:C:169:GLU:HG3	2.20	0.42
1:C:5:ILE:HD13	1:C:5:ILE:HA	1.95	0.42
1:C:238:LYS:HE3	1:C:238:LYS:HB2	1.83	0.42
1:A:269:GLN:O	1:A:351:THR:N	2.48	0.41
1:A:304:ALA:O	1:A:308[A]:GLU:HG2	2.20	0.41
1:A:361:HIS:CE1	1:A:513:SER:HG	2.38	0.41
2:D:241:VAL:HG12	2:D:350:LYS:HG2	2.01	0.41
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:GLU:O	1:C:482:ILE:HG12	2.19	0.41
2:D:12:LEU:HD23	2:D:12:LEU:HA	1.90	0.41
1:C:261:VAL:HG13	1:C:276:VAL:HB	2.01	0.41
1:C:122:GLU:HA	1:C:125:ARG:HD2	2.03	0.41
2:D:106:VAL:HA	2:D:190:GLY:HA2	2.03	0.41
1:A:246:LEU:CB	1:A:307:ARG:HE	2.34	0.41
1:C:58:THR:N	1:C:129:ALA:O	2.54	0.41
1:C:350:LYS:HE3	1:C:378:GLU:OE2	2.20	0.41
2:D:85:GLN:NE2	2:D:154:LYS:HB2	2.36	0.41
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.31	0.41
2:D:386:THR:HA	2:D:387:PRO:HD3	1.86	0.41
2:B:53:GLU:OE1	2:B:53:GLU:N	2.45	0.41
2:B:301:LEU:HD22	2:B:301:LEU:HA	1.95	0.41
1:A:362:THR:HG22	1:A:363:ASN:H	1.86	0.40
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.40
1:C:198:HIS:O	1:C:202:ILE:HG12	2.21	0.40
2:D:257:ILE:O	2:D:261:VAL:HG23	2.21	0.40
1:C:460:ASN:ND2	2:D:288:ALA:HB2	2.33	0.40
2:D:24[B]:TRP:CH2	2:D:399:GLU:HG2	2.56	0.40
2:D:263:LYS:HG2	2:D:425:LEU:CD2	2.50	0.40
1:A:77:PHE:O	1:A:81:ASN:N	2.40	0.40
1:A:458:VAL:HG22	1:A:464:GLN:HG2	2.03	0.40
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.56	0.40
1:A:406:TRP:CG	2:B:420:PRO:HB3	2.57	0.40
2:B:282:LEU:HD11	2:B:296:THR:HG23	2.02	0.40
2:D:42:GLU:HA	2:D:47:ILE:O	2.21	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	544/558 (98%)	533 (98%)	11 (2%)	0	100	100
1	C	535/558 (96%)	525 (98%)	10 (2%)	0	100	100
2	B	399/428 (93%)	392 (98%)	7 (2%)	0	100	100
2	D	396/428 (92%)	387 (98%)	9 (2%)	0	100	100
All	All	1874/1972 (95%)	1837 (98%)	37 (2%)	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	421/495 (85%)	402 (96%)	19 (4%)	27	50
1	C	431/495 (87%)	390 (90%)	41 (10%)	8	15
2	B	351/390 (90%)	338 (96%)	13 (4%)	34	58
2	D	300/390 (77%)	276 (92%)	24 (8%)	12	23
All	All	1503/1770 (85%)	1406 (94%)	97 (6%)	17	33

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	30	LYS
1	A	58	THR
1	A	68	SER
1	A	94	ILE
1	A	108	VAL
1	A	220	LYS
1	A	223	LYS
1	A	228	LEU
1	A	244	ILE
1	A	245	VAL
1	A	290	THR
1	A	350	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	362	THR
1	A	402	TRP
1	A	428	GLN
1	A	452	LEU
1	A	473	THR
1	A	551	LEU
2	B	22	LYS
2	B	61	PHE
2	B	64	LYS
2	B	68	SER
2	B	69	THR
2	B	86	ASP
2	B	88	TRP
2	B	89	GLU
2	B	92	LEU
2	B	301	LEU
2	B	326	ILE
2	B	338	THR
2	B	417	VAL
1	C	5	ILE
1	C	20	LYS
1	C	57	ASN
1	C	58	THR
1	C	73	LYS
1	C	101	LYS
1	C	103	LYS
1	C	110[A]	ASP
1	C	110[B]	ASP
1	C	113	ASP
1	C	132	ILE
1	C	146	TYR
1	C	183	TYR
1	C	185	ASP
1	C	199	ARG
1	C	216	THR
1	C	220	LYS
1	C	221	HIS
1	C	223	LYS
1	C	228	LEU
1	C	238	LYS
1	C	250	ASP
1	C	255	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	286	THR
1	C	295	LEU
1	C	351	THR
1	C	361	HIS
1	C	363	ASN
1	C	396	GLU
1	C	402	TRP
1	C	405	TYR
1	C	442	VAL
1	C	443	ASP
1	C	449	GLU
1	C	459	THR
1	C	463	ARG
1	C	465	LYS
1	C	509	GLN
1	C	547	GLN
1	C	548	VAL
1	C	549	ASP
2	D	5	ILE
2	D	6	GLU
2	D	21	VAL
2	D	72	ARG
2	D	85	GLN
2	D	91	GLN
2	D	121	ASP
2	D	212	TRP
2	D	232	TYR
2	D	238	LYS
2	D	246	LEU
2	D	249	LYS
2	D	286	THR
2	D	291	GLU
2	D	305	GLU
2	D	315	HIS
2	D	330	GLN
2	D	348	ASN
2	D	354	TYR
2	D	362	THR
2	D	374	LYS
2	D	405	TYR
2	D	414	TRP
2	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	29T	A	602	-	30,32,32	0.47	0	35,44,44	0.67	0
4	29T	C	602	-	30,32,32	0.75	1 (3%)	35,44,44	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	29T	A	602	-	-	0/10/12/12	0/4/4/4
4	29T	C	602	-	-	1/10/12/12	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	29T	C11-C14	2.82	1.40	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	602	29T	C05-C04-O0A-C0C

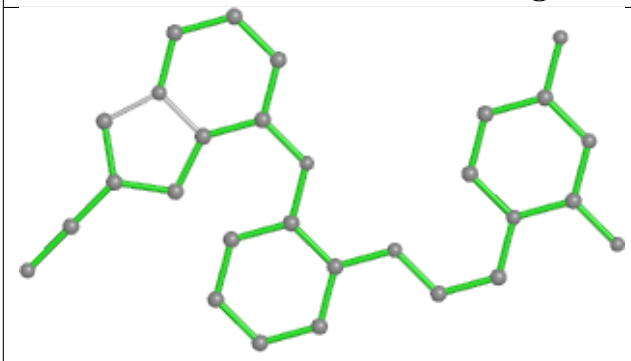
There are no ring outliers.

1 monomer is involved in 1 short contact:

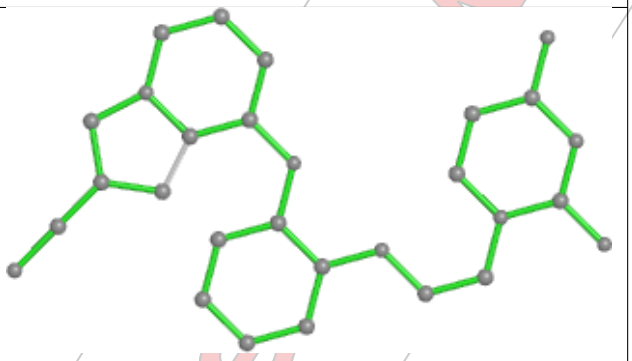
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	602	29T	1	0

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.

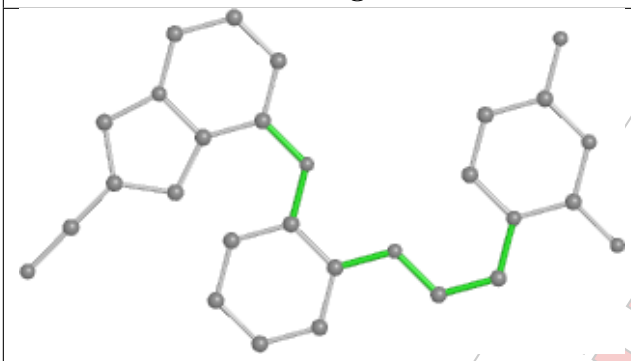
Ligand 29T A 602



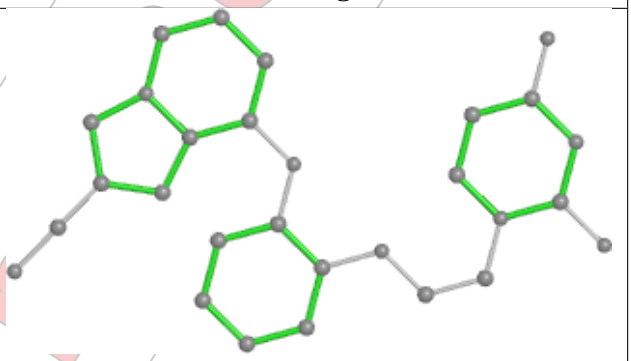
Bond lengths



Bond angles

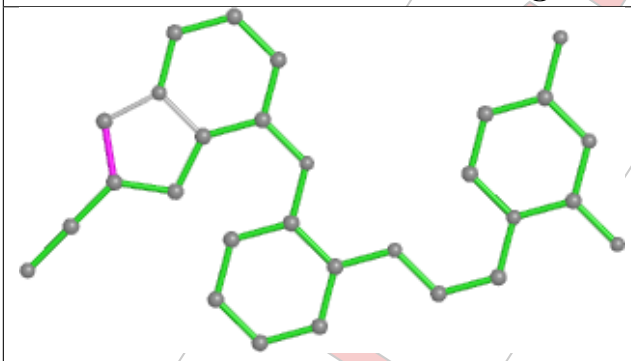


Torsions

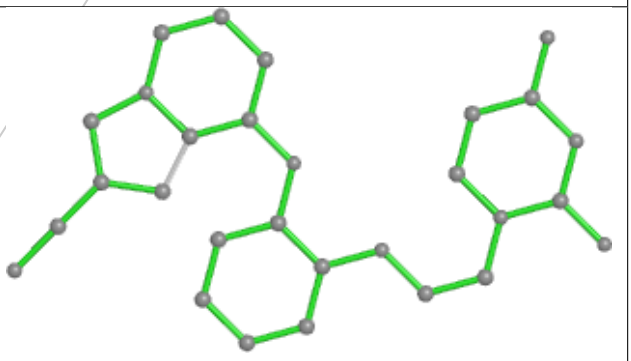


Rings

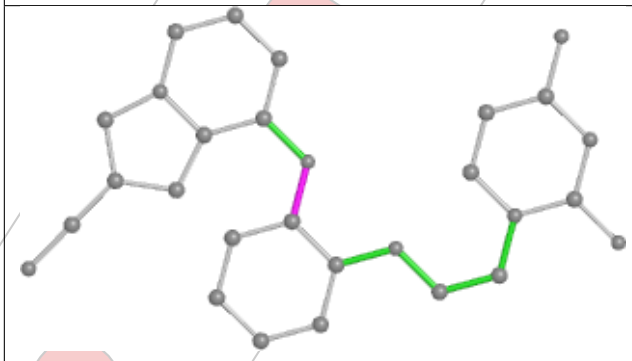
Ligand 29T C 602



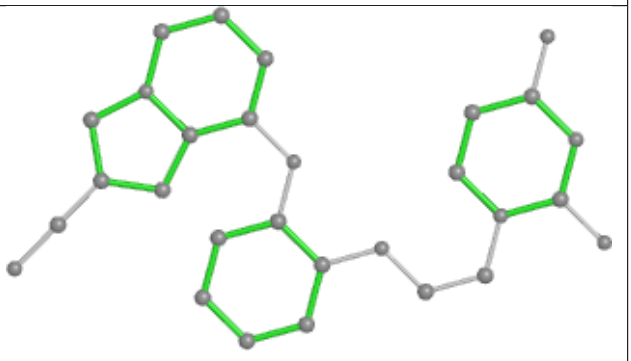
Bond lengths



Bond angles



Torsions



Rings

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	547/558 (98%)	0.23	24 (4%) 34 28	39, 76, 139, 160	0
1	C	544/558 (97%)	0.58	46 (8%) 10 7	68, 100, 134, 159	0
2	B	405/428 (94%)	0.18	9 (2%) 62 57	43, 69, 105, 134	7 (1%)
2	D	401/428 (93%)	0.68	43 (10%) 6 4	76, 114, 141, 155	5 (1%)
All	All	1897/1972 (96%)	0.42	122 (6%) 19 15	39, 92, 137, 160	12 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	245	VAL	4.9
1	A	225	PRO	4.9
1	C	246	LEU	4.8
1	C	556	ILE	4.7
2	D	212	TRP	4.5
1	C	286	THR	4.4
1	A	223	LYS	4.4
1	C	26	LEU	4.3
1	C	290	THR	4.3
1	C	276	VAL	4.2
1	C	225	PRO	4.1
2	D	24[A]	TRP	4.1
2	B	362	THR	4.1
2	D	272	PRO	4.0
1	A	294	PRO	3.9
1	C	244	ILE	3.9
2	D	174	GLN	3.7
1	C	297	GLU	3.7
1	C	131	THR	3.6
2	D	303	LEU	3.6
1	A	282	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	245	VAL	3.6
2	D	67	ASP	3.5
1	C	21	VAL	3.5
2	D	168	LEU	3.4
2	D	10	VAL	3.4
2	D	116	PHE	3.4
1	C	260	LEU	3.3
2	D	214	LEU	3.3
2	D	299	ALA	3.3
1	C	132	ILE	3.3
1	C	402	TRP	3.3
1	A	290	THR	3.2
1	C	75	VAL	3.2
1	A	71	TRP	3.2
2	B	361	HIS	3.2
1	C	304	ALA	3.2
1	A	303	LEU	3.2
1	C	136	ASN	3.2
2	D	95	PRO	3.2
1	A	246	LEU	3.2
2	D	5	ILE	3.1
1	C	61	PHE	3.1
1	C	128	THR	3.1
1	C	142	ILE	3.1
1	C	252	TRP	3.0
2	D	252	TRP	3.0
1	C	359	GLY	3.0
1	C	299	ALA	3.0
2	D	304	ALA	3.0
2	D	238	LYS	3.0
1	C	292	VAL	3.0
2	D	115	TYR	2.9
2	D	251	SER	2.9
1	A	299	ALA	2.9
2	D	306	ASN	2.9
1	A	300	GLU	2.9
1	A	452	LEU	2.9
1	C	130	PHE	2.8
1	A	253	THR	2.8
1	C	15	GLY	2.8
1	A	297	GLU	2.8
2	D	96	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	427	TYR	2.8
1	A	24	TRP	2.8
1	A	279	LEU	2.8
2	D	109	LEU	2.8
2	D	319	TYR	2.8
1	A	542	ILE	2.8
2	D	111	VAL	2.7
2	D	308	GLU	2.7
1	A	69	THR	2.7
1	A	252	TRP	2.7
1	C	309	ILE	2.7
1	C	223	LYS	2.7
2	B	14	PRO	2.6
1	C	283	LEU	2.6
1	C	310	LEU	2.6
1	C	58	THR	2.5
1	A	292	VAL	2.5
1	C	34	LEU	2.5
2	D	317	VAL	2.5
2	B	284	ARG	2.5
1	A	295	LEU	2.5
1	C	221	HIS	2.5
1	C	332[A]	GLN	2.4
1	C	20	LYS	2.4
1	C	554	ALA	2.4
1	A	260	LEU	2.4
2	D	286	THR	2.4
2	B	88	TRP	2.4
2	D	189	VAL	2.4
2	D	248	GLU	2.4
1	C	80	LEU	2.4
2	B	86	ASP	2.4
2	D	247	PRO	2.3
2	D	92	LEU	2.3
1	C	90	VAL	2.3
2	D	159	ILE	2.3
1	A	146	TYR	2.3
1	C	358	ARG	2.3
2	D	325	LEU	2.3
1	C	59	PRO	2.2
1	C	296	THR	2.2
1	C	282	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	366	LYS	2.2
1	C	275	LYS	2.2
2	B	85	GLN	2.2
2	D	296	THR	2.2
2	D	202	ILE	2.1
2	D	273	GLY	2.1
2	B	357	MET	2.1
2	D	154	LYS	2.1
2	D	101	LYS	2.1
2	D	341	ILE	2.1
1	A	302	GLU	2.1
2	D	97	PRO	2.1
1	C	291	GLU	2.1
2	B	283	LEU	2.0
1	A	298	GLU	2.0
1	C	16	MET	2.0
2	D	188	TYR	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.

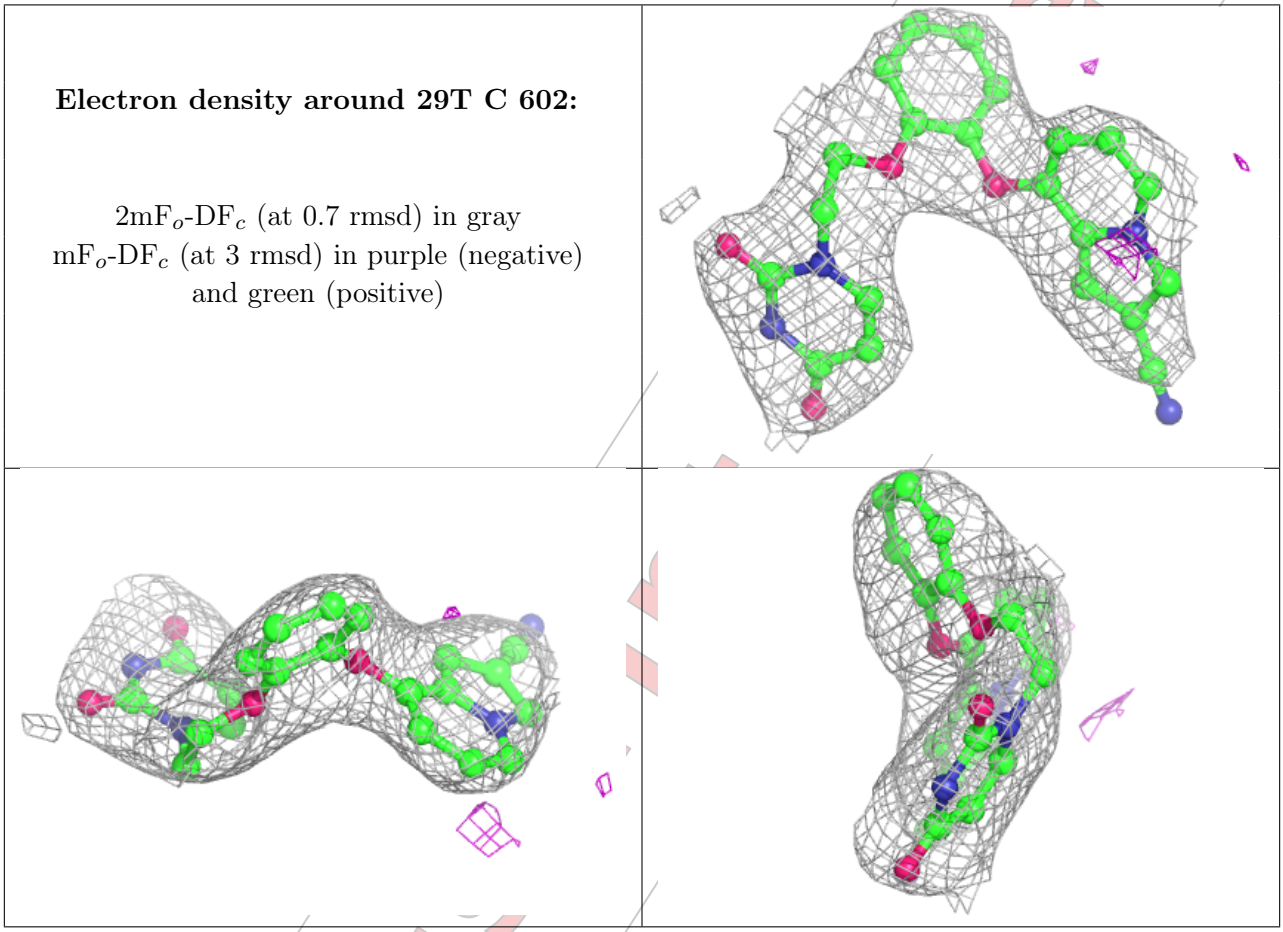
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	601	1/1	0.85	0.25	86,86,86,86	0
3	MG	A	601	1/1	0.90	0.23	85,85,85,85	0
4	29T	C	602	29/29	0.92	0.26	75,82,95,98	0
4	29T	A	602	29/29	0.97	0.18	48,58,66,69	0

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.

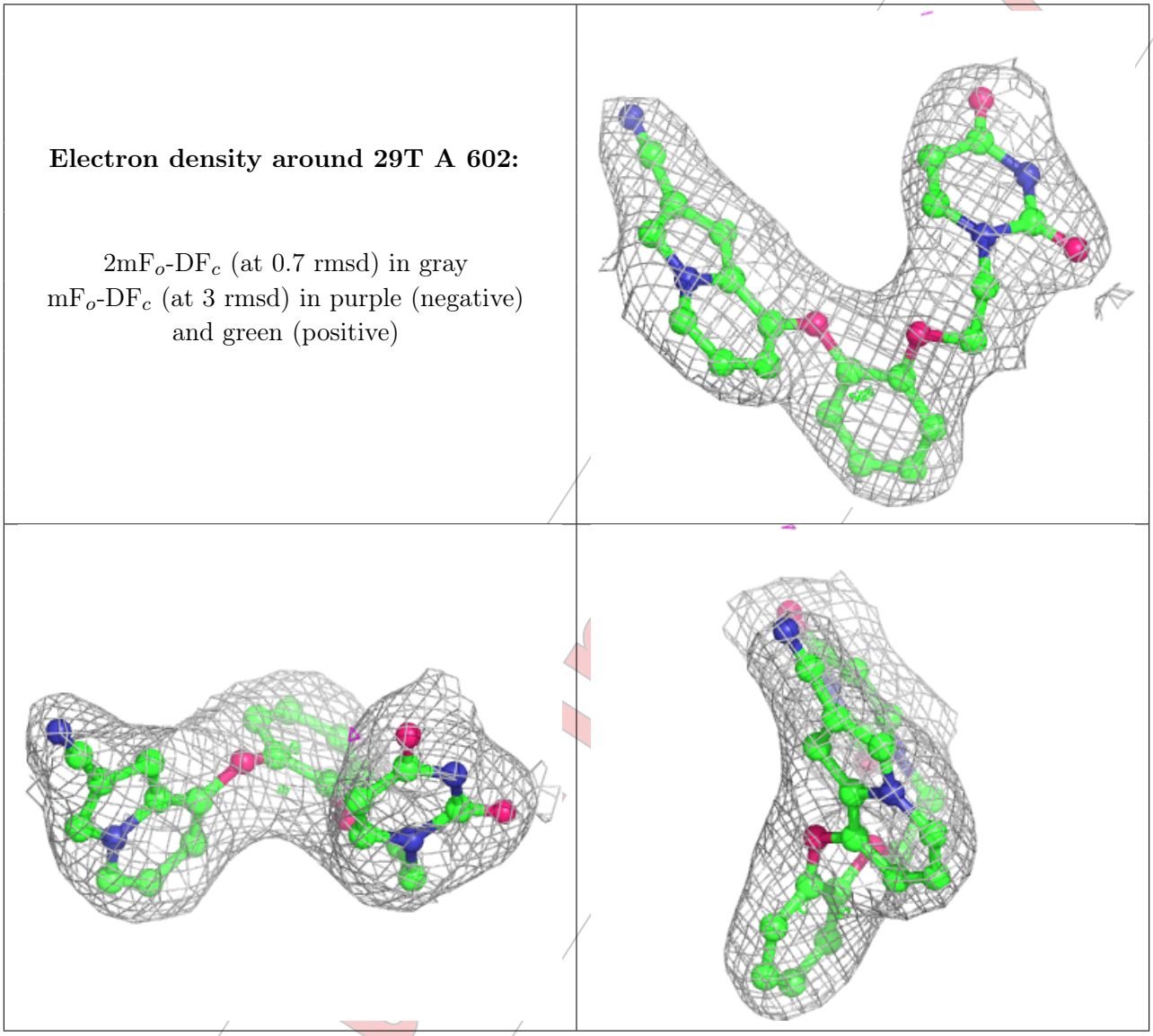
Electron density around 29T C 602:

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



Electron density around 29T A 602:

$2mF_o$-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.

Full wwPDB X-ray Structure Validation Report (i)

May 12, 2023 – 03:46 PM EDT

PDB ID	:	8STU
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (Y181C, V106A) variant in Complex with 8-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)-4-fluorophenoxy)-6-fluoroindolizine-2-carbonitrile (JLJ578), a non-nucleoside inhibitor
Deposited on	:	2023-05-11
Resolution	:	2.76 Å(reported)

This wwPDB validation report is for manuscript review

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

This report is produced by the wwPDB biocuration pipeline after 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

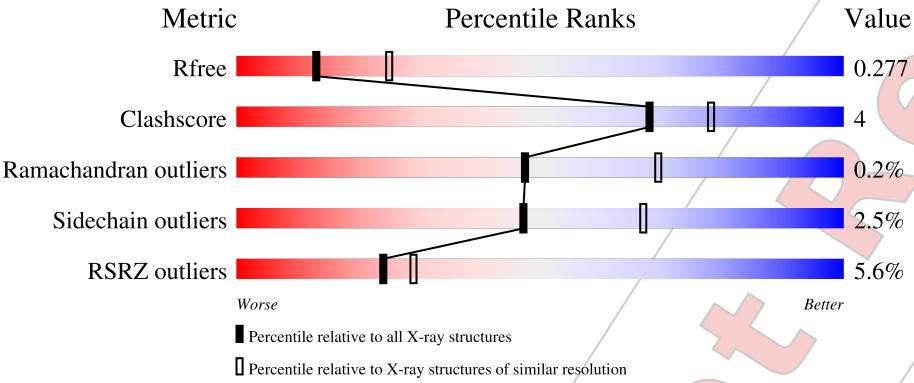
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

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 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	557	4% 86% 10% .
2	B	428	7% 81% 13% 6%

CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7368 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	539	4179	2692	699	780	8	0	3	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	106	ALA	VAL	engineered mutation	UNP P03366
A	172	ALA	LYS	conflict	UNP P03366
A	173	ALA	LYS	conflict	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	403	3130	2028	516	581	5	0	1	0

There is a discrepancy between the modelled and reference sequences:

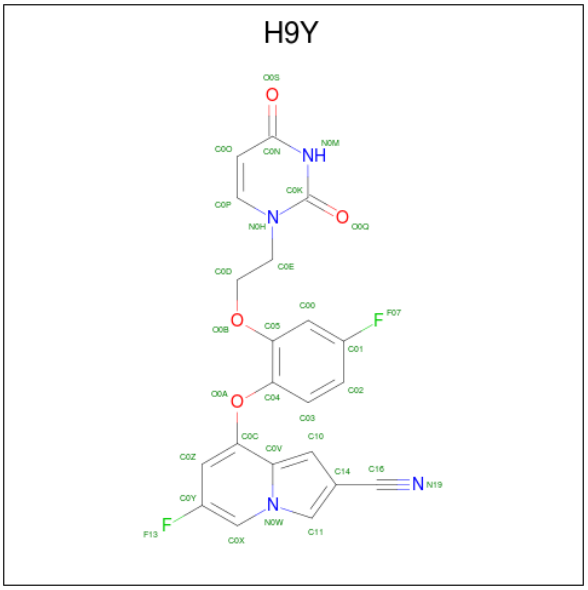
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is 8-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]-4-fluorophenoxy}-6

-fluoroindolizine-2-carbonitrile (three-letter code: H9Y) (formula: $C_{21}H_{14}F_2N_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	31	21	2	4	4	0	0

- Molecule 5 is water.

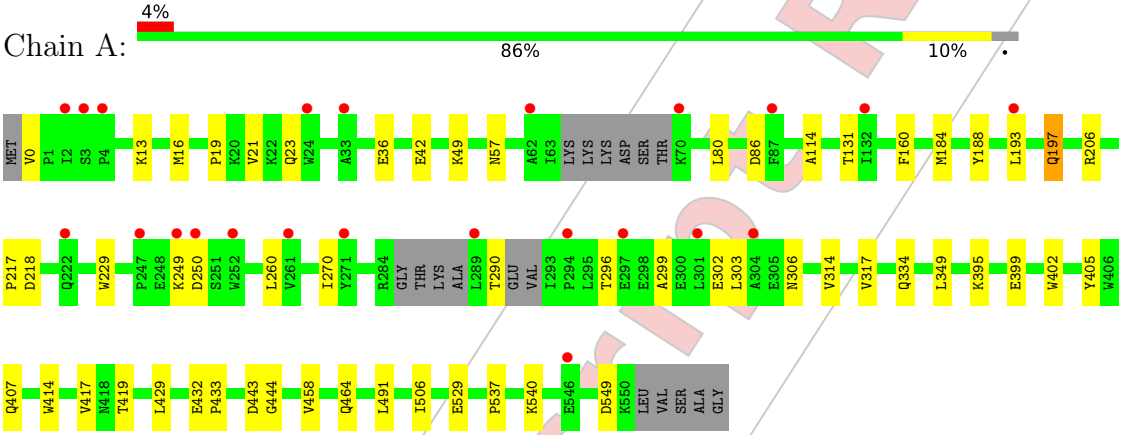
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	17	17	17	0	0
			Total	O		
5	B	10	10	10	0	0

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.

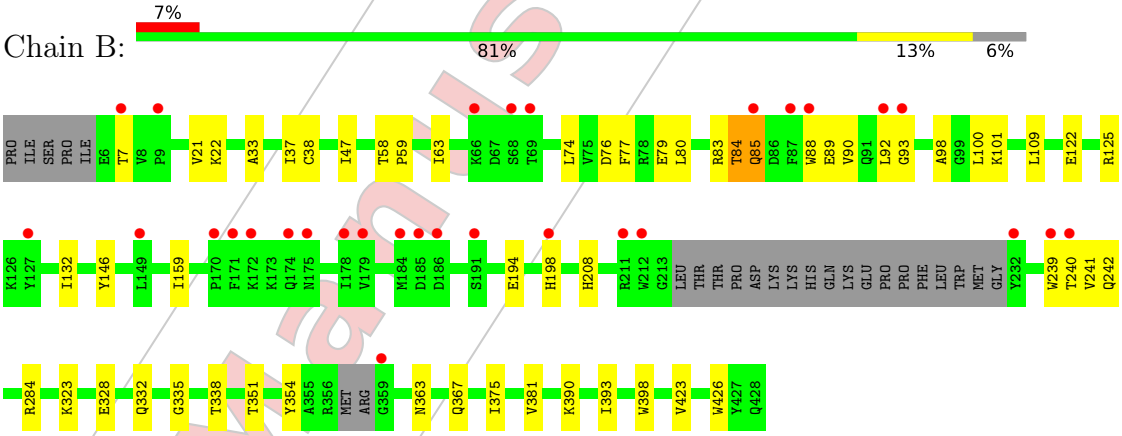
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



• Molecule 2: p51 RT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.61Å 73.98Å 109.09Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	29.62 – 2.76 29.62 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.62-2.76) 99.5 (29.62-2.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.226 , 0.280 0.227 , 0.277	Depositor DCC
R_{free} test set	1632 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7368	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: MG, H9Y

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	0.24	0/4299	0.44	0/5872
2	B	0.24	0/3221	0.45	0/4405
All	All	0.24	0/7520	0.44	0/10277

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	4179	0	3956	25	0
2	B	3130	0	2946	29	0
3	A	1	0	0	0	0
4	A	31	0	0	0	0
5	A	17	0	0	0	0
5	B	10	0	0	1	0
All	All	7368	0	6902	54	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 4.

All (54) 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:90:VAL:HA	2:B:92:LEU:H	1.29	0.97
2:B:90:VAL:HA	2:B:92:LEU:N	2.05	0.67
2:B:80:LEU:O	2:B:84:THR:N	2.26	0.66
2:B:89:GLU:O	2:B:93:GLY:N	2.30	0.62
2:B:79:GLU:OE2	2:B:83:ARG:NE	2.39	0.56
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.88	0.55
2:B:354[B]:TYR:CE2	2:B:375:ILE:HG13	2.42	0.55
2:B:194:GLU:O	2:B:198:HIS:N	2.35	0.53
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.44	0.53
2:B:354[B]:TYR:HE2	2:B:375:ILE:HG13	1.75	0.52
1:A:260:LEU:HD21	1:A:303:LEU:HD21	1.92	0.52
2:B:85:GLN:HG3	2:B:88:TRP:CB	2.40	0.52
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.93	0.51
1:A:395:LYS:NZ	1:A:414:TRP:O	2.44	0.49
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.95	0.49
2:B:100:LEU:HG	2:B:381:VAL:HG13	1.95	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.48	0.48
1:A:443:ASP:OD1	1:A:444:GLY:N	2.47	0.47
1:A:193:LEU:HD23	1:A:197:GLN:HB2	1.96	0.47
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.97	0.47
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.97	0.47
2:B:323:LYS:HA	2:B:323:LYS:HD3	1.78	0.46
2:B:33:ALA:O	2:B:37:ILE:HG12	2.17	0.45
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.16	0.45
1:A:23:GLN:HG2	1:A:131:THR:HB	1.98	0.45
1:A:296:THR:HG23	1:A:299:ALA:H	1.81	0.45
1:A:270:ILE:HG13	1:A:314:VAL:HG23	1.97	0.45
2:B:22:LYS:NZ	5:B:503:HOH:O	2.41	0.45
1:A:491:LEU:HB3	1:A:529:GLU:CG	2.47	0.45
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.99	0.44
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.18	0.44
2:B:242:GLN:NE2	2:B:351:THR:O	2.50	0.44
2:B:423:VAL:HA	2:B:426:TRP:CE3	2.52	0.44
2:B:363:ASN:O	2:B:367:GLN:HG3	2.17	0.44
1:A:249:LYS:HA	1:A:250:ASP:HA	1.71	0.44
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.99	0.44
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.98	0.44
2:B:98:ALA:O	2:B:101:LYS:HG2	2.18	0.44
1:A:317:VAL:HG23	1:A:349:LEU:HD23	2.00	0.44
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.99	0.43
1:A:303:LEU:HA	1:A:306:ASN:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.54	0.42
2:B:58:THR:HG21	2:B:77:PHE:CD1	2.54	0.42
1:A:21:VAL:O	1:A:57:ASN:ND2	2.52	0.42
1:A:188:TYR:HH	1:A:229:TRP:HE1	1.66	0.42
2:B:328:GLU:HG2	2:B:390:LYS:HD3	2.02	0.41
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.03	0.41
1:A:13:LYS:HB2	1:A:16:MET:HG3	2.03	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.60	0.41
2:B:63:ILE:HG12	2:B:74:LEU:HD13	2.03	0.41
2:B:125:ARG:HG2	2:B:146:TYR:O	2.21	0.41
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.01	0.41
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.04	0.40
1:A:206:ARG:NE	1:A:217:PRO:O	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	534/557 (96%)	521 (98%)	13 (2%)	0	100	100
2	B	398/428 (93%)	391 (98%)	5 (1%)	2 (0%)	29	47
All	All	932/985 (95%)	912 (98%)	18 (2%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	239	TRP
2	B	240	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	419/494 (85%)	409 (98%)	10 (2%)	49 68
2	B	314/390 (80%)	306 (98%)	8 (2%)	47 67
All	All	733/884 (83%)	715 (98%)	18 (2%)	47 67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	VAL
1	A	36	GLU
1	A	86	ASP
1	A	184	MET
1	A	197	GLN
1	A	218	ASP
1	A	290	THR
1	A	302	GLU
1	A	334	GLN
1	A	549	ASP
2	B	7	THR
2	B	84	THR
2	B	85	GLN
2	B	109	LEU
2	B	159	ILE
2	B	208	HIS
2	B	241	VAL
2	B	284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 2 ligands modelled in this entry, 1 is monoatomic - 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	$\#\|Z\| > 2$
4	H9Y	A	602	-	32,34,34	2.13	8 (25%)	38,48,48	1.88	8 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H9Y	A	602	-	-	0/10/12/12	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	H9Y	O0S-C0N	7.49	1.39	1.24
4	A	602	H9Y	F07-C01	4.37	1.47	1.36
4	A	602	H9Y	C14-C16	2.81	1.50	1.44
4	A	602	H9Y	C0E-N0H	2.47	1.53	1.47
4	A	602	H9Y	C0N-N0M	-2.43	1.34	1.38
4	A	602	H9Y	C0K-N0H	-2.43	1.34	1.37
4	A	602	H9Y	C0C-C0V	-2.22	1.39	1.42
4	A	602	H9Y	C0K-N0M	-2.08	1.34	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	H9Y	N0M-C0K-N0H	5.82	120.18	114.86
4	A	602	H9Y	C0N-N0M-C0K	-4.05	121.24	126.58
4	A	602	H9Y	O0Q-C0K-N0H	-3.34	119.92	122.85
4	A	602	H9Y	C0O-C0P-N0H	-3.19	119.45	122.44
4	A	602	H9Y	C0O-C0N-N0M	3.18	119.60	114.84
4	A	602	H9Y	O0S-C0N-C0O	-2.84	120.17	125.16
4	A	602	H9Y	C02-C01-C00	-2.61	119.90	123.29
4	A	602	H9Y	C0X-C0Y-C0Z	-2.55	119.26	122.01

There are no chirality outliers.

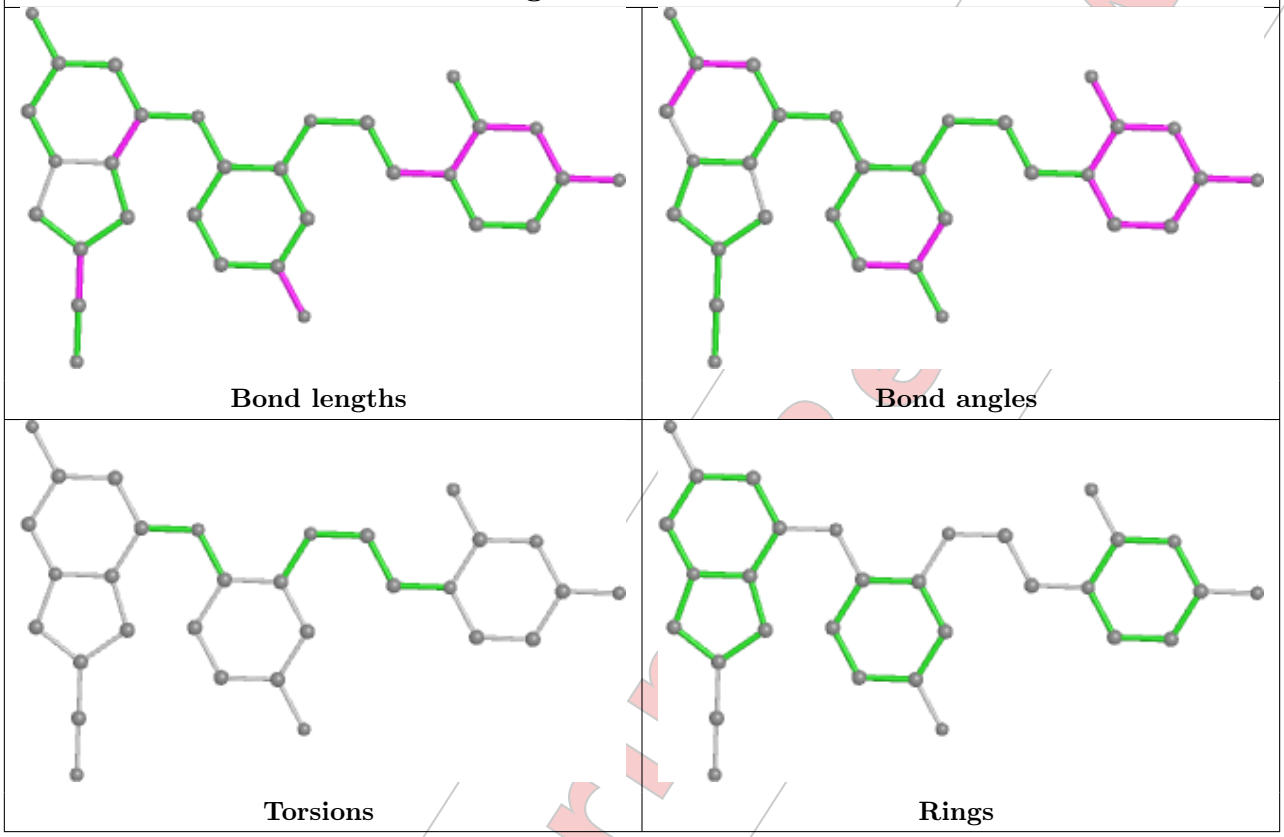
There are no torsion outliers.

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 H9Y A 602



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	539/557 (96%)	0.20	23 (4%) 35 42	43, 84, 127, 158	0
2	B	403/428 (94%)	0.30	30 (7%) 14 17	44, 80, 135, 150	0
All	All	942/985 (95%)	0.24	53 (5%) 24 29	43, 82, 132, 158	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	87	PHE	4.8
2	B	88	TRP	4.7
1	A	4	PRO	4.3
1	A	247	PRO	4.2
2	B	68	SER	4.2
2	B	240	THR	4.0
1	A	24	TRP	3.9
2	B	239	TRP	3.7
1	A	304	ALA	3.6
1	A	2	ILE	3.5
1	A	294	PRO	3.5
2	B	92	LEU	3.4
2	B	198	HIS	3.3
2	B	170	PRO	3.3
1	A	193	LEU	3.2
2	B	191	SER	3.2
1	A	33	ALA	3.2
2	B	172	LYS	3.2
2	B	174	GLN	3.2
2	B	171	PHE	3.1
1	A	252	TRP	3.0
2	B	178	ILE	3.0
2	B	186	ASP	2.8
2	B	185	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	211	ARG	2.7
1	A	297	GLU	2.6
2	B	212	TRP	2.6
1	A	301	LEU	2.6
2	B	9	PRO	2.6
1	A	271	TYR	2.5
1	A	261	VAL	2.5
1	A	70	LYS	2.5
1	A	249	LYS	2.5
1	A	62	ALA	2.5
2	B	232	TYR	2.5
2	B	7	THR	2.5
1	A	250	ASP	2.4
2	B	179	VAL	2.4
2	B	359	GLY	2.3
2	B	175	ASN	2.3
1	A	87	PHE	2.3
2	B	127	TYR	2.3
1	A	3	SER	2.2
1	A	546[A]	GLU	2.2
2	B	69	THR	2.2
2	B	184	MET	2.2
1	A	289	LEU	2.2
1	A	132	ILE	2.1
2	B	149	LEU	2.1
2	B	93	GLY	2.1
2	B	85	GLN	2.1
1	A	222	GLN	2.0
2	B	66	LYS	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

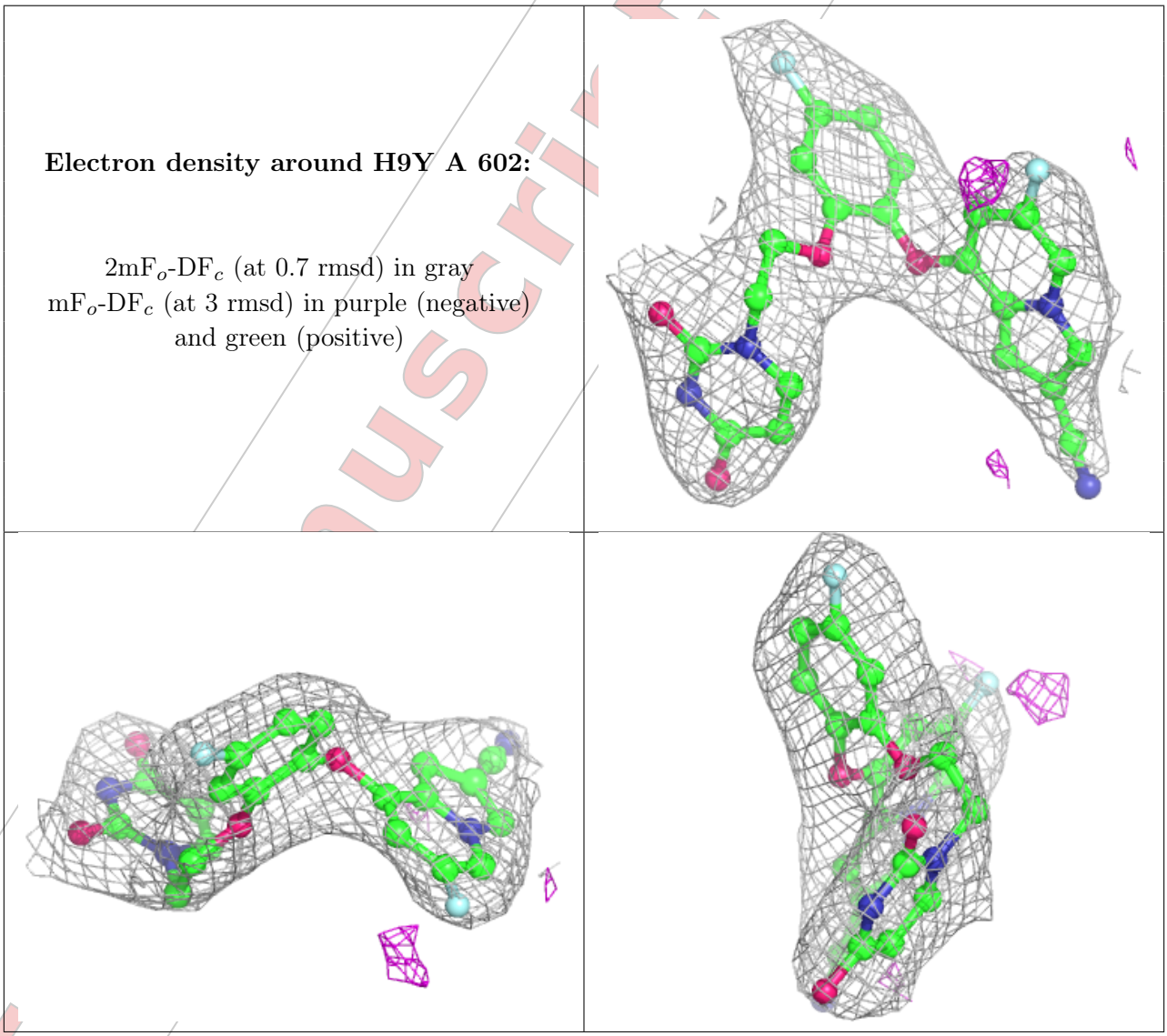
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MG	A	601	1/1	0.94	0.19	58,58,58,58	0
4	H9Y	A	602	31/31	0.94	0.19	55,69,78,79	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 H9Y A 602:

$2mF_o$-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.

Full wwPDB X-ray Structure Validation Report (i)

May 23, 2023 – 12:41 PM EDT

PDB ID	:	8STV
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (Y181C, V106A) variant in Complex with 5-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)-2-naphthonitrile (JLJ600), a non-nucleoside inhibitor
Deposited on	:	2023-05-11
Resolution	:	2.78 Å(reported)

This wwPDB validation report is for manuscript review

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

This report is produced by the wwPDB biocuration pipeline after 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

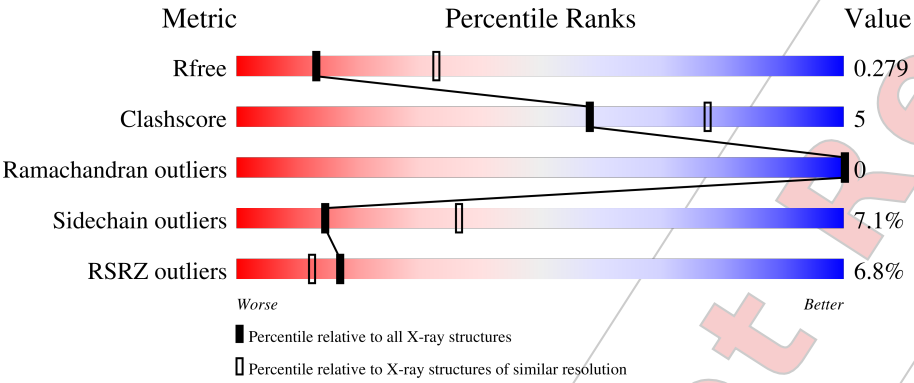
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

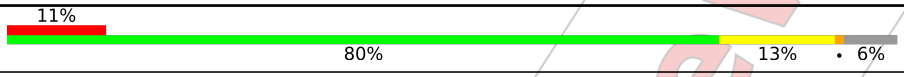
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	558	5% 80% 16%
1	C	558	8% 79% 18%
2	B	428	3% 83% 11% 5%

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	428	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14571 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	1	0
			4195	2703	695	790	7			
1	C	542	Total	C	N	O	S	0	2	0
			4072	2609	674	782	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	106	ALA	VAL	engineered mutation	UNP P03366
A	172	ALA	LYS	conflict	UNP P03366
A	173	ALA	LYS	conflict	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	106	ALA	VAL	engineered mutation	UNP P03366
C	172	ALA	LYS	conflict	UNP P03366
C	173	ALA	LYS	conflict	UNP P03366
C	181	CYS	TYR	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

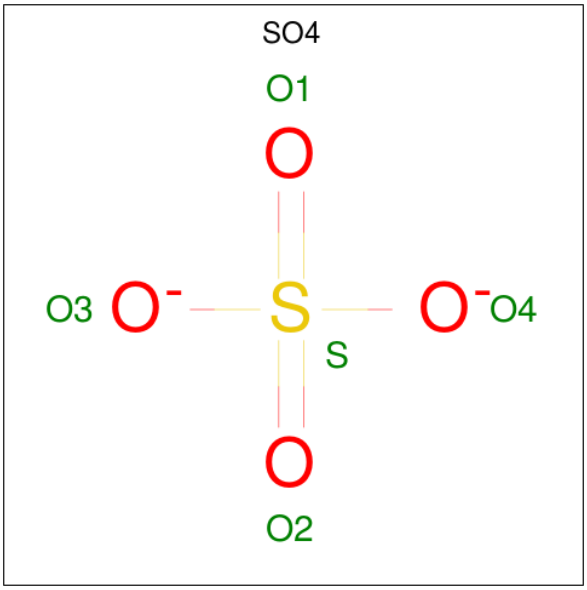
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	408	Total	C	N	O	S	19	1	0
			3285	2137	532	611	5			
2	D	401	Total	C	N	O	S	10	1	0
			2869	1838	488	540	3			

There are 2 discrepancies between the modelled and reference sequences:

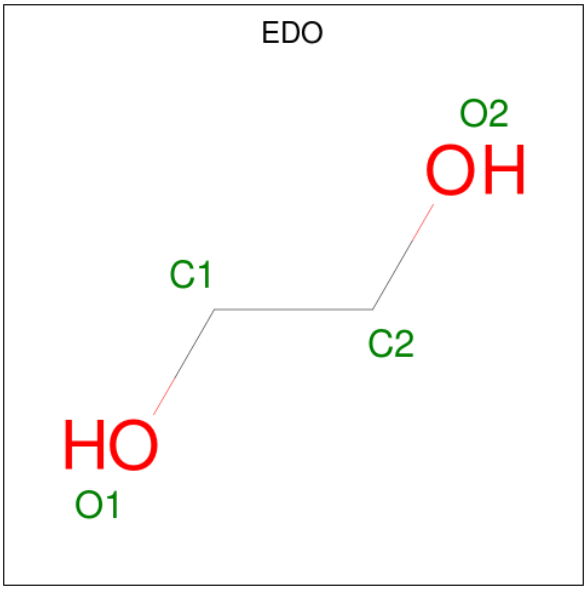
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



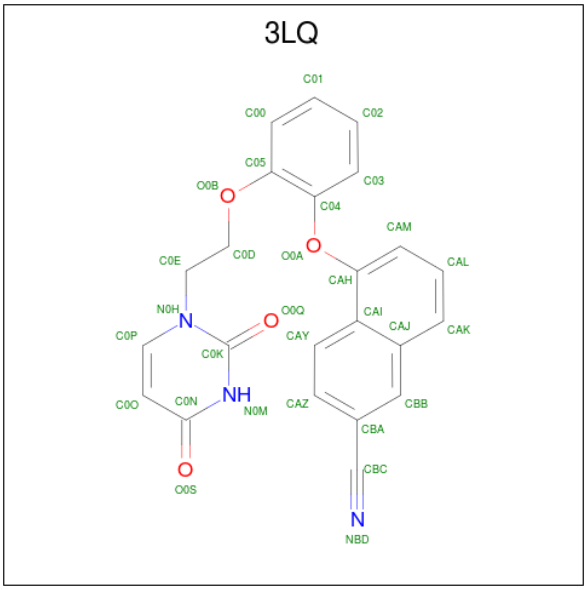
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is 5-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}naphthalene-2-carbonitrile (three-letter code: 3LQ) (formula: $C_{23}H_{17}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 30 23 3 4	0	0
5	C	1	Total C N O 30 23 3 4	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Mg 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	31	Total O 31 31	0	0

Continued on next page...

Continued from previous page...

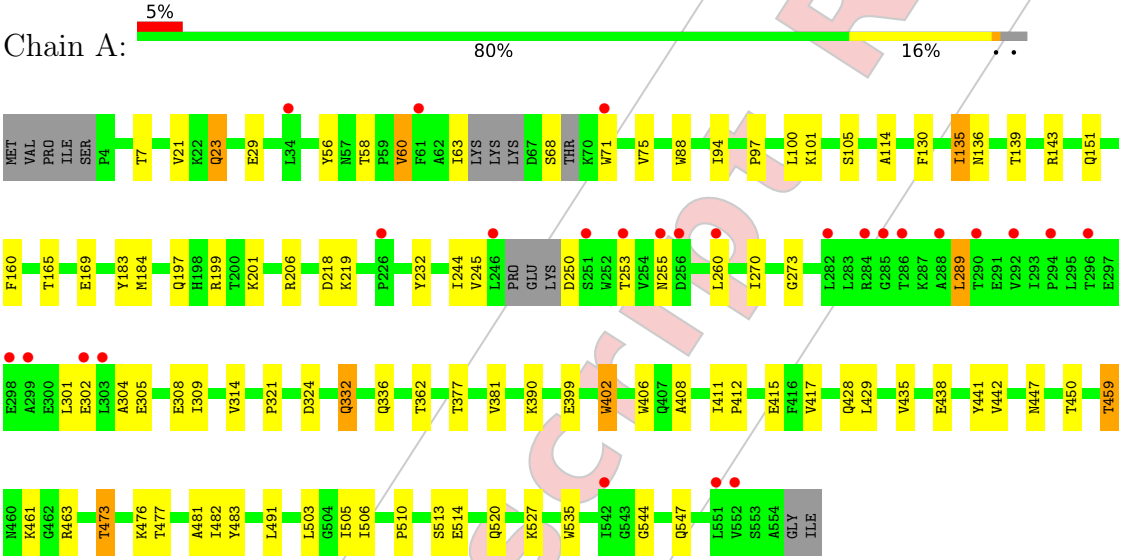
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	29	Total O 29 29	0	0
7	C	3	Total O 3 3	0	0
7	D	8	Total O 8 8	0	0

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.

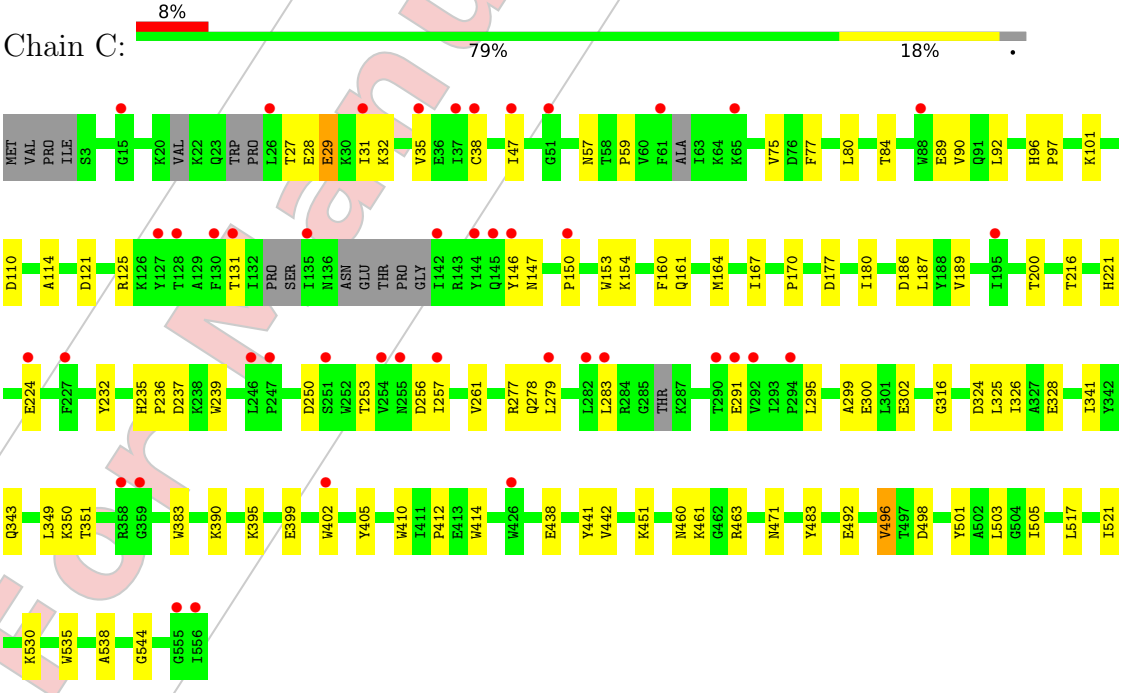
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



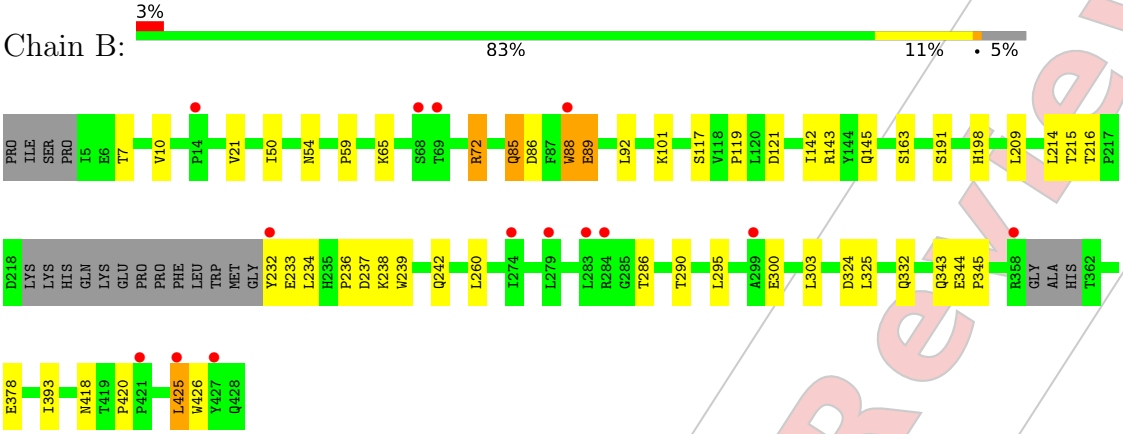
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain C:



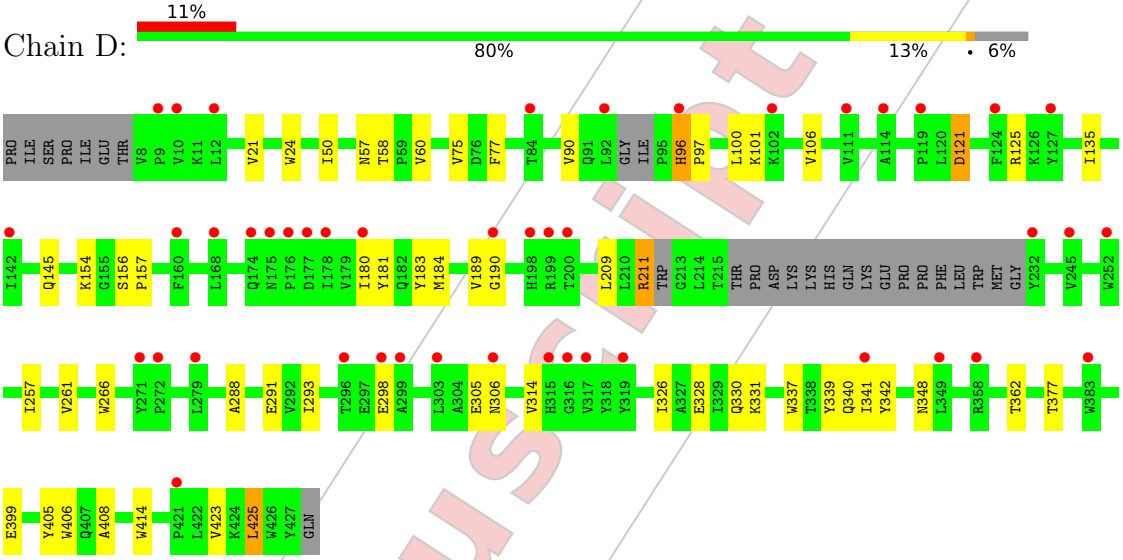
• Molecule 2: p51 RT

Chain B:



• Molecule 2: p51 RT

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.59Å 73.22Å 170.66Å 90.00° 97.73° 90.00°	Depositor
Resolution (Å)	37.83 – 2.78 37.83 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.83-2.78) 99.8 (37.83-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.232 , 0.276 0.235 , 0.279	Depositor DCC
R_{free} test set	3390 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	86.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 79.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14571	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: MG, EDO, 3LQ, SO4

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	0.25	0/4306	0.45	0/5884
1	C	0.25	0/4175	0.43	0/5710
2	B	0.25	0/3381	0.45	0/4617
2	D	0.26	0/2949	0.45	0/4065
All	All	0.25	0/14811	0.45	0/20276

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	4195	0	3982	45	0
1	C	4072	0	3724	43	0
2	B	3285	0	3200	24	0
2	D	2869	0	2419	25	0
3	A	10	0	0	0	0
4	A	4	0	6	0	0
4	C	4	0	6	1	0
5	A	30	0	17	1	0
5	C	30	0	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
7	A	31	0	0	1	0
7	B	29	0	0	0	0
7	C	3	0	0	0	0
7	D	8	0	0	0	0
All	All	14571	0	13371	132	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 (132) 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:451:LYS:HA	1:C:471:ASN:H	1.64	0.63
1:C:328:GLU:HG2	1:C:390:LYS:HB2	1.79	0.63
1:A:135:ILE:HD12	1:A:136:ASN:H	1.63	0.62
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.82	0.61
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.39	0.57
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.04	0.55
1:C:235:HIS:HB3	1:C:236:PRO:HD2	1.88	0.55
2:B:85:GLN:O	2:B:89:GLU:N	2.39	0.55
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.42	0.54
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.90	0.53
1:A:23:GLN:HE21	1:A:60:VAL:H	1.57	0.53
1:A:459:THR:HG23	1:A:461:LYS:H	1.73	0.53
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.92	0.52
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.44	0.52
1:A:332:GLN:O	1:A:336:GLN:HB2	2.10	0.52
1:C:89:GLU:HG2	1:C:92:LEU:HG	1.92	0.52
2:D:50:ILE:HG21	2:D:145:GLN:HB3	1.92	0.52
1:C:460:ASN:HD22	2:D:288:ALA:HB2	1.74	0.51
1:A:60:VAL:HG13	1:A:75:VAL:HG22	1.93	0.51
1:A:56:TYR:O	1:A:143:ARG:NH2	2.44	0.51
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.93	0.51
2:B:232:TYR:CG	2:B:233:GLU:N	2.78	0.51
1:C:150:PRO:HB2	1:C:153:TRP:HB2	1.92	0.51
2:D:180:ILE:HD13	2:D:189:VAL:HA	1.92	0.51
2:D:406:TRP:NE1	2:D:408:ALA:HB3	2.26	0.51
1:C:498:ASP:HB2	1:C:538:ALA:HB2	1.93	0.51
1:A:459:THR:HG22	1:A:463:ARG:H	1.76	0.50
1:C:438:GLU:OE2	1:C:463:ARG:HD3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.46	0.50
2:D:156:SER:HB2	2:D:157:PRO:HD3	1.94	0.50
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.49
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.94	0.49
1:A:273:GLY:N	7:A:703:HOH:O	2.44	0.49
1:C:239:TRP:O	1:C:316:GLY:N	2.45	0.49
2:D:106:VAL:HA	2:D:190:GLY:HA2	1.94	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.47	0.49
1:A:206:ARG:CZ	1:A:218:ASP:HB2	2.43	0.49
2:D:209:LEU:C	2:D:211:ARG:N	2.63	0.49
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.48	0.48
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.95	0.48
1:A:100:LEU:HB3	5:A:604:3LQ:H6	1.96	0.48
2:B:191:SER:OG	2:B:198:HIS:ND1	2.40	0.47
1:A:402:TRP:C	1:A:402:TRP:CD1	2.87	0.47
1:C:57:ASN:HD21	1:C:131:THR:HB	1.79	0.47
2:D:60:VAL:HG12	2:D:75:VAL:HG22	1.96	0.47
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.14	0.47
2:B:54:ASN:O	2:B:143:ARG:NH2	2.47	0.47
1:C:253:THR:HG23	1:C:256:ASP:H	1.80	0.47
1:C:59:PRO:O	1:C:75:VAL:HG13	2.15	0.47
1:C:77:PHE:HB3	1:C:80:LEU:HB3	1.97	0.47
1:C:89:GLU:OE1	1:C:90:VAL:N	2.47	0.47
2:D:96:HIS:N	2:D:97:PRO:HD2	2.30	0.47
2:D:266:TRP:CD2	2:D:425:LEU:HD13	2.50	0.46
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.46
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.97	0.46
2:B:332:GLN:HE22	2:B:425:LEU:HB2	1.80	0.46
1:C:164:MET:SD	1:C:187:LEU:HD21	2.55	0.46
1:A:505:ILE:O	1:A:510:PRO:HD3	2.16	0.46
2:D:154:LYS:O	2:D:157:PRO:HD2	2.17	0.45
1:A:428:GLN:HE21	1:A:428:GLN:HB3	1.63	0.44
1:C:517:LEU:H	4:C:602:EDO:H22	1.81	0.44
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.53	0.44
2:B:50:ILE:HG21	2:B:145:GLN:HB3	2.00	0.44
1:C:257:ILE:O	1:C:261:VAL:HG23	2.17	0.44
1:C:325:LEU:HD21	1:C:383:TRP:CE3	2.53	0.44
1:A:305:GLU:O	1:A:309:ILE:HG13	2.18	0.44
1:A:473:THR:O	1:A:477:THR:HG23	2.18	0.44
1:C:278:GLN:H	1:C:302:GLU:CD	2.21	0.44
1:C:501:TYR:CZ	1:C:505:ILE:HD11	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.99	0.44
1:A:88:TRP:CZ2	2:B:143:ARG:HD3	2.53	0.44
1:A:408:ALA:O	2:B:393:ILE:HG13	2.18	0.44
1:A:60:VAL:HG22	1:A:130:PHE:HB2	2.00	0.43
1:A:304:ALA:O	1:A:308[A]:GLU:HG2	2.16	0.43
1:A:411:ILE:HG22	1:A:412:PRO:O	2.18	0.43
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.43
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.99	0.43
2:B:324:ASP:O	2:B:343:GLN:HG2	2.18	0.43
1:C:97:PRO:HG2	1:C:232:TYR:CD1	2.53	0.43
2:B:344:GLU:HB3	2:B:345:PRO:HD2	2.01	0.43
1:C:180:ILE:HG12	1:C:189:VAL:HG22	1.99	0.43
1:C:483:TYR:HB2	1:C:521:ILE:HG12	2.00	0.43
2:D:24:TRP:CH2	2:D:399:GLU:HG2	2.54	0.43
1:C:492:GLU:OE2	1:C:530:LYS:HD3	2.19	0.43
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.53	0.43
1:C:38:CYS:HA	1:C:47:ILE:HD11	2.01	0.43
2:B:101:LYS:O	2:B:236:PRO:HB2	2.19	0.42
1:A:301:LEU:O	1:A:305:GLU:HG3	2.18	0.42
1:C:96:HIS:CE1	1:C:350:LYS:HD2	2.54	0.42
1:A:165:THR:O	1:A:169:GLU:HG3	2.20	0.42
1:C:29:GLU:H	1:C:29:GLU:HG3	1.43	0.42
1:A:255:ASN:HB2	1:A:289:LEU:HB3	2.01	0.42
1:A:406:TRP:NE1	2:B:420:PRO:HG3	2.35	0.42
2:B:325:LEU:HD23	2:B:343:GLN:HG3	2.00	0.42
1:C:501:TYR:CE2	1:C:505:ILE:HD11	2.54	0.42
1:A:270:ILE:HG13	1:A:314:VAL:HG12	2.02	0.42
1:C:167:ILE:O	1:C:170:PRO:HD2	2.19	0.42
2:D:135:ILE:HD13	2:D:135:ILE:HA	1.84	0.42
1:C:410:TRP:CZ2	1:C:412:PRO:HA	2.55	0.42
2:D:342:TYR:HB3	2:D:348:ASN:HA	2.02	0.42
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.55	0.41
2:D:157:PRO:HG2	2:D:184:MET:HA	2.01	0.41
1:A:135:ILE:H	1:A:135:ILE:HG13	1.49	0.41
2:D:305:GLU:HG2	2:D:306:ASN:N	2.36	0.41
1:C:84:THR:HB	1:C:154:LYS:HD3	2.02	0.41
1:C:121:ASP:O	1:C:125:ARG:HG3	2.21	0.41
1:A:197:GLN:O	1:A:201:LYS:HG2	2.20	0.41
2:D:181:TYR:CZ	2:D:183:TYR:HB2	2.55	0.41
2:D:209:LEU:C	2:D:211:ARG:H	2.24	0.41
1:A:94:ILE:HG22	1:A:183:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LYS:HB3	1:A:417:VAL:HG21	2.02	0.41
1:A:476:LYS:HE3	1:A:476:LYS:HB2	1.82	0.41
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.56	0.41
2:B:237:ASP:OD1	2:B:238:LYS:N	2.54	0.41
1:A:377:THR:O	1:A:381:VAL:HG23	2.21	0.41
2:B:65:LYS:HD2	2:B:72:ARG:HD2	2.03	0.41
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.56	0.41
1:C:279:LEU:HD13	1:C:299:ALA:HB1	2.02	0.41
1:C:438:GLU:HG3	1:C:461:LYS:HG2	2.03	0.41
1:C:441:TYR:HA	1:C:496:VAL:HG22	2.02	0.41
2:D:328:GLU:O	2:D:339:TYR:HA	2.21	0.41
2:D:121:ASP:O	2:D:125:ARG:HG3	2.21	0.40
2:D:326:ILE:O	2:D:341:ILE:HA	2.22	0.40
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.51	0.40
2:D:21:VAL:O	2:D:57:ASN:ND2	2.54	0.40
2:D:257:ILE:O	2:D:261:VAL:HG23	2.21	0.40
1:C:295:LEU:HB3	1:C:300:GLU:OE1	2.22	0.40
1:A:435:VAL:HA	2:B:290:THR:HG21	2.04	0.40
2:B:142:ILE:HD12	2:B:142:ILE:H	1.86	0.40
1:C:295:LEU:HB3	1:C:300:GLU:CD	2.42	0.40
1:C:326:ILE:O	1:C:341:ILE:HA	2.22	0.40
1:C:395:LYS:HD3	1:C:414:TRP:CZ2	2.56	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	537/558 (96%)	530 (99%)	7 (1%)	0	100	100
1	C	530/558 (95%)	524 (99%)	6 (1%)	0	100	100
2	B	403/428 (94%)	397 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	394/428 (92%)	386 (98%)	8 (2%)	0	100	100
All	All	1864/1972 (94%)	1837 (99%)	27 (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	425/495 (86%)	389 (92%)	36 (8%)	10	28
1	C	393/495 (79%)	363 (92%)	30 (8%)	13	33
2	B	350/390 (90%)	333 (95%)	17 (5%)	25	54
2	D	242/390 (62%)	224 (93%)	18 (7%)	13	34
All	All	1410/1770 (80%)	1309 (93%)	101 (7%)	14	36

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	21	VAL
1	A	23	GLN
1	A	29	GLU
1	A	58	THR
1	A	60	VAL
1	A	63	ILE
1	A	68	SER
1	A	71	TRP
1	A	105	SER
1	A	135	ILE
1	A	139	THR
1	A	151	GLN
1	A	184	MET
1	A	199	ARG
1	A	219	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	244	ILE
1	A	245	VAL
1	A	250	ASP
1	A	253	THR
1	A	260	LEU
1	A	289	LEU
1	A	302	GLU
1	A	324	ASP
1	A	332	GLN
1	A	362	THR
1	A	402	TRP
1	A	415	GLU
1	A	459	THR
1	A	473	THR
1	A	482	ILE
1	A	491	LEU
1	A	513	SER
1	A	514	GLU
1	A	527	LYS
1	A	547	GLN
2	B	72	ARG
2	B	85	GLN
2	B	86	ASP
2	B	88	TRP
2	B	89	GLU
2	B	92	LEU
2	B	117	SER
2	B	121	ASP
2	B	163	SER
2	B	215	THR
2	B	216	THR
2	B	234	LEU
2	B	242	GLN
2	B	286	THR
2	B	418	ASN
2	B	425	LEU
2	B	426	TRP
1	C	27	THR
1	C	28	GLU
1	C	29	GLU
1	C	31	ILE
1	C	32	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	35	VAL
1	C	101	LYS
1	C	110[A]	ASP
1	C	110[B]	ASP
1	C	146	TYR
1	C	147	ASN
1	C	161	GLN
1	C	177	ASP
1	C	186	ASP
1	C	200	THR
1	C	216	THR
1	C	221	HIS
1	C	224	GLU
1	C	237	ASP
1	C	250	ASP
1	C	277	ARG
1	C	283	LEU
1	C	291	GLU
1	C	324	ASP
1	C	351	THR
1	C	399	GLU
1	C	402	TRP
1	C	405	TYR
1	C	442	VAL
1	C	496	VAL
2	D	90	VAL
2	D	96	HIS
2	D	100	LEU
2	D	101	LYS
2	D	121	ASP
2	D	211	ARG
2	D	291	GLU
2	D	293	ILE
2	D	298	GLU
2	D	314	VAL
2	D	330	GLN
2	D	340	GLN
2	D	362	THR
2	D	377	THR
2	D	405	TYR
2	D	414	TRP
2	D	423	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	394	GLN

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.05	0
5	3LQ	A	604	-	33,33,33	0.45	0	44,45,45	0.52	0
4	EDO	A	603	-	3,3,3	0.47	0	2,2,2	0.25	0
3	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.05	0
5	3LQ	C	603	-	33,33,33	0.48	0	44,45,45	0.60	0
4	EDO	C	602	-	3,3,3	0.43	0	2,2,2	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3LQ	A	604	-	-	0/12/12/12	0/4/4/4
4	EDO	A	603	-	-	1/1/1/1	-
5	3LQ	C	603	-	-	5/12/12/12	0/4/4/4
4	EDO	C	602	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	603	3LQ	O0B-C0D-C0E-N0H
5	C	603	3LQ	C0E-C0D-O0B-C05
5	C	603	3LQ	C00-C05-O0B-C0D
5	C	603	3LQ	C04-C05-O0B-C0D
5	C	603	3LQ	C05-C04-O0A-CAH
4	A	603	EDO	O1-C1-C2-O2

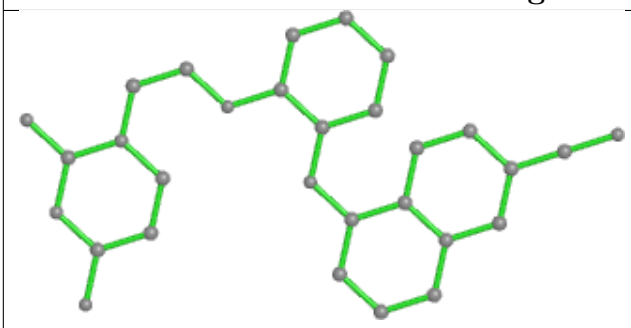
There are no ring outliers.

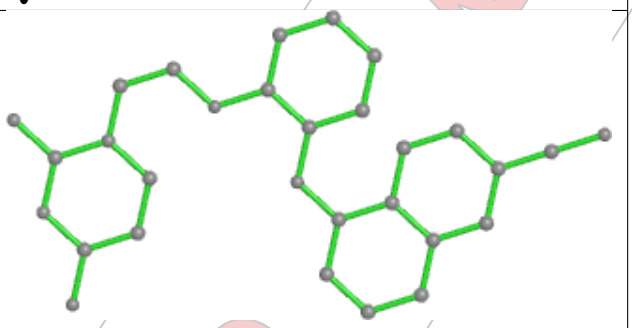
2 monomers are involved in 2 short contacts:

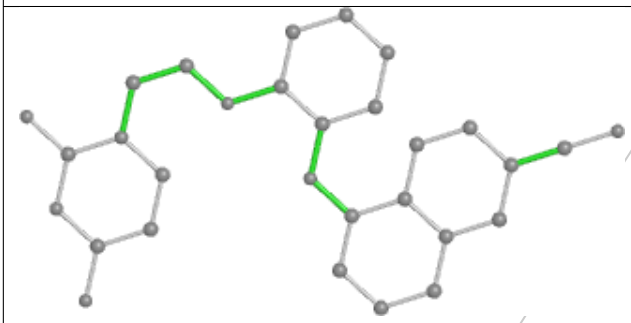
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	3LQ	1	0
4	C	602	EDO	1	0

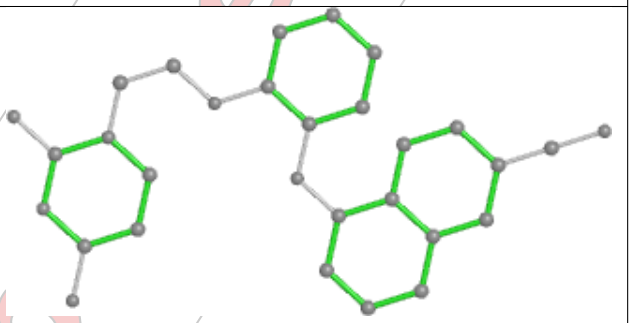
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 3LQ A 604

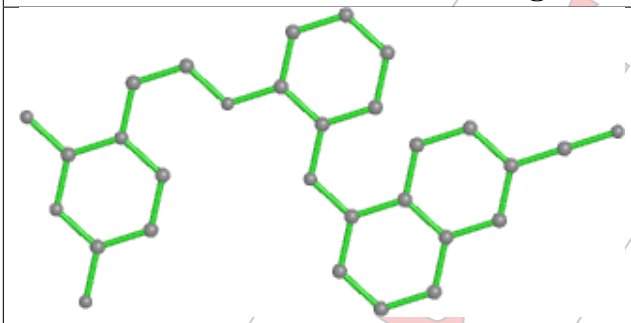

Bond lengths

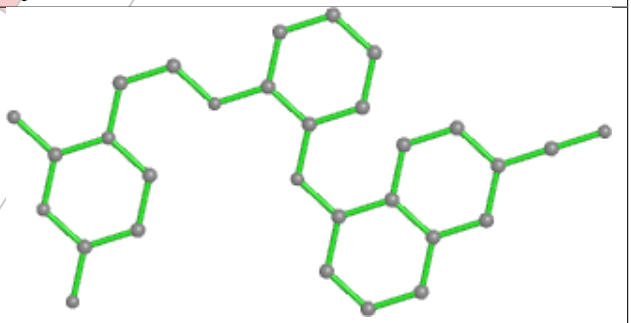

Bond angles

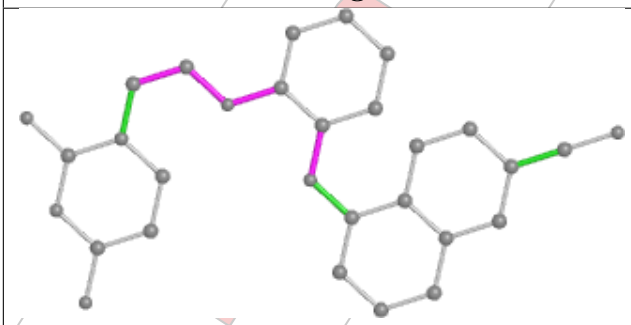

Torsions

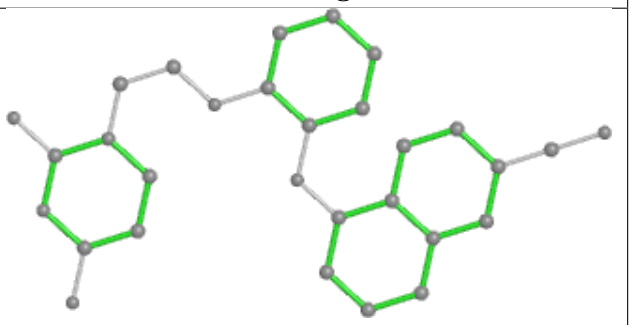

Rings

Ligand 3LQ C 603


Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers (i)

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	544/558 (97%)	0.30	26 (4%)	30	24	47, 84, 134, 161	0
1	C	542/558 (97%)	0.50	43 (7%)	12	9	74, 111, 148, 171	0
2	B	408/428 (95%)	0.33	14 (3%)	45	39	48, 78, 121, 139	6 (1%)
2	D	401/428 (93%)	0.55	45 (11%)	5	3	81, 125, 159, 170	4 (0%)
All	All	1895/1972 (96%)	0.41	128 (6%)	17	12	47, 100, 150, 171	10 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	283	LEU	4.6
2	D	272	PRO	4.6
2	D	299	ALA	4.5
2	D	232	TYR	4.5
1	A	292	VAL	4.5
1	C	247	PRO	4.4
1	C	142	ILE	4.4
1	A	552	VAL	4.3
1	C	290	THR	4.2
1	A	286	THR	4.2
1	C	282	LEU	4.2
2	D	200	THR	4.1
1	C	144	TYR	4.0
1	C	61	PHE	4.0
1	C	224	GLU	3.8
1	C	131	THR	3.8
1	A	282	LEU	3.6
1	C	402	TRP	3.6
1	A	251	SER	3.4
2	D	316	GLY	3.4
1	C	31	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	358	ARG	3.4
1	A	255	ASN	3.3
1	C	292	VAL	3.3
1	C	127	TYR	3.3
2	D	178	ILE	3.3
2	D	317	VAL	3.2
1	C	283	LEU	3.2
1	C	246	LEU	3.2
2	D	10	VAL	3.2
2	D	349	LEU	3.1
2	D	319	TYR	3.1
1	A	34	LEU	3.1
1	C	254	VAL	3.0
2	B	274	ILE	3.0
2	D	271	TYR	3.0
2	D	252	TRP	3.0
2	D	160	PHE	2.9
1	C	146	TYR	2.9
1	C	26	LEU	2.9
1	A	294	PRO	2.9
1	A	256	ASP	2.9
2	D	176	PRO	2.9
1	A	302	GLU	2.9
2	B	232	TYR	2.9
1	A	542	ILE	2.9
2	D	177	ASP	2.9
1	C	251	SER	2.8
1	C	130	PHE	2.8
1	C	279	LEU	2.8
1	C	37	ILE	2.8
2	D	421	PRO	2.8
1	A	290	THR	2.8
1	C	35	VAL	2.8
2	D	102	LYS	2.8
2	D	245	VAL	2.7
2	D	96	HIS	2.7
2	D	111	VAL	2.7
2	B	284	ARG	2.7
2	B	14	PRO	2.7
2	D	127	TYR	2.6
1	C	359	GLY	2.6
2	D	315	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	227	PHE	2.6
2	D	92	LEU	2.6
2	D	174	GLN	2.6
1	C	195	ILE	2.6
2	D	84	THR	2.6
1	A	260	LEU	2.5
2	D	114	ALA	2.5
2	D	142	ILE	2.5
2	D	341	ILE	2.5
2	D	199	ARG	2.5
2	D	296	THR	2.5
1	A	551	LEU	2.5
2	D	180	ILE	2.4
1	C	426	TRP	2.4
1	C	291	GLU	2.4
1	A	71	TRP	2.4
2	D	298	GLU	2.4
1	C	555	GLY	2.4
1	A	226	PRO	2.4
2	D	358	ARG	2.4
2	D	124	PHE	2.4
2	D	190	GLY	2.4
1	C	255	ASN	2.4
1	C	38	CYS	2.4
1	A	61	PHE	2.4
2	B	69	THR	2.3
1	C	257	ILE	2.3
1	C	15	GLY	2.3
1	C	556	ILE	2.3
1	A	285	GLY	2.3
1	C	135	ILE	2.3
2	D	168	LEU	2.3
1	A	246	LEU	2.2
1	C	294	PRO	2.2
1	C	145	GLN	2.2
1	C	88	TRP	2.2
1	A	288	ALA	2.2
2	B	299	ALA	2.2
1	C	51	GLY	2.2
2	D	12	LEU	2.2
2	D	303	LEU	2.2
1	A	296	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	284	ARG	2.2
1	C	65	LYS	2.1
1	C	358	ARG	2.1
2	D	383	TRP	2.1
1	C	47	ILE	2.1
2	B	88	TRP	2.1
2	D	9	PRO	2.1
2	D	119	PRO	2.1
1	A	253	THR	2.1
2	D	306	ASN	2.1
2	B	279	LEU	2.1
2	B	425	LEU	2.1
2	B	427	TYR	2.1
1	C	150	PRO	2.0
2	B	421	PRO	2.0
1	A	299	ALA	2.0
1	A	303	LEU	2.0
1	A	298	GLU	2.0
2	D	175	ASN	2.0
1	C	128	THR	2.0
2	D	279	LEU	2.0
2	D	198	HIS	2.0
2	B	68	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.

Continued on next page...

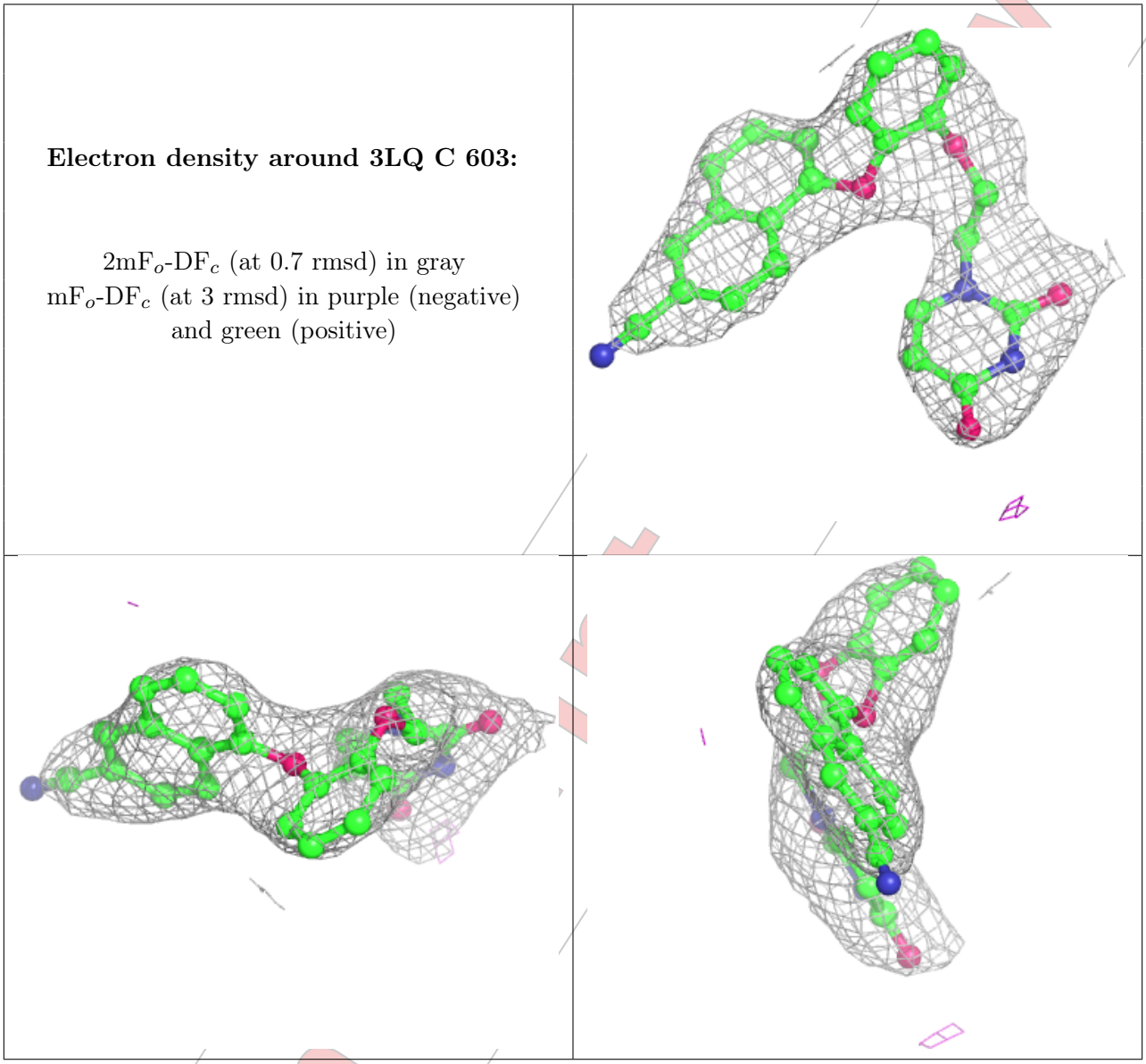
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	603	4/4	0.69	0.27	75,81,85,87	0
6	MG	C	601	1/1	0.84	0.30	100,100,100,100	0
4	EDO	C	602	4/4	0.88	0.19	99,100,105,117	0
3	SO4	A	602	5/5	0.92	0.12	107,119,130,140	0
5	3LQ	C	603	30/30	0.94	0.26	85,100,109,118	0
3	SO4	A	601	5/5	0.94	0.15	106,107,115,130	0
5	3LQ	A	604	30/30	0.97	0.20	51,64,77,86	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.

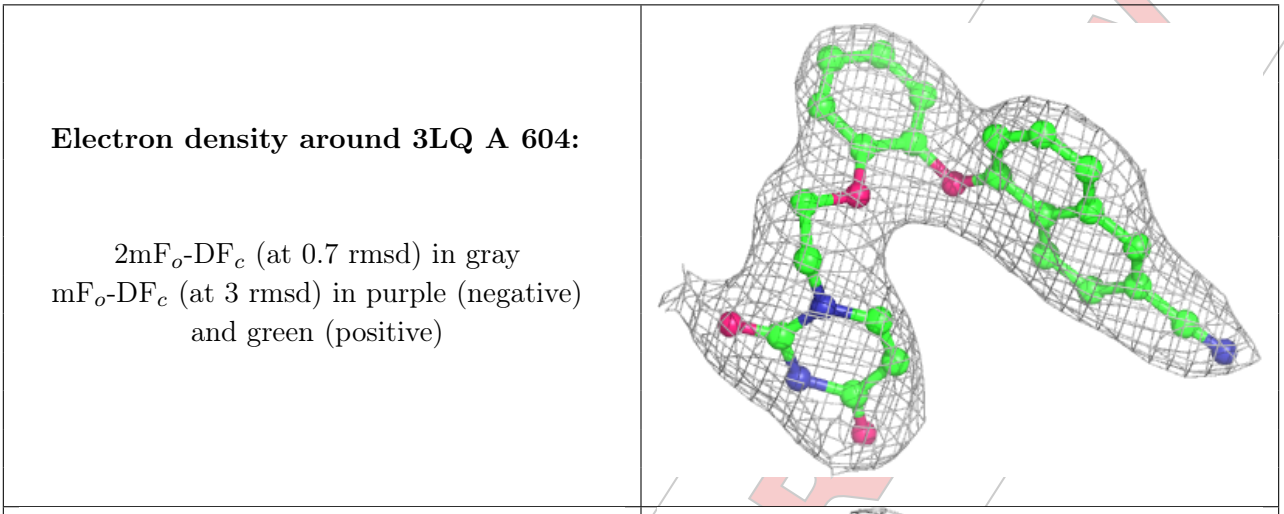
Electron density around 3LQ C 603:

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



Electron density around 3LQ A 604:

$2mF_o$-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.

Full wwPDB X-ray Structure Validation Report (i)

May 12, 2023 – 03:51 PM EDT

PDB ID	:	8STS
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (Y181C, V106A) varient in Complex with 5-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)-4-fluorophenoxy)-7-fluoro-2-naphthonitrile (JLJ636), a non-nucleoside inhibitor
Deposited on	:	2023-05-11
Resolution	:	3.02 Å(reported)

This wwPDB validation report is for manuscript review

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

This report is produced by the wwPDB biocuration pipeline after 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

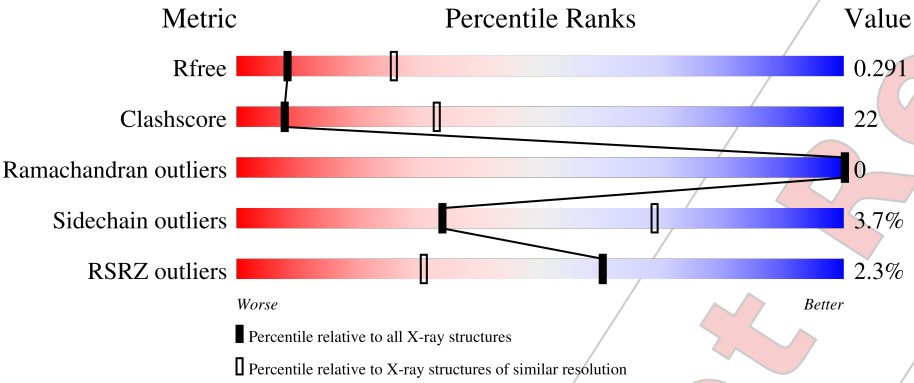
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

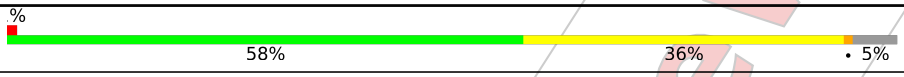
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	558	3% 54% 38%
1	C	558	3% 58% 38%
2	B	428	2% 55% 37% 6%

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	428	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14639 atoms, of which 30 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	546	Total	C	N	O	S	0	0	0
			4141	2658	688	788	7			
1	A	533	Total	C	N	O	S	0	0	0
			3972	2550	658	758	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	106	ALA	VAL	engineered mutation	UNP P03366
C	172	ALA	LYS	conflict	UNP P03366
C	173	ALA	LYS	conflict	UNP P03366
C	181	CYS	TYR	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	106	ALA	VAL	engineered mutation	UNP P03366
A	172	ALA	LYS	conflict	UNP P03366
A	173	ALA	LYS	conflict	UNP P03366
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

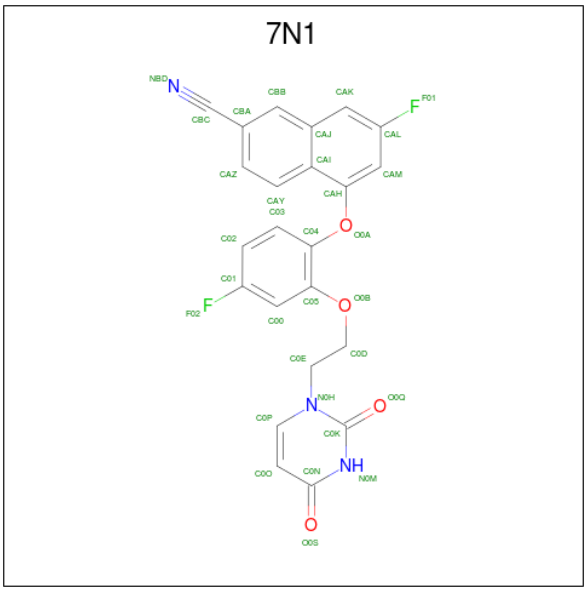
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	23	0	0
			3189	2071	522	591	5			
2	D	407	Total	C	N	O	S	0	0	0
			3229	2092	534	596	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 5-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]-4-fluorophenoxy}-7-fluoronaphthalene-2-carbonitrile (three-letter code: 7N1) (formula: $C_{23}H_{15}F_2N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	F	H	N	O	0	0
			47	23	2	15	3	4		
3	A	1	Total	C	F	H	N	O	0	0
			47	23	2	15	3	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

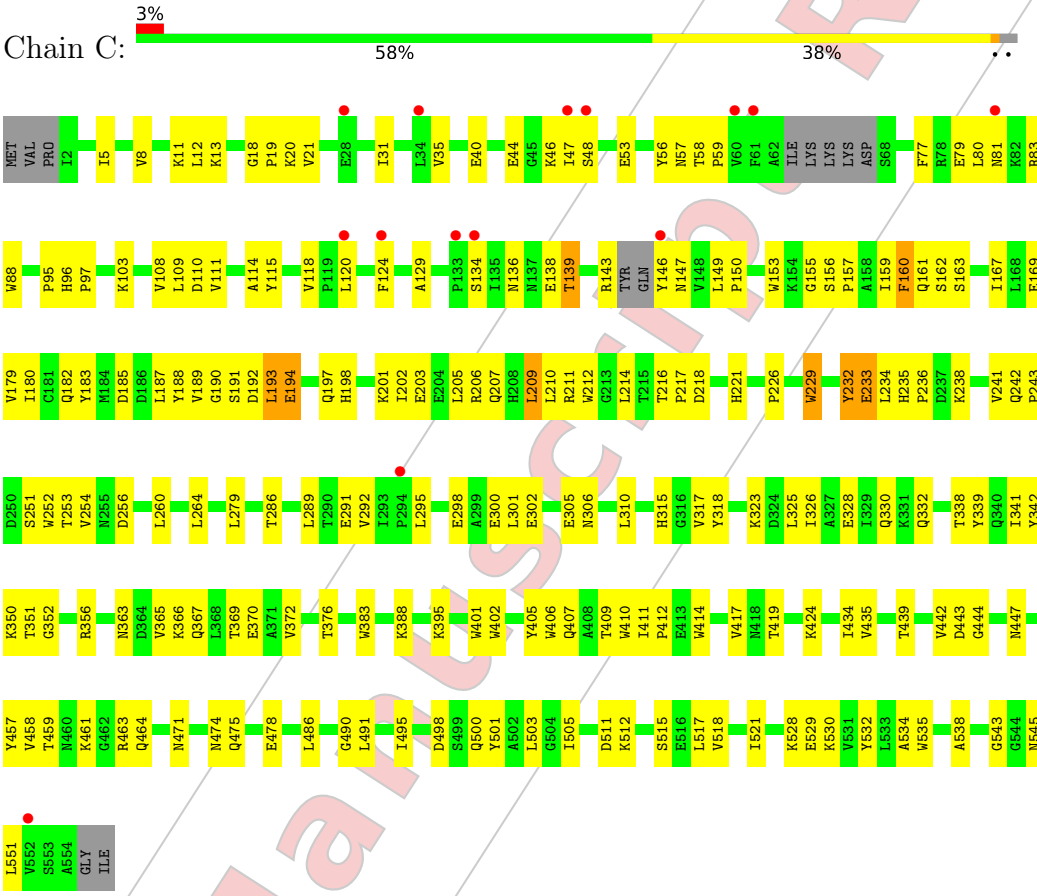
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	D	6	Total O 6 6	0	0

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.

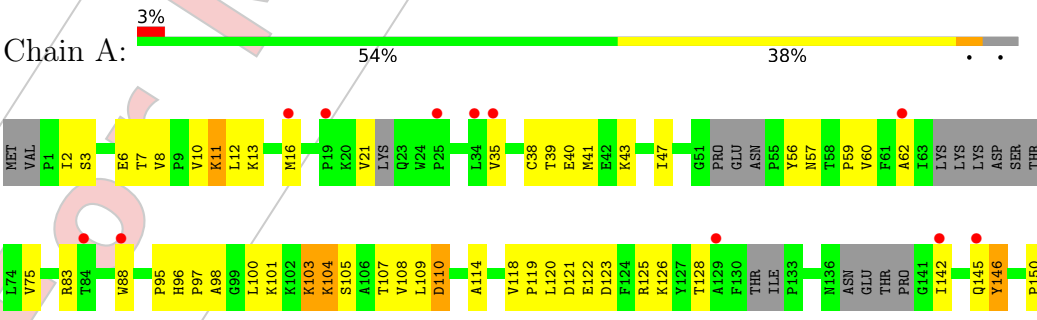
• Molecule 1: Reverse transcriptase/ribonuclease H

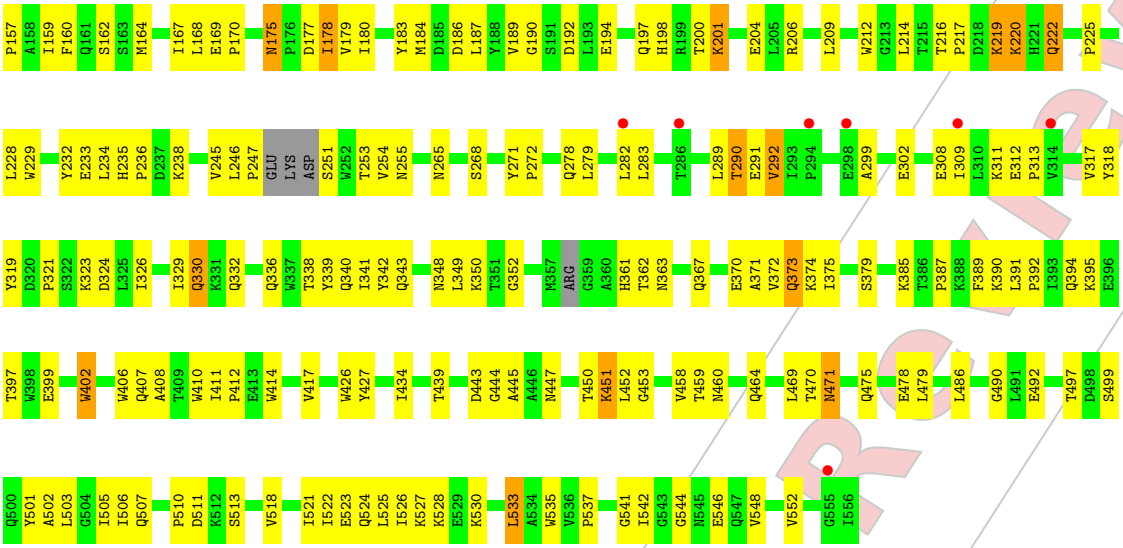
Chain C:



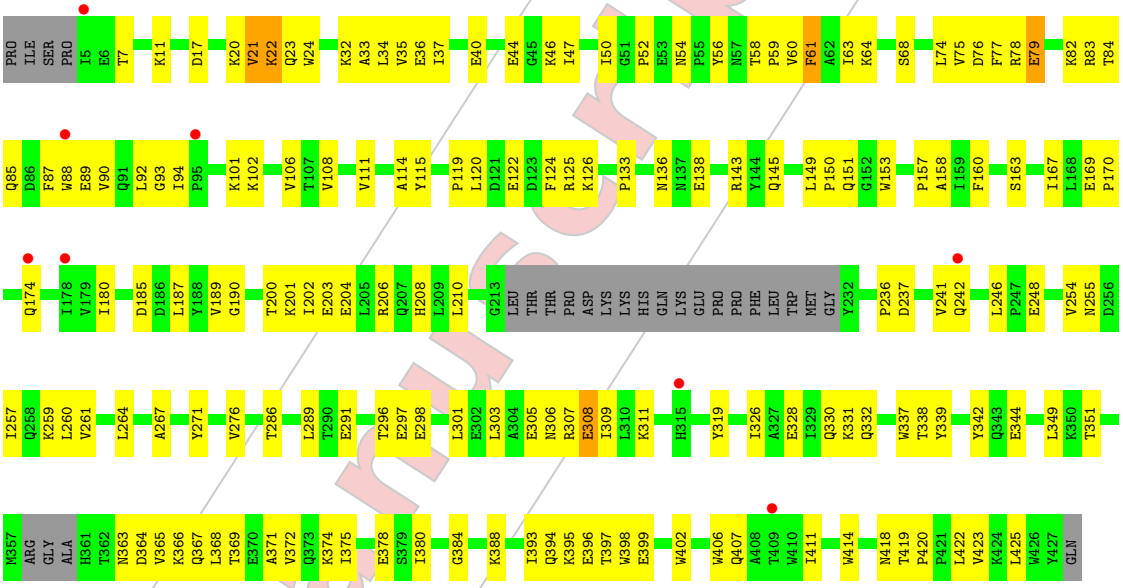
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:

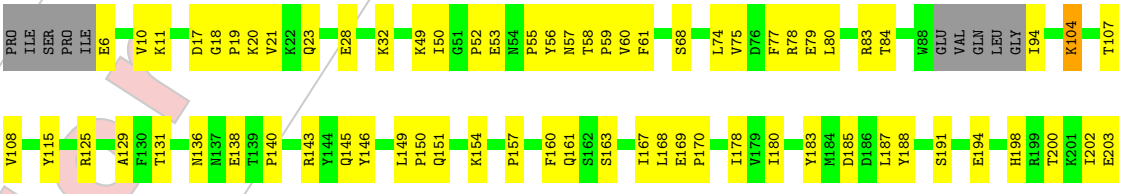


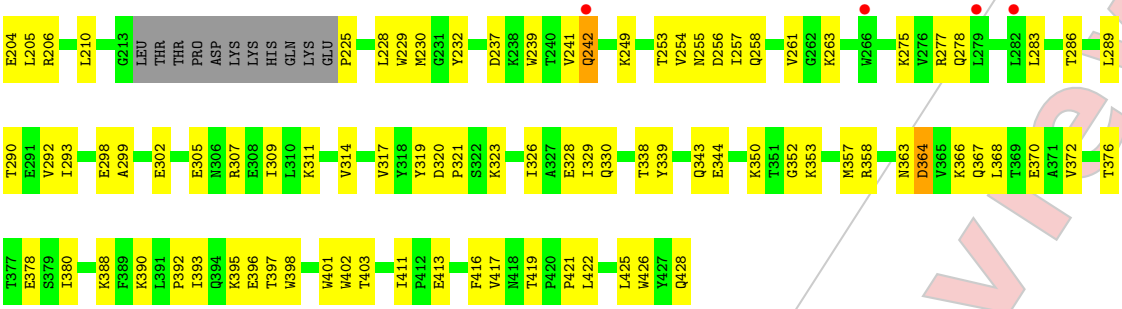


• Molecule 2: p51 RT



• Molecule 2: p51 RT





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.86Å 128.26Å 133.04Å 90.00° 105.32° 90.00°	Depositor
Resolution (Å)	38.11 – 3.02 38.12 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.11-3.02) 99.2 (38.12-3.02)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.240 , 0.285 0.247 , 0.291	Depositor DCC
R_{free} test set	2803 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	102.3	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 83.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14639	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: 7N1, MG

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	0.26	0/4067	0.41	0/5563
1	C	0.23	0/4250	0.41	0/5826
2	B	0.23	0/3278	0.41	0/4477
2	D	0.23	0/3323	0.41	0/4540
All	All	0.24	0/14918	0.41	0/20406

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	3972	0	3686	183	0
1	C	4141	0	3858	182	0
2	B	3189	0	3079	135	0
2	D	3229	0	3089	134	0
3	A	32	15	0	2	0
3	C	32	15	0	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	0	1	0
5	D	6	0	0	0	0
All	All	14609	30	13712	608	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 22.

All (608) 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:254:VAL:HG21	1:A:290:THR:HB	1.53	0.91
1:C:232:TYR:HB3	1:C:241:VAL:HA	1.54	0.90
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.63	0.81
1:C:253:THR:HG22	1:C:292:VAL:HG22	1.62	0.80
2:D:84:THR:HB	2:D:154:LYS:HD3	1.65	0.78
2:D:326:ILE:HD13	2:D:388:LYS:HB3	1.67	0.77
2:D:357:MET:O	2:D:358:ARG:HG3	1.85	0.77
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.66	0.76
1:C:178:ILE:HG22	1:C:180:ILE:HD11	1.67	0.76
2:D:20:LYS:HG2	2:D:56:TYR:HA	1.69	0.74
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.71	0.73
1:C:363:ASN:HA	1:C:511:ASP:OD1	1.89	0.72
1:A:219:LYS:HD2	1:A:220:LYS:H	1.54	0.72
2:D:393:ILE:HD11	2:D:397:THR:HG22	1.69	0.72
1:A:506:ILE:HD12	1:A:533:LEU:HD11	1.71	0.72
2:D:104:LYS:HE2	2:D:237:ASP:HB3	1.71	0.72
2:D:242:GLN:NE2	2:D:428:GLN:OXT	2.23	0.72
1:A:229:TRP:HB2	3:A:601:7N1:NBD	2.05	0.71
2:B:78:ARG:O	2:B:82:LYS:HG3	1.91	0.71
1:A:121:ASP:O	1:A:125:ARG:HG3	1.90	0.71
1:C:163:SER:O	1:C:167:ILE:HG12	1.90	0.70
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.26	0.70
2:B:111:VAL:CG1	2:B:114:ALA:HB3	2.22	0.69
2:B:305:GLU:O	2:B:309:ILE:HG13	1.93	0.69
1:A:370:GLU:O	1:A:374:LYS:HG2	1.92	0.69
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.75	0.69
1:C:182:GLN:HB2	2:D:140:PRO:HD3	1.75	0.69
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.73	0.69
2:D:358:ARG:O	2:D:367:GLN:HG2	1.92	0.69
2:B:115:TYR:O	2:B:149:LEU:HB2	1.93	0.68
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:LEU:CB	2:B:158:ALA:HB1	2.23	0.68
2:D:115:TYR:O	2:D:149:LEU:HB2	1.93	0.68
2:D:242:GLN:HB3	2:D:352:GLY:HA2	1.74	0.68
1:C:13:LYS:N	1:C:83:ARG:O	2.20	0.68
2:B:101:LYS:O	2:B:236:PRO:HB2	1.94	0.68
2:B:246:LEU:O	2:B:307:ARG:NH2	2.28	0.67
1:A:391:LEU:CD1	1:A:411:ILE:HD11	2.25	0.67
2:D:275:LYS:HZ1	2:D:277:ARG:HH11	1.40	0.67
1:A:219:LYS:HD2	1:A:220:LYS:N	2.10	0.67
2:D:357:MET:HB3	2:D:370:GLU:HG2	1.77	0.67
2:D:323:LYS:O	2:D:343:GLN:NE2	2.27	0.67
1:C:19:PRO:HB3	1:C:79:GLU:HG3	1.76	0.67
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.76	0.67
2:B:303:LEU:O	2:B:307:ARG:HG3	1.94	0.67
2:D:20:LYS:HE2	2:D:56:TYR:CD1	2.30	0.66
1:A:98:ALA:HB1	1:A:349:LEU:HD13	1.77	0.66
2:B:368:LEU:O	2:B:372:VAL:HG23	1.95	0.66
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.77	0.66
1:C:410:TRP:CH2	1:C:412:PRO:HA	2.31	0.66
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.77	0.66
1:C:372:VAL:HG11	1:C:412:PRO:HD2	1.76	0.66
2:B:330:GLN:HB2	2:B:338:THR:OG1	1.95	0.66
2:D:19:PRO:HG3	2:D:80:LEU:HB2	1.77	0.65
1:C:18:GLY:HA3	1:C:56:TYR:CE1	2.31	0.65
1:C:326:ILE:HD13	1:C:388:LYS:HB2	1.79	0.65
2:D:358:ARG:NH1	2:D:370:GLU:OE1	2.26	0.65
1:C:171:PHE:CD2	1:C:205:LEU:HD13	2.31	0.65
2:B:40:GLU:O	2:B:44:GLU:HG3	1.97	0.65
1:A:254:VAL:HG21	1:A:290:THR:CB	2.27	0.65
2:B:328:GLU:O	2:B:339:TYR:HA	1.96	0.65
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
1:C:134:SER:HB2	1:C:139:THR:HG23	1.79	0.64
2:D:194:GLU:OE1	2:D:194:GLU:N	2.29	0.64
1:C:543:GLY:HA2	2:D:283:LEU:O	1.97	0.64
1:A:271:TYR:OH	1:A:313:PRO:HA	1.98	0.64
1:C:21:VAL:HB	1:C:59:PRO:HD3	1.78	0.64
1:A:167:ILE:O	1:A:170:PRO:HD2	1.98	0.64
1:A:363:ASN:HA	1:A:511:ASP:OD1	1.98	0.64
2:B:363:ASN:O	2:B:367:GLN:HG3	1.99	0.63
1:A:175:ASN:HB2	1:A:178:ILE:HD13	1.80	0.63
1:A:479:LEU:O	1:A:521:ILE:HD11	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HE2	1:A:47:ILE:HG13	1.81	0.63
1:C:206:ARG:NH1	1:C:216:THR:O	2.30	0.62
1:A:272:PRO:O	1:A:309:ILE:HD13	1.97	0.62
2:B:326:ILE:HG22	2:B:388:LYS:HB3	1.79	0.62
1:C:136:ASN:HB2	1:C:138:GLU:HG3	1.82	0.62
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.82	0.62
1:C:114:ALA:O	1:C:118:VAL:HG23	2.00	0.61
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.82	0.61
2:D:328:GLU:O	2:D:339:TYR:HA	2.00	0.61
1:C:511:ASP:O	1:C:512:LYS:HG3	2.00	0.61
2:B:425:LEU:HD23	2:B:425:LEU:O	2.00	0.61
2:D:314:VAL:HG13	2:D:317:VAL:HG21	1.81	0.61
2:D:198:HIS:O	2:D:202:ILE:HG12	2.01	0.61
2:B:23:GLN:HG2	2:B:133:PRO:HD3	1.83	0.61
2:B:248:GLU:OE1	2:B:307:ARG:NH1	2.33	0.61
1:C:207:GLN:O	1:C:211:ARG:HG3	2.01	0.61
1:A:479:LEU:HD21	1:A:518:VAL:HG22	1.83	0.61
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.82	0.60
2:D:225:PRO:HB3	2:D:228:LEU:HB2	1.81	0.60
1:C:376:THR:HG21	2:D:401:TRP:CH2	2.35	0.60
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.83	0.60
2:B:396:GLU:OE1	2:B:396:GLU:N	2.35	0.60
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.36	0.60
2:D:368:LEU:O	2:D:372:VAL:HG23	2.02	0.60
1:C:202:ILE:O	1:C:206:ARG:HG3	2.02	0.60
1:A:7:THR:HG22	1:A:119:PRO:O	2.02	0.60
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.37	0.60
2:D:210:LEU:HD21	2:D:228:LEU:HD23	1.83	0.60
1:A:233:GLU:HG2	1:A:235:HIS:CE1	2.36	0.60
1:C:226:PRO:HB3	1:C:235:HIS:CD2	2.36	0.59
1:C:203:GLU:O	1:C:207:GLN:HG2	2.02	0.59
1:A:427:TYR:OH	1:A:510:PRO:HD2	2.02	0.59
1:C:20:LYS:HA	1:C:57:ASN:H	1.66	0.59
1:C:226:PRO:HB3	1:C:235:HIS:HD2	1.65	0.59
1:C:317:VAL:HG23	1:C:318:TYR:O	2.02	0.59
1:C:206:ARG:HD2	1:C:216:THR:O	2.01	0.59
1:C:395:LYS:HD3	1:C:414:TRP:CZ2	2.38	0.59
1:C:97:PRO:HD3	1:C:232:TYR:CE1	2.37	0.59
2:B:398:TRP:O	2:B:402:TRP:HB3	2.01	0.59
2:D:398:TRP:O	2:D:402:TRP:HB3	2.03	0.59
1:A:60:VAL:HG12	1:A:75:VAL:CB	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:VAL:CG1	2:D:317:VAL:HG21	2.32	0.59
1:C:180:ILE:HG13	1:C:189:VAL:HG22	1.85	0.59
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.37	0.59
1:C:253:THR:HA	1:C:292:VAL:HA	1.84	0.58
1:C:350:LYS:HG2	1:C:351:THR:N	2.18	0.58
2:D:200:THR:O	2:D:204:GLU:HG3	2.03	0.58
1:C:178:ILE:HG22	1:C:180:ILE:CD1	2.32	0.58
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.85	0.58
1:A:522:ILE:O	1:A:526:ILE:HG13	2.02	0.58
1:A:108:VAL:O	1:A:109:LEU:HD23	2.03	0.58
1:C:118:VAL:HB	1:C:149:LEU:HD12	1.84	0.58
1:A:35:VAL:O	1:A:39:THR:HG23	2.04	0.58
1:A:103:LYS:NZ	1:A:103:LYS:HA	2.18	0.58
1:C:238:LYS:HD3	1:C:315:HIS:ND1	2.19	0.58
1:A:329:ILE:O	1:A:392:PRO:HD3	2.04	0.58
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.84	0.58
1:A:186:ASP:O	1:A:187:LEU:HD22	2.04	0.58
1:C:221:HIS:HA	5:C:702:HOH:O	2.02	0.58
1:C:503:LEU:HD23	2:D:422:LEU:HD22	1.84	0.58
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.39	0.58
2:D:78:ARG:HD3	2:D:411:ILE:O	2.02	0.58
2:D:229:TRP:CZ3	2:D:230:MET:HG2	2.39	0.58
1:C:233:GLU:C	1:C:234:LEU:HD12	2.25	0.57
2:D:307:ARG:HG2	2:D:311:LYS:HE3	1.85	0.57
2:B:88:TRP:HE1	2:B:158:ALA:HB3	1.68	0.57
1:C:491:LEU:HB3	1:C:529:GLU:HG3	1.84	0.57
1:A:40:GLU:HA	1:A:43:LYS:HD2	1.86	0.57
1:A:324:ASP:O	1:A:343:GLN:HG2	2.04	0.57
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.86	0.57
2:B:203:GLU:HA	2:B:206:ARG:HD3	1.85	0.57
1:C:547:GLN:O	1:C:551:LEU:HG	2.05	0.57
2:D:20:LYS:HE2	2:D:56:TYR:HD1	1.69	0.57
1:C:210:LEU:HD22	1:C:214:LEU:O	2.03	0.57
2:D:169:GLU:HB3	2:D:170:PRO:HD3	1.86	0.57
2:D:53:GLU:O	2:D:55:PRO:HD3	2.04	0.57
1:A:190:GLY:HA2	1:A:198:HIS:HE1	1.70	0.57
2:B:255:ASN:O	2:B:259:LYS:HG3	2.05	0.57
2:D:320:ASP:HB3	2:D:323:LYS:HD3	1.87	0.57
2:D:163:SER:O	2:D:167:ILE:HG13	2.04	0.56
1:A:153:TRP:HB3	1:A:156:SER:OG	2.05	0.56
2:B:54:ASN:O	2:B:143:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:PHE:CD2	2:D:403:THR:HG23	2.40	0.56
1:C:344:GLU:HG3	1:C:345:PRO:HD2	1.87	0.56
1:A:162:SER:CB	2:B:52:PRO:HD3	2.35	0.56
2:B:85:GLN:HG3	2:B:89:GLU:HB2	1.87	0.56
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.05	0.56
2:D:421:PRO:O	2:D:422:LEU:HB3	2.06	0.56
1:C:110:ASP:O	1:C:216:THR:HA	2.05	0.56
2:B:203:GLU:HA	2:B:206:ARG:HB2	1.86	0.56
1:C:236:PRO:HA	3:C:601:7N1:C0N	2.35	0.56
1:A:323:LYS:O	1:A:343:GLN:NE2	2.39	0.56
2:B:371:ALA:O	2:B:375:ILE:HG13	2.04	0.56
1:C:167:ILE:O	1:C:170:PRO:HD2	2.05	0.56
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.39	0.56
2:D:229:TRP:CH2	2:D:230:MET:HG2	2.41	0.56
1:C:233:GLU:OE2	1:C:243:PRO:HD3	2.06	0.56
1:C:236:PRO:HA	3:C:601:7N1:O0S	2.05	0.56
2:D:180:ILE:CG2	2:D:187:LEU:HD11	2.36	0.56
1:A:120:LEU:CD2	1:A:128:THR:HG21	2.37	0.55
2:D:257:ILE:O	2:D:261:VAL:HG23	2.06	0.55
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.87	0.55
2:B:85:GLN:HA	2:B:88:TRP:HB3	1.88	0.55
1:C:443:ASP:OD1	1:C:444:GLY:N	2.39	0.55
1:C:19:PRO:HG3	1:C:80:LEU:HB2	1.89	0.55
2:B:419:THR:HG22	2:B:420:PRO:O	2.06	0.55
1:C:194:GLU:HG3	1:C:197:GLN:H	1.72	0.55
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.40	0.55
1:A:426:TRP:CD1	1:A:511:ASP:HB2	2.42	0.55
1:C:252:TRP:HE3	1:C:256:ASP:HB3	1.71	0.55
1:A:35:VAL:HG22	1:A:142:ILE:HD11	1.89	0.55
2:D:10:VAL:O	2:D:11:LYS:HD2	2.07	0.55
1:A:8:VAL:O	1:A:10:VAL:HG23	2.07	0.55
1:C:253:THR:HG22	1:C:292:VAL:CG2	2.33	0.55
1:A:13:LYS:HE2	1:A:16:MET:HG2	1.88	0.54
1:C:87:PHE:CD1	2:D:53:GLU:HA	2.42	0.54
1:C:501:TYR:O	1:C:505:ILE:HG12	2.07	0.54
2:B:32:LYS:O	2:B:35:VAL:HG22	2.07	0.54
2:D:146:TYR:CG	2:D:150:PRO:HB3	2.42	0.54
1:A:200:THR:O	1:A:204:GLU:HG3	2.07	0.54
1:A:220:LYS:O	1:A:220:LYS:HG2	2.06	0.54
2:B:257:ILE:O	2:B:261:VAL:HG23	2.07	0.54
2:B:395:LYS:HE3	2:B:399:GLU:OE2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ILE:HD11	2:D:145:GLN:HB3	1.89	0.54
1:A:206:ARG:CB	1:A:217:PRO:HB3	2.37	0.54
2:B:202:ILE:HG22	2:B:206:ARG:CD	2.37	0.54
2:D:363:ASN:O	2:D:367:GLN:HG3	2.07	0.54
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.88	0.54
2:B:101:LYS:HG3	2:B:102:LYS:HD3	1.89	0.54
1:C:253:THR:CG2	1:C:292:VAL:HG22	2.33	0.54
1:C:515:SER:HB3	1:C:518:VAL:HG23	1.90	0.54
1:A:122:GLU:HA	1:A:125:ARG:CD	2.37	0.54
2:D:131:THR:HG22	2:D:143:ARG:NE	2.22	0.54
1:A:228:LEU:HD22	1:A:232:TYR:O	2.07	0.54
2:B:111:VAL:HG13	2:B:114:ALA:HB3	1.89	0.54
2:D:6:GLU:N	2:D:6:GLU:OE1	2.40	0.54
2:D:388:LYS:HD2	2:D:413:GLU:HB3	1.90	0.54
1:A:62:ALA:HA	1:A:73:LYS:N	2.23	0.54
1:C:160:PHE:HZ	1:C:185:ASP:H	1.55	0.53
1:C:474:ASN:O	1:C:478:GLU:HG3	2.07	0.53
1:A:408:ALA:O	2:B:393:ILE:HG13	2.08	0.53
1:C:178:ILE:HG23	1:C:189:VAL:HG13	1.90	0.53
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.44	0.53
1:A:16:MET:HG3	1:A:83:ARG:HA	1.90	0.53
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.43	0.53
1:C:12:LEU:HD12	1:C:124:PHE:CE2	2.43	0.53
2:D:79:GLU:OE2	2:D:83:ARG:NE	2.35	0.53
1:C:21:VAL:O	1:C:57:ASN:ND2	2.42	0.53
1:A:11:LYS:HG2	1:A:12:LEU:O	2.09	0.53
1:A:350:LYS:O	1:A:350:LYS:HG3	2.09	0.53
1:A:451:LYS:HB3	1:A:471:ASN:HA	1.90	0.53
2:B:24:TRP:HE1	2:B:61:PHE:HB3	1.74	0.53
1:A:47:ILE:HG23	1:A:145:GLN:O	2.09	0.53
1:A:371:ALA:O	1:A:375:ILE:HG13	2.09	0.53
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.44	0.52
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.91	0.52
1:C:365:VAL:HG11	1:C:401:TRP:CG	2.45	0.52
1:C:463:ARG:O	1:C:464:GLN:HG3	2.09	0.52
1:C:232:TYR:HA	1:C:242:GLN:OE1	2.09	0.52
1:A:253:THR:HA	1:A:292:VAL:HB	1.92	0.52
2:D:275:LYS:HE2	2:D:277:ARG:HD3	1.92	0.52
1:A:460:ASN:HA	2:B:286:THR:HG22	1.92	0.52
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.44	0.52
1:A:164:MET:O	1:A:168:LEU:HG	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:330:GLN:HB2	2:D:338:THR:OG1	2.09	0.52
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.92	0.52
2:D:358:ARG:HB3	2:D:366:LYS:HE3	1.92	0.52
1:A:39:THR:O	1:A:43:LYS:HG3	2.09	0.52
1:C:156:SER:HB2	1:C:157:PRO:HD3	1.91	0.52
1:C:323:LYS:O	1:C:343:GLN:NE2	2.43	0.52
1:A:391:LEU:HD12	1:A:411:ILE:HD11	1.91	0.51
2:D:239:TRP:CZ3	2:D:378:GLU:HA	2.45	0.51
1:C:253:THR:HG22	1:C:292:VAL:HG13	1.92	0.51
2:B:79:GLU:OE1	2:B:83:ARG:NH1	2.43	0.51
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.91	0.51
2:B:330:GLN:HE21	2:B:422:LEU:HD23	1.76	0.51
2:D:249:LYS:HE2	2:D:256:ASP:OD2	2.10	0.51
2:D:302:GLU:O	2:D:305:GLU:HG3	2.11	0.51
1:C:149:LEU:HD11	1:C:159:ILE:CG2	2.40	0.51
1:C:326:ILE:O	1:C:341:ILE:HA	2.11	0.51
1:A:265:ASN:O	1:A:268:SER:OG	2.22	0.51
1:A:123:ASP:O	1:A:126:LYS:HG2	2.11	0.51
2:B:32:LYS:O	2:B:36:GLU:HG3	2.11	0.51
2:D:286:THR:HG23	2:D:286:THR:O	2.11	0.51
1:C:451:LYS:HB3	1:C:471:ASN:HA	1.93	0.51
1:C:149:LEU:HD11	1:C:159:ILE:HG22	1.93	0.51
1:C:187:LEU:HD23	1:C:189:VAL:HG23	1.91	0.51
1:C:248:GLU:O	1:C:248:GLU:HG2	2.10	0.51
1:C:500:GLN:HG2	1:C:535:TRP:NE1	2.26	0.51
1:A:216:THR:N	1:A:217:PRO:HD2	2.26	0.51
1:A:324:ASP:HA	1:A:385:LYS:NZ	2.26	0.51
2:B:61:PHE:N	2:B:61:PHE:HD1	2.08	0.51
2:B:61:PHE:N	2:B:61:PHE:CD1	2.78	0.51
1:C:110:ASP:OD1	1:C:217:PRO:HD2	2.11	0.50
1:A:56:TYR:HE2	1:A:126:LYS:HB2	1.76	0.50
2:D:275:LYS:CE	2:D:277:ARG:HD3	2.41	0.50
2:D:396:GLU:OE1	2:D:396:GLU:N	2.41	0.50
1:A:523:GLU:HB3	1:A:527:LYS:HZ1	1.76	0.50
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.12	0.50
2:D:298:GLU:HG2	2:D:299:ALA:N	2.26	0.50
2:D:319:TYR:CZ	2:D:321:PRO:HA	2.47	0.50
2:D:417:VAL:O	2:D:417:VAL:HG23	2.10	0.50
1:C:254:VAL:HG23	1:C:291:GLU:O	2.11	0.50
1:C:402:TRP:HB2	1:C:409:THR:HG23	1.92	0.50
1:A:478:GLU:CD	1:A:499:SER:HB2	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TYR:CE1	2:B:157:PRO:HA	2.46	0.50
2:B:201:LYS:O	2:B:204:GLU:HB3	2.11	0.50
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.92	0.50
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.93	0.50
2:D:275:LYS:NZ	2:D:277:ARG:HH11	2.07	0.50
1:C:458:VAL:HG22	1:C:464:GLN:HG2	1.92	0.50
2:B:64:LYS:O	2:B:407:GLN:NE2	2.45	0.50
1:C:366:LYS:O	1:C:370:GLU:HG3	2.12	0.50
1:A:60:VAL:HA	1:A:75:VAL:HA	1.94	0.50
2:D:239:TRP:CH2	2:D:378:GLU:HA	2.47	0.50
1:C:58:THR:HG23	1:C:59:PRO:HD2	1.94	0.50
1:A:3:SER:OG	1:A:212:TRP:HA	2.11	0.50
2:B:93:GLY:O	2:B:94:ILE:HD13	2.12	0.50
2:D:68:SER:HB2	2:D:230:MET:CE	2.42	0.50
1:C:48:SER:OG	1:C:147:ASN:ND2	2.45	0.49
1:A:330:GLN:HE21	1:A:338:THR:HG23	1.77	0.49
1:A:407:GLN:OE1	2:B:394:GLN:HG2	2.13	0.49
2:B:332:GLN:CD	2:B:423:VAL:HG23	2.32	0.49
2:D:146:TYR:CD2	2:D:150:PRO:HB3	2.48	0.49
2:D:154:LYS:O	2:D:157:PRO:HD2	2.13	0.49
1:C:115:TYR:O	1:C:149:LEU:HB2	2.11	0.49
2:B:202:ILE:HG22	2:B:206:ARG:HD2	1.93	0.49
2:D:263:LYS:HE3	2:D:426:TRP:HA	1.93	0.49
1:C:302:GLU:O	1:C:306:ASN:ND2	2.44	0.49
1:A:229:TRP:HB2	3:A:601:7N1:CBC	2.41	0.49
1:A:459:THR:O	2:B:286:THR:HG21	2.11	0.49
1:C:5:ILE:HD11	1:C:212:TRP:O	2.13	0.49
1:C:191:SER:OG	1:C:198:HIS:ND1	2.36	0.49
1:C:410:TRP:CZ2	1:C:412:PRO:HA	2.48	0.49
1:A:391:LEU:HD11	1:A:411:ILE:HD11	1.94	0.49
2:B:206:ARG:O	2:B:210:LEU:HD13	2.12	0.49
2:D:254:VAL:HG22	2:D:293:ILE:CD1	2.42	0.49
1:C:235:HIS:HB2	1:C:238:LYS:HG2	1.94	0.49
1:C:326:ILE:CD1	1:C:388:LYS:HB2	2.42	0.49
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.48	0.49
2:D:94:ILE:HG12	2:D:161:GLN:NE2	2.28	0.49
2:D:125:ARG:O	2:D:145:GLN:HG3	2.12	0.49
1:C:417:VAL:HG22	1:C:419:THR:HG23	1.95	0.49
2:B:260:LEU:O	2:B:264:LEU:HD13	2.13	0.49
1:C:209:LEU:HB3	1:C:214:LEU:HB2	1.94	0.49
1:C:249:LYS:HG2	1:C:252:TRP:CE2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.48	0.49
1:A:406:TRP:CE3	2:B:419:THR:HB	2.48	0.48
1:A:184:MET:O	1:A:184:MET:HG3	2.13	0.48
1:A:308:GLU:O	1:A:311:LYS:HG2	2.13	0.48
2:B:326:ILE:HG12	2:B:342:TYR:O	2.13	0.48
1:A:443:ASP:OD1	1:A:444:GLY:N	2.44	0.48
2:B:200:THR:O	2:B:204:GLU:N	2.40	0.48
1:C:517:LEU:O	1:C:521:ILE:HG13	2.14	0.48
1:A:183:TYR:CE2	1:A:184:MET:HG2	2.48	0.48
1:A:390:LYS:HB3	1:A:417:VAL:HG11	1.95	0.48
1:C:486:LEU:HD23	1:C:495:ILE:HD11	1.95	0.48
1:A:101:LYS:HE3	1:A:319:TYR:CD2	2.49	0.48
2:B:24:TRP:HZ2	2:B:61:PHE:CD1	2.31	0.48
1:A:361:HIS:CE1	1:A:518:VAL:HG21	2.49	0.48
1:A:426:TRP:CE3	1:A:426:TRP:HA	2.49	0.48
2:B:163:SER:O	2:B:167:ILE:HG13	2.14	0.48
2:D:168:LEU:HD22	2:D:205:LEU:HD11	1.95	0.48
1:C:87:PHE:CE1	2:D:53:GLU:HA	2.48	0.48
1:A:478:GLU:OE1	1:A:499:SER:OG	2.22	0.48
2:B:33:ALA:O	2:B:37:ILE:HG13	2.14	0.48
2:B:170:PRO:HG2	2:B:208:HIS:NE2	2.28	0.48
1:C:180:ILE:N	1:C:180:ILE:HD12	2.28	0.47
1:C:490:GLY:O	1:C:528:LYS:HD2	2.14	0.47
1:A:279:LEU:O	1:A:283:LEU:HD23	2.14	0.47
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.14	0.47
1:A:120:LEU:HD21	1:A:128:THR:HG21	1.97	0.47
1:C:365:VAL:HG11	1:C:401:TRP:CD1	2.49	0.47
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.49	0.47
2:B:363:ASN:HB3	2:B:366:LYS:HB3	1.96	0.47
1:C:19:PRO:CB	1:C:79:GLU:HG3	2.45	0.47
1:C:171:PHE:CG	1:C:205:LEU:HD13	2.49	0.47
1:C:356:ARG:HG3	1:C:367:GLN:NE2	2.29	0.47
2:D:242:GLN:OE1	2:D:353:LYS:HE3	2.13	0.47
1:A:254:VAL:HB	1:A:289:LEU:HD12	1.96	0.47
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.45	0.47
1:A:537:PRO:HD2	1:A:542:ILE:CD1	2.45	0.47
2:D:329:ILE:HA	2:D:338:THR:O	2.15	0.47
1:C:187:LEU:CD2	1:C:189:VAL:HG23	2.44	0.47
1:C:260:LEU:O	1:C:264:LEU:HG	2.13	0.47
1:A:332:GLN:O	1:A:332:GLN:HG3	2.15	0.47
1:A:21:VAL:HG21	1:A:59:PRO:CD	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:O	1:A:118:VAL:HG23	2.14	0.47
2:B:125:ARG:O	2:B:145:GLN:HG3	2.15	0.47
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.45	0.47
2:B:170:PRO:O	2:B:174:GLN:HG3	2.14	0.47
2:D:129:ALA:HB1	2:D:143:ARG:NH2	2.29	0.47
2:D:376:THR:O	2:D:380:ILE:HG13	2.15	0.47
1:C:56:TYR:O	1:C:129:ALA:HB3	2.15	0.47
2:B:64:LYS:HG3	2:B:68:SER:O	2.15	0.47
2:B:202:ILE:HG22	2:B:206:ARG:HH11	1.78	0.47
1:C:439:THR:O	1:C:459:THR:HA	2.14	0.47
2:B:319:TYR:HA	2:B:349:LEU:HD21	1.97	0.47
2:B:332:GLN:NE2	2:B:423:VAL:HG23	2.30	0.47
1:A:220:LYS:H	1:A:220:LYS:HD2	1.79	0.47
1:C:97:PRO:HD3	1:C:232:TYR:HE1	1.81	0.46
1:A:104:LYS:CB	1:A:192:ASP:HA	2.45	0.46
1:C:77:PHE:O	1:C:81:ASN:N	2.41	0.46
1:C:153:TRP:HB3	1:C:156:SER:OG	2.15	0.46
1:C:295:LEU:HD21	1:C:300:GLU:CB	2.45	0.46
1:A:278:GLN:O	1:A:282:LEU:HD13	2.16	0.46
1:A:452:LEU:HA	1:A:470:THR:HA	1.97	0.46
2:D:203:GLU:HA	2:D:206:ARG:HD2	1.97	0.46
2:D:364:ASP:OD1	2:D:364:ASP:N	2.45	0.46
1:C:206:ARG:NE	1:C:218:ASP:HB2	2.31	0.46
1:A:544:GLY:O	1:A:548:VAL:HG12	2.15	0.46
2:D:20:LYS:HE2	2:D:56:TYR:CE1	2.50	0.46
1:A:332:GLN:O	1:A:336:GLN:HB2	2.15	0.46
2:B:17:ASP:O	2:B:83:ARG:HD3	2.16	0.46
2:B:202:ILE:C	2:B:206:ARG:HD3	2.36	0.46
2:B:264:LEU:HD23	2:B:306:ASN:HD22	1.79	0.46
2:D:115:TYR:HE2	2:D:185:ASP:HA	1.80	0.46
2:D:307:ARG:O	2:D:311:LYS:HG3	2.15	0.46
2:D:357:MET:HE3	2:D:367:GLN:HB3	1.98	0.46
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.51	0.46
2:B:20:LYS:HD3	2:B:56:TYR:HD1	1.80	0.46
2:B:84:THR:HG1	2:B:124:PHE:HZ	1.64	0.46
1:C:95:PRO:HD2	1:C:229:TRP:HH2	1.81	0.46
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.80	0.46
1:C:120:LEU:HD13	1:C:149:LEU:HD23	1.97	0.45
1:C:328:GLU:HG2	1:C:330:GLN:NE2	2.31	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.50	0.45
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:VAL:HG13	2:B:351:THR:H	1.80	0.45
2:B:267:ALA:O	2:B:271:TYR:N	2.44	0.45
2:B:296:THR:HG22	2:B:298:GLU:H	1.81	0.45
2:D:19:PRO:HG3	2:D:80:LEU:CB	2.43	0.45
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.16	0.45
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.81	0.45
1:C:332:GLN:CG	1:C:338:THR:HG23	2.46	0.45
1:C:411:ILE:HG23	1:C:412:PRO:HD2	1.98	0.45
2:D:50:ILE:HG13	2:D:145:GLN:HB2	1.96	0.45
2:D:328:GLU:HG2	2:D:390:LYS:HG3	1.97	0.45
1:C:447:ASN:ND2	1:C:450:THR:OG1	2.48	0.45
1:A:201:LYS:HD2	1:A:201:LYS:HA	1.66	0.45
2:B:11:LYS:HG3	2:B:87:PHE:CE1	2.51	0.45
2:B:342:TYR:HD2	2:B:344:GLU:O	2.00	0.45
2:D:160:PHE:O	2:D:163:SER:OG	2.27	0.45
1:C:198:HIS:O	1:C:202:ILE:HG12	2.16	0.45
1:A:21:VAL:H	1:A:57:ASN:HB3	1.81	0.45
1:A:97:PRO:HA	1:A:100:LEU:HG	1.99	0.45
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.52	0.45
1:C:498:ASP:HB2	1:C:538:ALA:HB2	1.98	0.45
1:A:13:LYS:HB2	1:A:16:MET:HG2	1.99	0.45
2:D:183:TYR:HB2	2:D:188:TYR:HE1	1.82	0.45
2:D:210:LEU:CD2	2:D:228:LEU:HD23	2.47	0.45
1:C:58:THR:CG2	1:C:59:PRO:HD2	2.47	0.45
1:A:228:LEU:HA	1:A:232:TYR:O	2.17	0.45
1:A:341:ILE:O	1:A:349:LEU:HG	2.17	0.45
2:D:323:LYS:HE3	2:D:344:GLU:OE2	2.17	0.45
1:C:111:VAL:HG22	1:C:185:ASP:O	2.17	0.45
1:C:193:LEU:HD13	1:C:198:HIS:N	2.31	0.45
1:C:197:GLN:O	1:C:201:LYS:HG2	2.17	0.45
2:B:308:GLU:O	2:B:311:LYS:HG2	2.16	0.45
2:D:23:GLN:NE2	2:D:60:VAL:O	2.48	0.45
1:C:162:SER:OG	2:D:52:PRO:HD3	2.17	0.44
2:B:22:LYS:HE2	2:B:22:LYS:HB3	1.79	0.44
1:C:88:TRP:HB2	2:D:143:ARG:HH11	1.82	0.44
1:C:435:VAL:HG22	2:D:290:THR:OG1	2.17	0.44
2:B:406:TRP:O	2:B:407:GLN:NE2	2.34	0.44
2:D:395:LYS:HG3	2:D:416:PHE:CE2	2.52	0.44
1:C:247:PRO:HD2	1:C:252:TRP:HH2	1.82	0.44
1:A:311:LYS:HG3	1:A:312:GLU:N	2.33	0.44
1:A:361:HIS:CE1	1:A:513:SER:HG	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLN:C	1:A:225:PRO:HD2	2.38	0.44
2:B:365:VAL:O	2:B:369:THR:HG23	2.17	0.44
2:D:241:VAL:HG22	2:D:350:LYS:HG3	1.99	0.44
2:D:278:GLN:OE1	2:D:298:GLU:HG3	2.17	0.44
1:A:114:ALA:HB1	1:A:160:PHE:CD1	2.53	0.44
1:A:179:VAL:O	1:A:189:VAL:HA	2.17	0.44
1:A:180:ILE:HG23	1:A:189:VAL:HG22	2.00	0.44
2:B:111:VAL:HG12	2:B:114:ALA:HB3	1.97	0.44
2:D:78:ARG:NH1	2:D:411:ILE:HG22	2.32	0.44
1:C:31:ILE:O	1:C:35:VAL:HG12	2.17	0.44
1:C:95:PRO:HA	2:D:136:ASN:OD1	2.17	0.44
1:C:328:GLU:O	1:C:339:TYR:HA	2.17	0.44
1:C:463:ARG:C	1:C:464:GLN:HG3	2.37	0.44
1:A:88:TRP:CD1	2:B:143:ARG:HD3	2.52	0.44
1:A:96:HIS:CE1	1:A:350:LYS:HD3	2.52	0.44
1:A:290:THR:HG22	1:A:291:GLU:H	1.83	0.44
2:B:326:ILE:HD11	2:B:342:TYR:CE2	2.53	0.44
2:B:254:VAL:HG23	2:B:291:GLU:O	2.18	0.44
1:C:56:TYR:O	1:C:143:ARG:NH2	2.46	0.44
1:A:390:LYS:O	1:A:391:LEU:HD23	2.18	0.44
2:D:253:THR:O	2:D:257:ILE:HG12	2.18	0.44
1:A:330:GLN:HE21	1:A:330:GLN:HB2	1.49	0.44
2:D:17:ASP:OD1	2:D:56:TYR:OH	2.24	0.44
2:D:151:GLN:HB3	2:D:185:ASP:OD2	2.18	0.44
1:C:369:THR:HA	1:C:411:ILE:HD11	2.00	0.43
1:A:447:ASN:ND2	1:A:450:THR:H	2.16	0.43
1:A:523:GLU:HB3	1:A:527:LYS:NZ	2.33	0.43
2:B:34:LEU:HD23	2:B:34:LEU:HA	1.84	0.43
2:B:331:LYS:C	2:B:332:GLN:HG2	2.38	0.43
2:D:180:ILE:N	2:D:180:ILE:HD12	2.32	0.43
1:C:5:ILE:HG12	1:C:212:TRP:HE3	1.84	0.43
1:C:150:PRO:HG2	1:C:153:TRP:HB2	2.00	0.43
1:A:146:TYR:CE2	1:A:150:PRO:HA	2.53	0.43
1:A:234:LEU:HD12	1:A:234:LEU:N	2.33	0.43
1:A:439:THR:O	1:A:459:THR:HA	2.18	0.43
1:A:118:VAL:HG11	1:A:159:ILE:HG22	2.00	0.43
1:A:349:LEU:C	1:A:349:LEU:HD12	2.39	0.43
2:B:202:ILE:HG22	2:B:206:ARG:HD3	2.00	0.43
2:D:255:ASN:HB2	2:D:289:LEU:HB3	1.99	0.43
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.84	0.43
2:B:202:ILE:O	2:B:206:ARG:HD3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:LYS:O	2:D:104:LYS:HD3	2.19	0.43
1:C:332:GLN:HG3	1:C:338:THR:HG23	2.00	0.43
1:C:451:LYS:CB	1:C:471:ASN:HA	2.49	0.43
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.34	0.43
1:C:87:PHE:HD1	2:D:52:PRO:O	2.01	0.43
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.54	0.43
1:C:209:LEU:HD12	1:C:209:LEU:HA	1.86	0.43
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.84	0.43
1:C:40:GLU:O	1:C:44:GLU:HG3	2.19	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.43
2:B:11:LYS:HE3	2:B:87:PHE:CE1	2.54	0.43
2:B:106:VAL:HG22	2:B:190:GLY:HA3	2.01	0.43
2:B:150:PRO:HG2	2:B:153:TRP:HB3	2.00	0.43
2:D:108:VAL:HG22	2:D:188:TYR:CD2	2.54	0.43
1:C:442:VAL:HG12	1:C:457:TYR:HB3	2.00	0.43
1:A:317:VAL:HG12	1:A:318:TYR:N	2.34	0.43
1:A:326:ILE:O	1:A:341:ILE:HA	2.19	0.43
2:B:78:ARG:NH2	2:B:411:ILE:HG22	2.34	0.43
1:C:232:TYR:CB	1:C:241:VAL:HA	2.37	0.42
2:B:44:GLU:HB3	2:B:46:LYS:HE3	2.00	0.42
1:C:169:GLU:HB3	1:C:170:PRO:HD3	2.01	0.42
1:C:298:GLU:H	1:C:298:GLU:CD	2.21	0.42
1:C:543:GLY:H	2:D:283:LEU:HB3	1.84	0.42
2:D:28:GLU:HG2	2:D:32:LYS:HE3	2.01	0.42
2:D:393:ILE:HD11	2:D:397:THR:CG2	2.43	0.42
1:C:11:LYS:O	1:C:85:GLN:HB3	2.18	0.42
1:C:18:GLY:HA3	1:C:56:TYR:CD1	2.54	0.42
1:C:108:VAL:HG13	1:C:188:TYR:CD1	2.55	0.42
1:C:344:GLU:CG	1:C:345:PRO:HD2	2.48	0.42
1:C:545:ASN:HA	1:C:548:VAL:HG12	2.01	0.42
1:A:219:LYS:HE3	1:A:219:LYS:HB3	1.73	0.42
1:A:399:GLU:HG3	1:A:402:TRP:HZ3	1.84	0.42
2:D:19:PRO:HG3	2:D:80:LEU:HD13	2.01	0.42
1:A:21:VAL:HG23	1:A:57:ASN:OD1	2.19	0.42
1:A:235:HIS:HB2	1:A:238:LYS:O	2.19	0.42
1:A:279:LEU:HD23	1:A:299:ALA:HB1	2.02	0.42
1:A:444:GLY:CA	1:A:552:VAL:HG11	2.50	0.42
1:A:445:ALA:HB3	1:A:552:VAL:HG12	2.02	0.42
2:B:237:ASP:OD1	2:B:237:ASP:N	2.52	0.42
1:C:8:VAL:HG11	2:D:52:PRO:HG2	2.00	0.42
1:C:46:LYS:HE2	1:C:46:LYS:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TYR:HB3	1:C:188:TYR:HE2	1.85	0.42
1:A:453:GLY:O	1:A:469:LEU:N	2.47	0.42
2:D:178:ILE:HG12	2:D:191:SER:HB3	2.02	0.42
1:A:47:ILE:HG12	1:A:146:TYR:HA	2.02	0.42
1:A:490:GLY:O	1:A:528:LYS:HD2	2.20	0.42
2:D:49:LYS:O	2:D:50:ILE:HD13	2.20	0.42
2:B:108:VAL:HA	2:B:187:LEU:O	2.20	0.42
2:B:380:ILE:O	2:B:384:GLY:N	2.52	0.42
1:C:306:ASN:O	1:C:310:LEU:HG	2.20	0.42
1:C:434:ILE:HD13	1:C:530:LYS:HB2	2.01	0.42
1:C:486:LEU:CD2	1:C:495:ILE:HD11	2.50	0.42
1:A:101:LYS:HD2	1:A:101:LYS:N	2.34	0.42
1:A:427:TYR:CE2	1:A:525:LEU:HD13	2.55	0.42
1:A:110:ASP:O	1:A:216:THR:HA	2.20	0.41
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.68	0.41
1:A:372:VAL:HG13	1:A:389:PHE:CE2	2.55	0.41
2:B:180:ILE:HG23	2:B:189:VAL:HG22	2.02	0.41
1:C:8:VAL:HG13	2:D:53:GLU:OE1	2.20	0.41
1:C:235:HIS:HB2	1:C:238:LYS:CG	2.51	0.41
1:A:486:LEU:O	1:A:528:LYS:NZ	2.50	0.41
1:C:103:LYS:HA	1:C:192:ASP:OD1	2.20	0.41
1:C:249:LYS:HG3	1:C:251:SER:O	2.20	0.41
1:C:301:LEU:O	1:C:305:GLU:HG3	2.20	0.41
1:A:362:THR:HG21	1:A:367:GLN:HE21	1.86	0.41
1:A:379:SER:CB	1:A:387:PRO:HD3	2.51	0.41
1:A:478:GLU:OE1	1:A:499:SER:CB	2.68	0.41
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.85	0.41
2:D:18:GLY:HA3	2:D:56:TYR:CE2	2.56	0.41
1:C:344:GLU:HA	1:C:344:GLU:OE1	2.21	0.41
2:D:136:ASN:HB3	2:D:138:GLU:HG3	2.03	0.41
1:C:53:GLU:CD	1:C:53:GLU:H	2.23	0.41
1:C:406:TRP:CE2	1:C:407:GLN:HG3	2.56	0.41
1:C:424:LYS:HB2	1:C:424:LYS:HE2	1.88	0.41
1:A:246:LEU:N	1:A:247:PRO:CD	2.83	0.41
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.20	0.41
2:D:254:VAL:O	2:D:258:GLN:HG3	2.21	0.41
2:D:305:GLU:O	2:D:309:ILE:HG13	2.21	0.41
1:C:325:LEU:HD21	1:C:383:TRP:CE3	2.54	0.41
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.85	0.41
1:A:108:VAL:C	1:A:109:LEU:HD23	2.41	0.41
2:B:393:ILE:HG12	2:B:394:GLN:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:HE2	1:C:46:LYS:CA	2.51	0.41
1:C:47:ILE:HG22	1:C:146:TYR:HA	2.02	0.41
1:A:492:GLU:HG2	1:A:530:LYS:HB2	2.03	0.41
2:B:11:LYS:O	2:B:87:PHE:HZ	2.03	0.41
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.55	0.41
2:B:261:VAL:HG13	2:B:276:VAL:HB	2.02	0.41
1:C:109:LEU:HB3	1:C:216:THR:HB	2.02	0.41
1:C:155:GLY:O	1:C:159:ILE:HG13	2.21	0.41
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.35	0.41
1:A:479:LEU:HD21	1:A:518:VAL:CG2	2.50	0.41
2:B:46:LYS:H	2:B:46:LYS:HG2	1.61	0.41
2:B:203:GLU:CA	2:B:206:ARG:HD3	2.51	0.41
1:C:452:LEU:HD12	1:C:452:LEU:O	2.20	0.41
1:A:502:ALA:O	1:A:506:ILE:HG13	2.21	0.41
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.51	0.41
2:B:297:GLU:O	2:B:301:LEU:HG	2.20	0.41
2:D:180:ILE:HG23	2:D:187:LEU:HD11	2.03	0.41
1:C:179:VAL:HG12	1:C:190:GLY:O	2.21	0.41
1:A:458:VAL:HG13	1:A:464:GLN:HG2	2.03	0.41
2:D:107:THR:HA	2:D:232:TYR:O	2.20	0.41
1:C:461:LYS:HE2	1:C:461:LYS:HB3	1.96	0.40
1:A:175:ASN:O	1:A:178:ILE:HD13	2.21	0.40
2:D:253:THR:HA	2:D:292:VAL:HA	2.03	0.40
1:C:87:PHE:HD1	2:D:53:GLU:HA	1.86	0.40
1:C:326:ILE:HB	1:C:342:TYR:O	2.21	0.40
1:C:532:TYR:CE2	1:C:534:ALA:HB2	2.56	0.40
2:B:122:GLU:CD	2:B:122:GLU:H	2.24	0.40
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.02	0.40
2:B:374:LYS:O	2:B:378:GLU:HG3	2.21	0.40
2:D:314:VAL:HG13	2:D:317:VAL:CG2	2.47	0.40
1:A:38:CYS:SG	1:A:142:ILE:HG21	2.62	0.40
2:B:50:ILE:HD12	2:B:54:ASN:HB3	2.03	0.40
2:D:20:LYS:HA	2:D:57:ASN:H	1.86	0.40
2:D:329:ILE:O	2:D:392:PRO:HG3	2.21	0.40
2:D:357:MET:CE	2:D:367:GLN:HB3	2.52	0.40
1:C:180:ILE:HG23	1:C:189:VAL:CG2	2.52	0.40
1:A:255:ASN:CG	1:A:289:LEU:HD22	2.42	0.40
1:A:329:ILE:CD1	1:A:375:ILE:HD12	2.48	0.40
1:C:118:VAL:CB	1:C:149:LEU:HD12	2.49	0.40
1:A:503:LEU:HD11	1:A:507:GLN:NE2	2.37	0.40
2:B:241:VAL:HG12	2:B:242:GLN:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:LEU:HD12	2:D:75:VAL:H	1.86	0.40
2:D:79:GLU:O	2:D:83:ARG:HD2	2.22	0.40
2:D:425:LEU:O	2:D:428:GLN:HB2	2.21	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	517/558 (93%)	511 (99%)	6 (1%)	0	100	100
1	C	540/558 (97%)	531 (98%)	9 (2%)	0	100	100
2	B	396/428 (92%)	388 (98%)	8 (2%)	0	100	100
2	D	401/428 (94%)	395 (98%)	6 (2%)	0	100	100
All	All	1854/1972 (94%)	1825 (98%)	29 (2%)	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	387/495 (78%)	359 (93%)	28 (7%)	14	44
1	C	412/495 (83%)	400 (97%)	12 (3%)	42	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	334/390 (86%)	323 (97%)	11 (3%)	38	72
2	D	335/390 (86%)	331 (99%)	4 (1%)	71	89
All	All	1468/1770 (83%)	1413 (96%)	55 (4%)	34	69

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	139	THR
1	C	160	PHE
1	C	161	GLN
1	C	193	LEU
1	C	194	GLU
1	C	209	LEU
1	C	229	TRP
1	C	232	TYR
1	C	233	GLU
1	C	279	LEU
1	C	286	THR
1	C	289	LEU
1	A	2	ILE
1	A	6	GLU
1	A	11	LYS
1	A	103	LYS
1	A	104	LYS
1	A	105	SER
1	A	107	THR
1	A	110	ASP
1	A	146	TYR
1	A	175	ASN
1	A	177	ASP
1	A	178	ILE
1	A	194	GLU
1	A	197	GLN
1	A	201	LYS
1	A	219	LYS
1	A	220	LYS
1	A	222	GLN
1	A	245	VAL
1	A	251	SER
1	A	290	THR
1	A	292	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	330	GLN
1	A	373	GLN
1	A	402	TRP
1	A	451	LYS
1	A	471	ASN
1	A	533	LEU
2	B	21	VAL
2	B	22	LYS
2	B	47	ILE
2	B	58	THR
2	B	61	PHE
2	B	63	ILE
2	B	79	GLU
2	B	90	VAL
2	B	308	GLU
2	B	364	ASP
2	B	414	TRP
2	D	104	LYS
2	D	242	GLN
2	D	364	ASP
2	D	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	373	GLN
2	B	348	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, 2 are monoatomic - leaving 2 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	7N1	A	601	-	35,35,35	1.60	7 (20%)	48,49,49	1.85	8 (16%)
3	7N1	C	601	-	35,35,35	1.61	7 (20%)	48,49,49	1.84	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7N1	A	601	-	-	0/12/12/12	0/4/4/4
3	7N1	C	601	-	-	0/12/12/12	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	7N1	CBA-CBC	3.85	1.53	1.44
3	A	601	7N1	CBA-CBC	3.83	1.53	1.44
3	A	601	7N1	C0O-C0N	-3.50	1.35	1.43
3	C	601	7N1	C0O-C0N	-3.49	1.35	1.43
3	C	601	7N1	C0N-N0M	-3.23	1.32	1.38
3	A	601	7N1	C0N-N0M	-3.22	1.32	1.38
3	C	601	7N1	C0P-N0H	-2.91	1.32	1.37
3	A	601	7N1	C0P-N0H	-2.90	1.32	1.37
3	C	601	7N1	O0S-C0N	-2.88	1.18	1.24
3	A	601	7N1	O0S-C0N	-2.87	1.18	1.24
3	C	601	7N1	O0B-C05	2.35	1.42	1.37
3	A	601	7N1	O0Q-C0K	-2.31	1.18	1.23
3	C	601	7N1	O0Q-C0K	-2.29	1.18	1.23
3	A	601	7N1	O0B-C05	2.24	1.42	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	7N1	N0M-C0K-N0H	5.60	119.98	114.86
3	C	601	7N1	N0M-C0K-N0H	5.53	119.92	114.86
3	A	601	7N1	C0N-N0M-C0K	-4.92	120.09	126.58
3	C	601	7N1	C0N-N0M-C0K	-4.90	120.11	126.58
3	A	601	7N1	CAK-CAL-CAM	-4.86	120.25	124.09
3	C	601	7N1	CAK-CAL-CAM	-4.58	120.47	124.09
3	C	601	7N1	C0O-C0N-N0M	3.41	119.95	114.84
3	A	601	7N1	C0O-C0N-N0M	3.39	119.92	114.84
3	A	601	7N1	O0Q-C0K-N0H	-3.19	120.05	122.85
3	C	601	7N1	O0S-C0N-C0O	-2.99	119.90	125.16
3	A	601	7N1	O0S-C0N-C0O	-2.97	119.94	125.16
3	C	601	7N1	O0Q-C0K-N0H	-2.85	120.35	122.85
3	A	601	7N1	C0O-C0P-N0H	-2.66	119.95	122.44
3	C	601	7N1	C02-C01-C00	-2.60	119.92	123.29
3	A	601	7N1	C02-C01-C00	-2.58	119.94	123.29
3	C	601	7N1	C0O-C0P-N0H	-2.53	120.07	122.44
3	C	601	7N1	CAH-CAI-CAJ	2.27	120.86	118.01

There are no chirality outliers.

There are no torsion outliers.

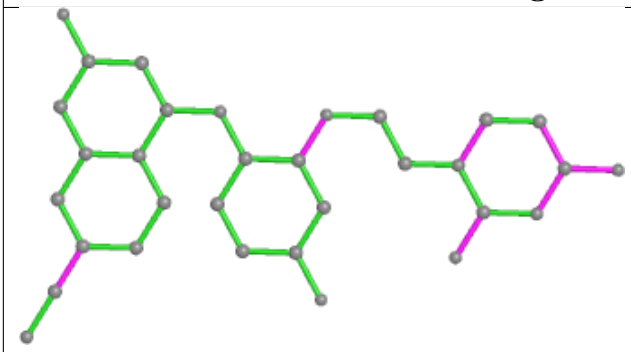
There are no ring outliers.

2 monomers are involved in 4 short contacts:

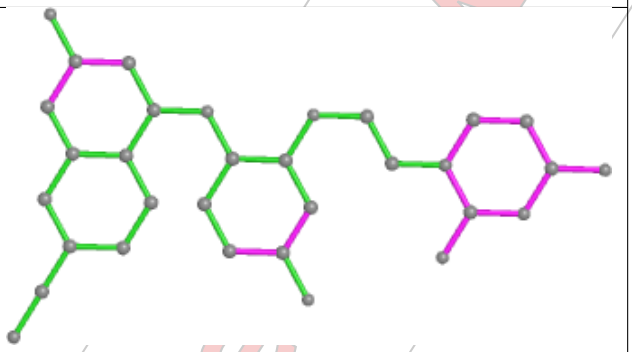
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	7N1	2	0
3	C	601	7N1	2	0

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.

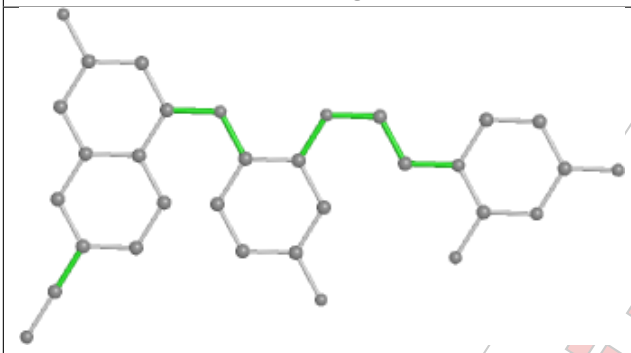
Ligand 7N1 A 601



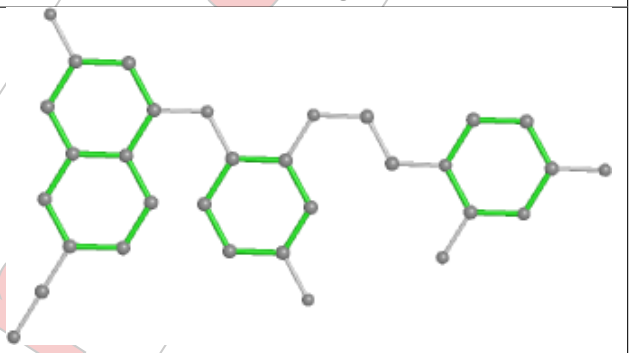
Bond lengths



Bond angles

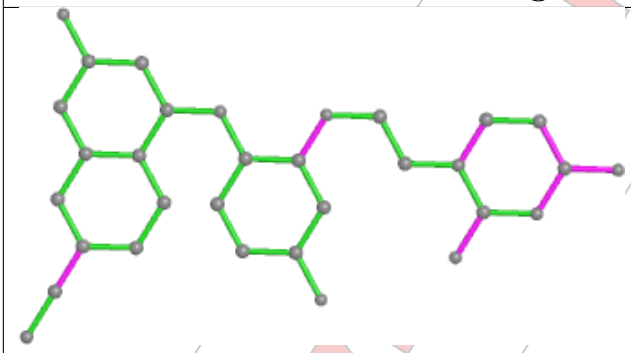


Torsions

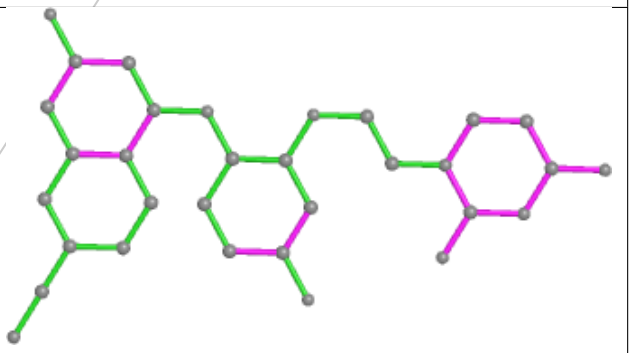


Rings

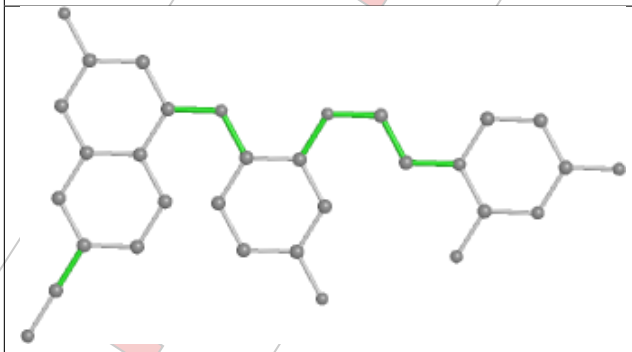
Ligand 7N1 C 601



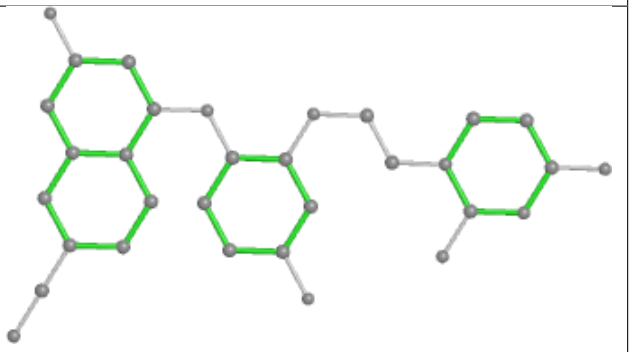
Bond lengths



Bond angles



Torsions



Rings

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	533/558 (95%)	0.01	18 (3%)	45	19	55, 123, 191, 216	0
1	C	546/558 (97%)	-0.09	14 (2%)	56	27	58, 120, 182, 239	0
2	B	402/428 (93%)	-0.13	8 (1%)	65	36	60, 108, 158, 211	7 (1%)
2	D	407/428 (95%)	-0.15	4 (0%)	82	58	53, 109, 156, 194	0
All	All	1888/1972 (95%)	-0.08	44 (2%)	60	31	53, 115, 182, 239	7 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	THR	4.4
1	A	34	LEU	4.2
1	C	146	TYR	4.1
1	A	62	ALA	3.8
2	B	242	GLN	3.6
1	A	25	PRO	3.4
1	A	309	ILE	3.3
1	C	34	LEU	3.2
2	B	5	ILE	3.2
1	C	552	VAL	3.1
1	A	142	ILE	3.1
1	C	61	PHE	3.0
1	A	282	LEU	3.0
1	A	84	THR	2.9
1	A	314	VAL	2.9
1	A	16	MET	2.8
1	C	47	ILE	2.8
1	C	60	VAL	2.7
1	C	134	SER	2.7
2	B	88	TRP	2.6
2	B	95	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	294	PRO	2.6
1	C	81	ASN	2.5
1	A	129	ALA	2.5
2	B	174	GLN	2.4
1	A	19	PRO	2.4
1	A	35	VAL	2.4
1	C	133	PRO	2.4
1	A	555	GLY	2.4
1	C	28	GLU	2.3
1	C	48	SER	2.3
2	D	242	GLN	2.3
1	C	120	LEU	2.3
2	D	266	TRP	2.2
1	A	294	PRO	2.2
1	A	145	GLN	2.2
2	B	178	ILE	2.2
1	A	88	TRP	2.2
1	A	298	GLU	2.1
2	B	315	HIS	2.1
2	D	279	LEU	2.1
2	B	409	THR	2.0
2	D	282	LEU	2.0
1	C	124	PHE	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.

Continued on next page...

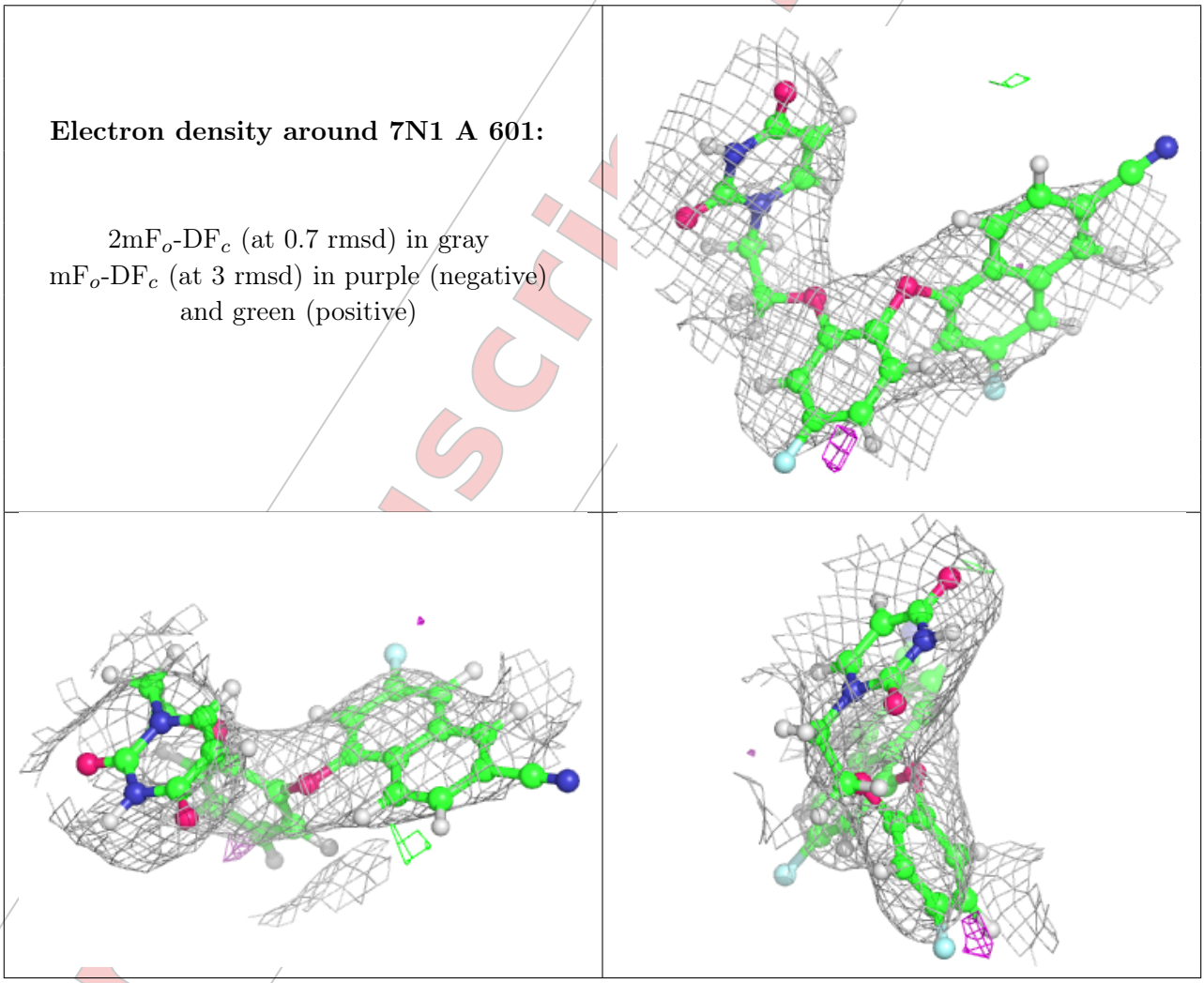
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	602	1/1	0.76	0.36	86,86,86,86	0
3	7N1	A	601	32/32	0.91	0.24	111,130,156,160	0
3	7N1	C	601	32/32	0.91	0.30	88,107,132,134	0
4	MG	C	602	1/1	0.97	0.14	87,87,87,87	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.

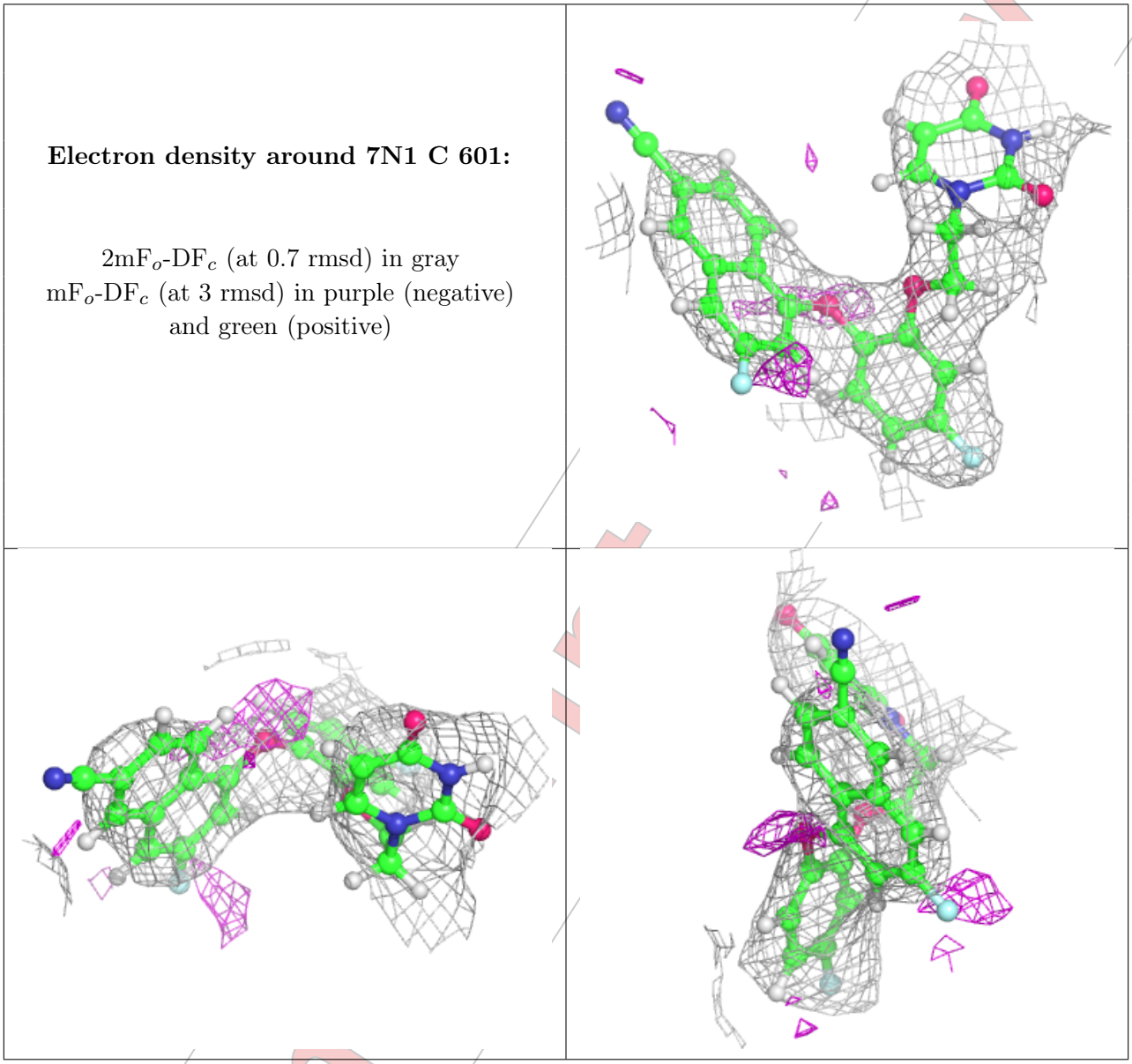
Electron density around 7N1 A 601:

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



Electron density around 7N1 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

There are no such residues in this entry.