



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:21 AM UTC

PDB ID : 3SFG / pdb_00003sfg
Title : crystal structure of murine norovirus RNA dependent RNA polymerase in complex with 2thiouridine(2TU)
Authors : Kim, K.H.; Alam, I.
Deposited on : 2011-06-13
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

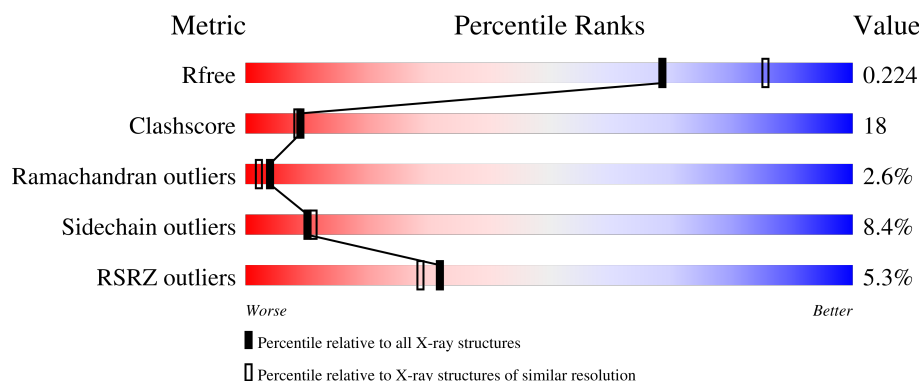
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	517	6% 64% 20% 7% 7%
1	B	517	5% 64% 23% 5% 8%
1	C	517	3% 66% 24% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2TU	C	601	-	-	X	-
3	SO4	B	607	-	-	X	-
4	GOL	A	613	-	-	X	-
4	GOL	A	615	-	-	X	-
4	GOL	B	614	-	-	X	-
4	GOL	B	616	-	-	X	-
4	GOL	C	613	-	-	X	-
4	GOL	C	617	-	-	X	-
4	GOL	C	618	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12359 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 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3826	2421	674	706	25			
1	B	474	Total	C	N	O	S	0	1	0
			3774	2390	663	696	25			
1	C	488	Total	C	N	O	S	0	0	0
			3872	2448	681	718	25			

There are 33 discrepancies between the modelled and reference sequences:

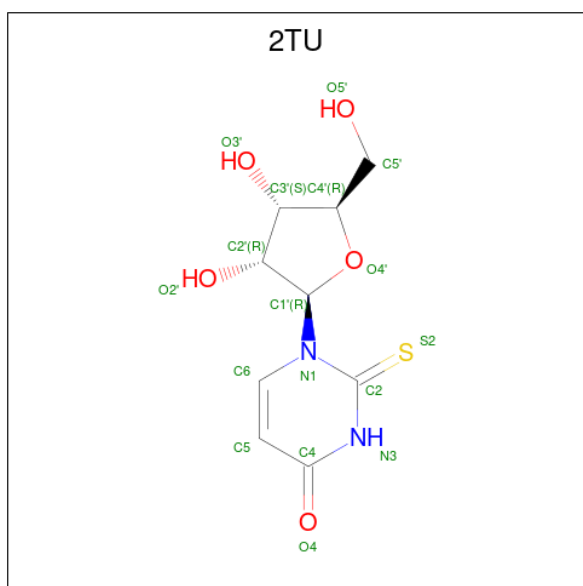
Chain	Residue	Modelled	Actual	Comment	Reference
A	510	ALA	-	expression tag	UNP Q80J95
A	511	ALA	-	expression tag	UNP Q80J95
A	512	ALA	-	expression tag	UNP Q80J95
A	513	LEU	-	expression tag	UNP Q80J95
A	514	GLU	-	expression tag	UNP Q80J95
A	515	HIS	-	expression tag	UNP Q80J95
A	516	HIS	-	expression tag	UNP Q80J95
A	517	HIS	-	expression tag	UNP Q80J95
A	518	HIS	-	expression tag	UNP Q80J95
A	519	HIS	-	expression tag	UNP Q80J95
A	520	HIS	-	expression tag	UNP Q80J95
B	510	ALA	-	expression tag	UNP Q80J95
B	511	ALA	-	expression tag	UNP Q80J95
B	512	ALA	-	expression tag	UNP Q80J95
B	513	LEU	-	expression tag	UNP Q80J95
B	514	GLU	-	expression tag	UNP Q80J95
B	515	HIS	-	expression tag	UNP Q80J95
B	516	HIS	-	expression tag	UNP Q80J95
B	517	HIS	-	expression tag	UNP Q80J95
B	518	HIS	-	expression tag	UNP Q80J95
B	519	HIS	-	expression tag	UNP Q80J95
B	520	HIS	-	expression tag	UNP Q80J95
C	510	ALA	-	expression tag	UNP Q80J95

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Chain	Residue	Modelled	Actual	Comment	Reference
C	511	ALA	-	expression tag	UNP Q80J95
C	512	ALA	-	expression tag	UNP Q80J95
C	513	LEU	-	expression tag	UNP Q80J95
C	514	GLU	-	expression tag	UNP Q80J95
C	515	HIS	-	expression tag	UNP Q80J95
C	516	HIS	-	expression tag	UNP Q80J95
C	517	HIS	-	expression tag	UNP Q80J95
C	518	HIS	-	expression tag	UNP Q80J95
C	519	HIS	-	expression tag	UNP Q80J95
C	520	HIS	-	expression tag	UNP Q80J95

- Molecule 2 is 1-(beta-D-ribofuranosyl)-2-thioxo-2,3-dihydropyrimidin-4(1H)-one (CCD ID: 2TU) (formula: C₉H₁₂N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
2	B	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
2	C	1	Total	C	N	O	S	0	0
			17	9	2	5	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	1	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	1	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

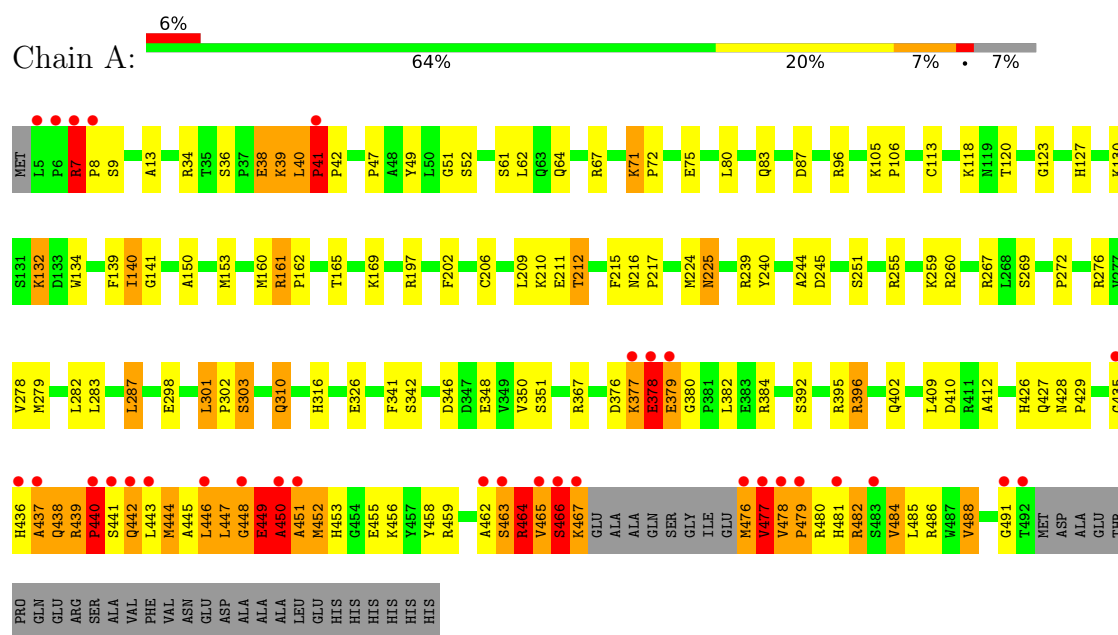
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	212	Total O 212 212	0	0
6	B	168	Total O 168 168	0	0
6	C	163	Total O 163 163	0	0

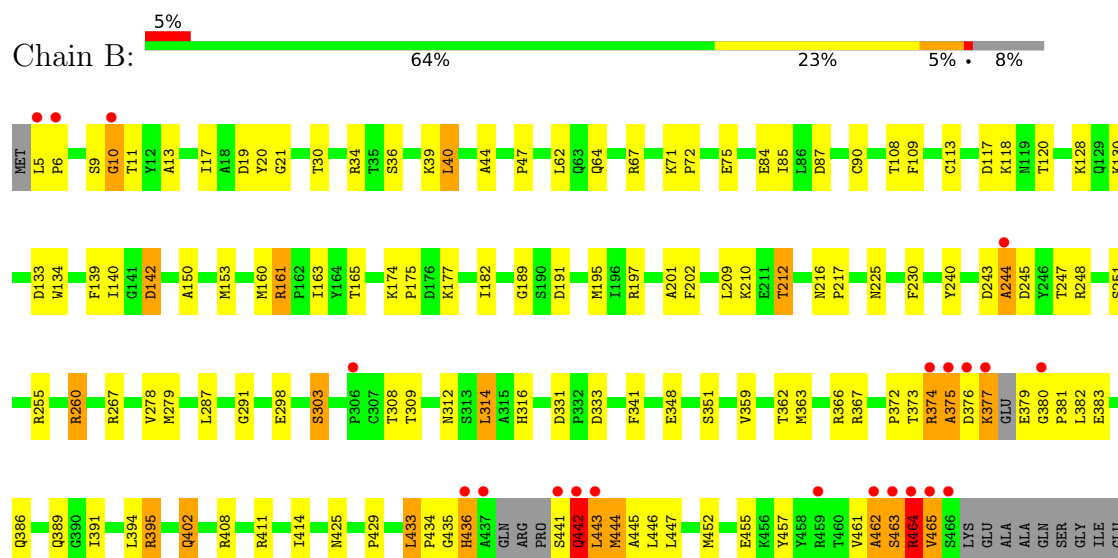
3 Residue-property plots

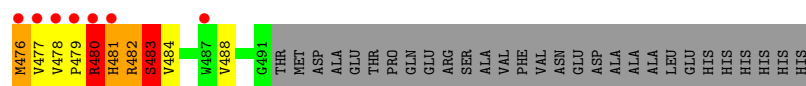
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: RNA polymerase

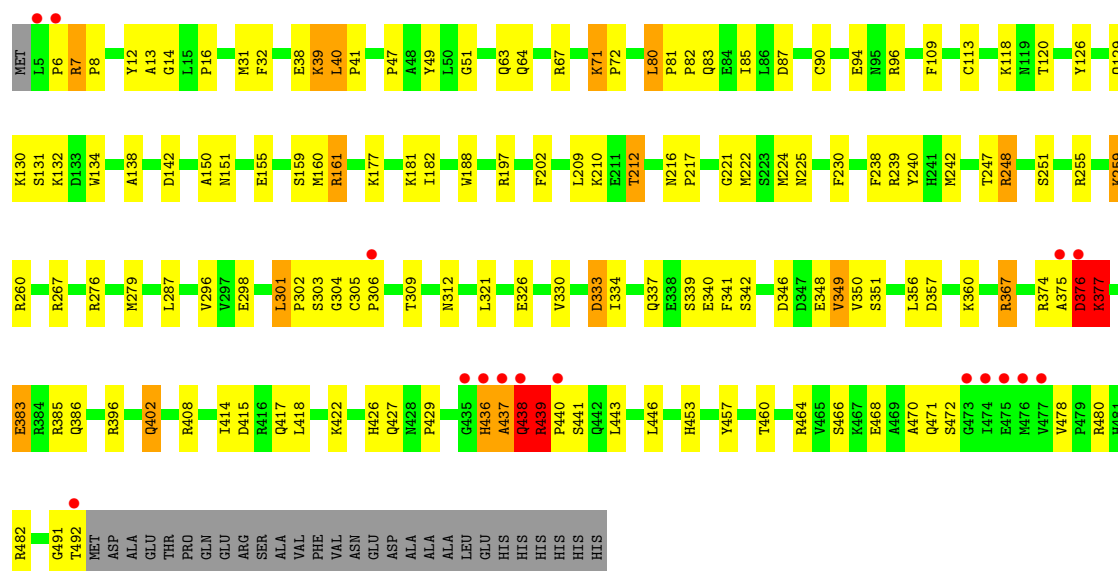


• Molecule 1: RNA polymerase





● Molecule 1: RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.79Å 195.97Å 109.33Å 90.00° 114.86° 90.00°	Depositor
Resolution (Å)	31.62 – 2.21 31.62 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.62-2.21) 98.8 (31.62-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.46	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.203 , 0.253 (Not available) , 0.224	Depositor DCC
R_{free} test set	2000 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12359	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO4, 2TU, GOL, 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	0.57	0/3921	0.90	9/5313 (0.2%)
1	B	0.51	0/3866	0.83	0/5236
1	C	0.52	0/3968	0.84	1/5378 (0.0%)
All	All	0.53	0/11755	0.86	10/15927 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	1
All	All	0	7

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	SER	N-CA-C	-8.46	99.77	112.54
1	A	484	VAL	N-CA-C	-8.43	100.79	112.50
1	A	444	MET	N-CA-C	-7.86	104.12	112.93
1	A	466	SER	N-CA-C	7.76	119.75	108.34
1	C	437	ALA	N-CA-C	-6.99	104.25	114.39
1	A	450	ALA	N-CA-C	5.81	122.19	114.12
1	A	449	GLU	N-CA-C	-5.79	98.46	110.80
1	A	447	LEU	N-CA-C	-5.61	98.85	110.80
1	A	7	ARG	N-CA-C	5.27	121.47	109.81
1	A	446	LEU	N-CA-C	-5.02	102.34	110.32

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	LEU	Peptide
1	A	41	PRO	Peptide
1	A	439	ARG	Peptide
1	A	440	PRO	Peptide
1	A	450	ALA	Peptide
1	A	465	VAL	Peptide
1	B	442	GLN	Peptide

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	3826	0	3786	175	1
1	B	3774	0	3730	142	0
1	C	3872	0	3829	112	0
2	A	17	0	12	1	0
2	B	17	0	12	3	0
2	C	17	0	12	7	0
3	A	45	0	0	4	0
3	B	40	0	0	4	0
3	C	55	0	0	1	0
4	A	72	0	96	19	1
4	B	42	0	56	20	0
4	C	36	0	48	14	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	212	0	0	15	0
6	B	168	0	0	7	0
6	C	163	0	0	3	0
All	All	12359	0	11581	431	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (431) 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:440:PRO:CB	1:A:441:SER:HB2	1.76	1.16
1:A:466:SER:CB	1:A:467:LYS:HA	1.80	1.11
1:A:39:LYS:HD3	1:A:40:LEU:H	1.06	1.10
1:A:466:SER:HB2	1:A:467:LYS:CA	1.87	1.04
1:A:466:SER:HB2	1:A:467:LYS:HA	1.07	1.03
1:A:440:PRO:HB3	1:A:441:SER:HB2	1.05	1.02
1:A:456:LYS:H	1:A:456:LYS:HD2	1.21	1.01
1:B:376:ASP:H	1:B:377:LYS:HA	1.26	1.01
1:A:448:GLY:HA2	1:A:451:ALA:HB3	1.45	0.98
1:B:376:ASP:N	1:B:377:LYS:HA	1.76	0.97
1:A:451:ALA:H	1:A:458:TYR:HD2	1.13	0.96
1:A:150:ALA:HA	1:A:160:MET:HE1	1.47	0.95
1:B:373:THR:O	1:B:374:ARG:HG2	1.67	0.94
1:C:367:ARG:HD2	6:C:703:HOH:O	1.68	0.94
1:A:153:MET:HB2	1:A:160:MET:HE2	1.49	0.94
1:C:437:ALA:HA	1:C:472:SER:HB2	1.50	0.91
1:A:440:PRO:HB3	1:A:441:SER:CB	1.98	0.90
1:A:39:LYS:HD3	1:A:40:LEU:N	1.84	0.90
1:A:378:GLU:O	1:A:380:GLY:HA3	1.73	0.89
1:A:160:MET:HE3	1:A:197:ARG:HD3	1.53	0.89
1:B:109:PHE:HB2	4:B:616:GOL:H11	1.55	0.89
1:A:13:ALA:H	4:A:613:GOL:H2	1.37	0.89
1:B:267:ARG:NH1	3:B:607:SO4:O1	2.07	0.88
1:A:448:GLY:CA	1:A:451:ALA:HB3	2.04	0.87
1:A:448:GLY:HA2	1:A:451:ALA:CB	2.05	0.87
1:A:482:ARG:HG3	1:A:482:ARG:O	1.75	0.87
1:C:267:ARG:NH1	4:C:617:GOL:H2	1.89	0.86
1:C:417:GLN:O	1:C:439:ARG:NH2	2.09	0.85
1:A:113:CYS:HG	4:A:617:GOL:HO3	1.20	0.84
1:A:438:GLN:HB2	1:A:440:PRO:O	1.79	0.82
1:C:312:ASN:HD22	2:C:601:2TU:H1'	1.45	0.82
1:C:138:ALA:HB1	4:C:613:GOL:H2	1.61	0.81
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.45	0.81
1:C:309:THR:HA	2:C:601:2TU:O2'	1.79	0.81
1:B:109:PHE:HB3	4:B:616:GOL:H32	1.62	0.81
1:B:462:ALA:HA	1:B:463:SER:C	2.05	0.79
1:A:7:ARG:HA	1:A:8:PRO:C	2.08	0.78
1:B:165:THR:HB	4:B:614:GOL:H2	1.66	0.77
1:C:32:PHE:O	1:C:426:HIS:HE1	1.68	0.77
1:C:267:ARG:HH12	4:C:617:GOL:H2	1.49	0.77
1:C:375:ALA:O	1:C:376:ASP:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PHE:H	4:B:616:GOL:H2	1.51	0.76
1:B:153:MET:HB2	1:B:160:MET:HE2	1.68	0.75
1:A:451:ALA:O	1:A:453:HIS:N	2.18	0.75
1:B:34:ARG:HD2	1:B:40:LEU:HD13	1.68	0.75
1:A:377:LYS:O	1:A:378:GLU:HB2	1.86	0.75
1:A:67:ARG:NH1	4:A:613:GOL:O2	2.20	0.74
1:B:443:LEU:C	1:B:445:ALA:H	1.94	0.74
1:C:385:ARG:NH1	3:C:604:SO4:O4	2.19	0.73
1:C:113:CYS:SG	4:C:613:GOL:H11	2.28	0.73
1:A:160:MET:CE	1:A:197:ARG:HD3	2.19	0.73
1:B:461:VAL:O	1:B:462:ALA:HB2	1.89	0.72
1:A:160:MET:HE3	1:A:197:ARG:CD	2.18	0.72
1:B:153:MET:CB	1:B:160:MET:HE2	2.19	0.72
1:B:482:ARG:HA	1:B:484:VAL:H	1.54	0.72
1:A:479:PRO:HD2	1:A:480:ARG:HA	1.72	0.72
1:A:448:GLY:O	1:A:449:GLU:HB2	1.88	0.71
1:A:62:LEU:HG	4:A:615:GOL:H31	1.71	0.71
1:A:440:PRO:CB	1:A:441:SER:CB	2.64	0.71
1:A:153:MET:CB	1:A:160:MET:HE2	2.19	0.71
1:C:90:CYS:HB3	4:C:617:GOL:O1	1.90	0.70
1:B:476:MET:SD	1:B:477:VAL:N	2.65	0.70
1:C:31:MET:HE3	1:C:422:LYS:HE2	1.73	0.69
1:A:96:ARG:HE	1:A:216:ASN:ND2	1.89	0.69
1:B:435:GLY:O	1:B:436:HIS:ND1	2.26	0.69
1:A:396:ARG:HD2	6:A:831:HOH:O	1.93	0.69
1:B:433:LEU:HD22	1:B:434:PRO:HD2	1.74	0.69
1:A:456:LYS:H	1:A:456:LYS:CD	1.97	0.69
1:C:247:THR:HG22	1:C:248:ARG:HG2	1.74	0.69
1:C:436:HIS:NE2	1:C:439:ARG:HB2	2.08	0.68
1:A:161:ARG:HD2	1:A:287:LEU:HD22	1.75	0.68
1:C:87:ASP:OD1	1:C:260:ARG:NH2	2.27	0.68
1:A:467:LYS:HB2	1:A:476:MET:HE1	1.76	0.68
1:B:443:LEU:O	1:B:445:ALA:N	2.26	0.67
1:B:476:MET:SD	1:B:478:VAL:N	2.64	0.67
1:A:479:PRO:CD	1:A:480:ARG:HA	2.25	0.67
1:B:13:ALA:HB2	1:B:67:ARG:HG2	1.76	0.67
1:B:359:VAL:HG22	1:B:381:PRO:HG3	1.77	0.67
1:A:165:THR:HG21	4:A:619:GOL:H2	1.77	0.67
1:A:150:ALA:CA	1:A:160:MET:HE1	2.24	0.67
1:B:163:ILE:HG13	1:B:287:LEU:HD23	1.75	0.67
1:A:132:LYS:HB3	1:A:132:LYS:HZ2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:HG3	1:A:378:GLU:N	2.11	0.66
1:A:440:PRO:HB2	1:A:442:GLN:N	2.11	0.66
1:A:465:VAL:HG22	1:A:466:SER:H	1.60	0.66
1:C:309:THR:HG23	2:C:601:2TU:H2'	1.77	0.66
1:C:342:SER:HB2	1:C:349:VAL:HG13	1.77	0.66
1:C:480:ARG:HG3	1:C:482:ARG:HG2	1.78	0.66
1:B:109:PHE:H	4:B:616:GOL:C2	2.09	0.65
1:C:138:ALA:CB	4:C:613:GOL:H2	2.25	0.65
1:A:96:ARG:HE	1:A:216:ASN:HD22	1.43	0.65
1:A:377:LYS:HG3	1:A:378:GLU:H	1.61	0.65
1:A:41:PRO:N	1:A:42:PRO:HD3	2.12	0.65
1:A:446:LEU:O	1:A:447:LEU:HB2	1.96	0.65
1:B:217:PRO:HB3	1:B:341:PHE:HB2	1.78	0.65
1:B:482:ARG:HA	1:B:484:VAL:N	2.12	0.65
1:C:386:GLN:HB2	4:C:616:GOL:H32	1.77	0.65
1:A:395:ARG:NH2	6:A:731:HOH:O	2.29	0.65
1:B:376:ASP:H	1:B:377:LYS:CA	2.08	0.64
1:A:41:PRO:CD	1:A:42:PRO:HD3	2.28	0.64
1:C:439:ARG:N	1:C:440:PRO:HD3	2.12	0.64
1:A:40:LEU:HB2	1:A:41:PRO:HA	1.80	0.64
1:A:376:ASP:OD2	1:A:377:LYS:N	2.30	0.64
1:B:316:HIS:CE1	1:B:348:GLU:HB3	2.33	0.64
1:A:480:ARG:NH2	6:A:894:HOH:O	2.31	0.63
1:A:455:GLU:OE1	1:A:459:ARG:NH2	2.32	0.63
1:B:209:LEU:O	1:B:212:THR:HG22	1.98	0.63
1:C:7:ARG:H	1:C:8:PRO:HD2	1.61	0.63
1:B:108:THR:HB	4:B:616:GOL:O3	1.97	0.63
1:C:160:MET:HE2	1:C:197:ARG:HD3	1.81	0.63
1:A:150:ALA:HA	1:A:160:MET:CE	2.27	0.63
1:C:94:GLU:OE2	1:C:267:ARG:NH1	2.25	0.63
1:A:113:CYS:SG	4:A:617:GOL:O3	2.43	0.62
1:B:9:SER:O	1:B:10:GLY:O	2.18	0.62
1:A:479:PRO:HD2	1:A:480:ARG:HD2	1.82	0.62
1:B:165:THR:CB	4:B:614:GOL:H2	2.30	0.61
1:B:479:PRO:O	1:B:480:ARG:HB3	1.99	0.61
1:A:34:ARG:NH2	6:A:719:HOH:O	2.33	0.61
1:A:435:GLY:O	1:A:437:ALA:N	2.33	0.61
1:B:90:CYS:HB3	3:B:607:SO4:O4	2.00	0.61
1:C:427:GLN:HB3	4:C:618:GOL:H11	1.81	0.61
1:A:239:ARG:HD3	1:A:240:TYR:CZ	2.35	0.61
1:B:150:ALA:HA	1:B:160:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:SER:HB2	6:A:726:HOH:O	2.00	0.61
1:B:463:SER:N	1:B:464:ARG:HB3	2.14	0.61
1:A:132:LYS:HB3	1:A:132:LYS:NZ	2.16	0.61
1:B:461:VAL:O	1:B:462:ALA:CB	2.49	0.61
1:B:212:THR:HG21	1:B:216:ASN:HD22	1.65	0.60
1:B:113:CYS:SG	4:B:613:GOL:H31	2.41	0.60
1:C:402:GLN:CD	1:C:402:GLN:H	2.10	0.60
1:B:375:ALA:HB1	1:B:380:GLY:HA2	1.83	0.60
1:B:386:GLN:HB2	3:B:609:SO4:O1	2.01	0.60
1:A:486:ARG:NH2	3:A:606:SO4:O4	2.30	0.60
1:B:160:MET:CE	1:B:197:ARG:HD3	2.31	0.60
1:C:383:GLU:HB2	1:C:385:ARG:NH1	2.16	0.60
1:C:376:ASP:HB3	1:C:377:LYS:HG2	1.84	0.60
1:A:439:ARG:HB2	1:A:464:ARG:HH12	1.66	0.60
1:C:427:GLN:H	4:C:618:GOL:H11	1.66	0.60
1:A:217:PRO:HB3	1:A:341:PHE:HB2	1.85	0.59
1:B:117:ASP:HB3	4:B:610:GOL:H32	1.83	0.59
1:C:415:ASP:HA	1:C:418:LEU:HD12	1.83	0.59
1:B:463:SER:CA	1:B:464:ARG:HB3	2.33	0.59
1:C:341:PHE:CE1	1:C:350:VAL:HG13	2.37	0.59
1:B:202:PHE:CZ	1:B:279:MET:HE2	2.38	0.59
1:C:333:ASP:O	1:C:337:GLN:HG3	2.02	0.58
1:A:479:PRO:CB	1:A:480:ARG:HA	2.33	0.58
1:A:396:ARG:HE	1:A:409:LEU:HD13	1.68	0.57
1:A:484:VAL:O	1:A:488:VAL:HG22	2.04	0.57
1:A:61:SER:HA	4:A:615:GOL:O3	2.04	0.57
1:A:367:ARG:HD3	6:A:714:HOH:O	2.04	0.57
1:A:426:HIS:CE1	1:A:428:ASN:O	2.58	0.57
1:A:255:ARG:HG3	1:A:298:GLU:O	2.05	0.57
1:A:447:LEU:H	1:A:450:ALA:HB3	1.70	0.56
1:B:108:THR:HB	4:B:616:GOL:H2	1.88	0.56
1:A:482:ARG:HG2	6:A:869:HOH:O	2.06	0.56
1:C:374:ARG:HE	1:C:377:LYS:HE2	1.71	0.56
1:A:206:CYS:SG	1:A:310:GLN:HG3	2.46	0.56
1:A:202:PHE:CZ	1:A:279:MET:HE2	2.40	0.56
1:B:464:ARG:HH21	1:B:465:VAL:HA	1.72	0.55
1:A:479:PRO:HB2	1:A:480:ARG:CA	2.36	0.55
1:B:19:ASP:OD1	1:B:20:TYR:N	2.39	0.55
1:A:224:MET:HE3	1:A:396:ARG:HG3	1.87	0.55
1:B:408:ARG:HG3	1:B:452:MET:HE3	1.89	0.55
1:B:463:SER:HA	1:B:464:ARG:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:N	3:A:607:SO4:O3	2.31	0.55
1:A:346:ASP:OD2	2:A:601:2TU:N3	2.35	0.55
1:A:477:VAL:HG22	1:A:478:VAL:N	2.21	0.55
1:A:479:PRO:HB2	1:A:480:ARG:HA	1.87	0.55
1:B:309:THR:HA	2:B:601:2TU:H5'A	1.89	0.55
1:A:87:ASP:OD1	1:A:260:ARG:NH2	2.39	0.54
1:A:259:LYS:NZ	6:A:885:HOH:O	2.35	0.54
1:C:80:LEU:HD12	1:C:81:PRO:HD2	1.89	0.54
1:C:217:PRO:HB3	1:C:341:PHE:HB2	1.89	0.54
1:A:47:PRO:HG2	1:A:429:PRO:HB3	1.90	0.54
1:B:402[A]:GLN:H	1:B:402[A]:GLN:CD	2.14	0.54
1:C:301:LEU:HD22	1:C:302:PRO:HD2	1.89	0.54
1:A:446:LEU:O	1:A:447:LEU:CB	2.55	0.54
1:B:243:ASP:HB3	1:B:391:ILE:HG23	1.89	0.54
1:C:49:TYR:CE2	1:C:51:GLY:HA2	2.42	0.54
1:A:463:SER:O	1:A:465:VAL:N	2.41	0.54
1:C:375:ALA:O	1:C:376:ASP:CB	2.53	0.54
1:A:482:ARG:O	1:A:482:ARG:CG	2.53	0.54
1:B:142:ASP:OD2	1:B:142:ASP:N	2.25	0.54
1:A:477:VAL:HG13	1:A:478:VAL:HG22	1.90	0.54
1:A:479:PRO:CD	1:A:480:ARG:HD2	2.39	0.53
1:B:247:THR:HG23	1:B:373:THR:HG21	1.90	0.53
1:C:342:SER:O	1:C:348:GLU:HA	2.08	0.53
1:C:312:ASN:ND2	2:C:601:2TU:H1'	2.20	0.53
1:B:44:ALA:O	1:B:175:PRO:HG3	2.09	0.53
1:A:448:GLY:CA	1:A:451:ALA:CB	2.77	0.53
1:B:443:LEU:C	1:B:445:ALA:N	2.63	0.53
1:A:212:THR:HG23	1:A:216:ASN:HB2	1.91	0.53
1:B:87:ASP:OD1	1:B:260:ARG:NH2	2.41	0.53
1:B:212:THR:CG2	1:B:216:ASN:HD22	2.22	0.52
1:C:177:LYS:O	1:C:182:ILE:HA	2.08	0.52
1:A:341:PHE:CE1	1:A:350:VAL:HG13	2.44	0.52
1:A:479:PRO:HD2	1:A:480:ARG:CD	2.39	0.52
1:A:437:ALA:HB1	1:A:438:GLN:HG2	1.91	0.52
1:B:479:PRO:O	1:B:480:ARG:CB	2.57	0.52
1:C:212:THR:HG23	1:C:216:ASN:HB2	1.92	0.52
1:B:260:ARG:NH1	3:B:607:SO4:O3	2.37	0.52
1:A:34:ARG:NH1	1:A:38:GLU:O	2.44	0.51
1:B:255:ARG:HG3	1:B:298:GLU:O	2.09	0.51
1:C:96:ARG:HE	1:C:216:ASN:ND2	2.07	0.51
1:C:150:ALA:HA	1:C:160:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PRO:HG2	1:B:429:PRO:HB3	1.93	0.51
1:C:212:THR:HG23	1:C:212:THR:O	2.10	0.51
1:B:443:LEU:HG	1:B:444:MET:H	1.76	0.51
1:A:96:ARG:NH2	1:A:215:PHE:O	2.44	0.51
1:C:470:ALA:C	1:C:472:SER:H	2.19	0.51
1:A:448:GLY:N	1:A:451:ALA:HB3	2.25	0.51
1:A:52:SER:H	4:A:615:GOL:C3	2.23	0.50
1:A:212:THR:HG23	1:A:212:THR:O	2.11	0.50
1:B:160:MET:HE3	1:B:197:ARG:HD3	1.92	0.50
1:B:362:THR:OG1	1:B:381:PRO:HB2	2.11	0.50
1:B:372:PRO:HB2	1:B:382:LEU:HD21	1.92	0.50
1:B:463:SER:HA	1:B:464:ARG:HB3	1.93	0.50
1:B:414:ILE:HG23	1:B:446:LEU:HD22	1.94	0.50
1:A:41:PRO:N	1:A:42:PRO:CD	2.75	0.50
1:A:210:LYS:C	1:A:212:THR:H	2.20	0.50
4:A:615:GOL:H12	6:A:897:HOH:O	2.10	0.50
1:C:374:ARG:HH21	1:C:377:LYS:HD3	1.77	0.49
1:A:427:GLN:H	4:A:620:GOL:H2	1.75	0.49
1:B:160:MET:HE3	1:B:197:ARG:NE	2.28	0.49
1:B:312:ASN:HD22	2:B:601:2TU:C5'	2.22	0.49
1:B:359:VAL:CG2	1:B:381:PRO:HG3	2.42	0.49
1:B:303:SER:HB2	6:B:806:HOH:O	2.13	0.49
1:A:160:MET:HE3	1:A:197:ARG:NE	2.27	0.49
1:A:13:ALA:HB2	1:A:67:ARG:HG2	1.95	0.49
1:B:71:LYS:HE2	6:B:837:HOH:O	2.12	0.49
1:B:72:PRO:HA	1:B:75:GLU:HG2	1.94	0.49
1:B:133:ASP:O	1:B:139:PHE:HA	2.12	0.49
1:B:161:ARG:HD3	6:B:732:HOH:O	2.11	0.49
1:A:41:PRO:HD2	1:A:42:PRO:HD3	1.94	0.49
1:A:209:LEU:O	1:A:212:THR:HG22	2.12	0.49
1:C:414:ILE:HG23	1:C:446:LEU:HD22	1.95	0.49
1:A:123:GLY:HA2	4:A:619:GOL:H31	1.95	0.49
1:B:436:HIS:HD1	1:B:436:HIS:C	2.21	0.49
1:B:442:GLN:CD	1:B:442:GLN:N	2.70	0.49
1:C:85:ILE:HD13	1:C:326:GLU:HG3	1.94	0.49
1:C:301:LEU:CD2	1:C:302:PRO:HD2	2.43	0.49
1:B:109:PHE:N	4:B:616:GOL:H2	2.25	0.48
1:B:462:ALA:HA	1:B:463:SER:O	2.13	0.48
1:C:374:ARG:HH21	1:C:377:LYS:CD	2.25	0.48
1:A:342:SER:O	1:A:348:GLU:HA	2.14	0.48
1:B:333:ASP:OD1	1:B:333:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PHE:HE1	1:C:350:VAL:HG13	1.78	0.48
1:C:39:LYS:HE3	1:C:39:LYS:H	1.78	0.48
1:C:40:LEU:HD12	1:C:41:PRO:HD2	1.95	0.48
1:C:126:TYR:CZ	1:C:142:ASP:HB3	2.48	0.48
1:C:357:ASP:CG	1:C:360:LYS:HG3	2.37	0.48
1:A:161:ARG:CD	1:A:287:LEU:HD22	2.43	0.48
1:B:464:ARG:NH2	1:B:465:VAL:HA	2.29	0.48
1:A:450:ALA:C	1:A:451:ALA:O	2.56	0.48
1:B:153:MET:HB2	1:B:160:MET:CE	2.40	0.48
1:C:383:GLU:HB2	1:C:385:ARG:HH12	1.77	0.48
1:A:52:SER:H	4:A:615:GOL:H32	1.79	0.48
1:A:61:SER:OG	1:A:64:GLN:HG3	2.14	0.48
1:A:105:LYS:HD2	1:A:106:PRO:HD2	1.95	0.48
1:A:478:VAL:HB	1:A:479:PRO:CA	2.44	0.48
1:B:120:THR:OG1	1:B:130:LYS:NZ	2.47	0.48
1:B:411:ARG:NH1	1:B:457:TYR:HB2	2.29	0.48
1:C:63:GLN:O	1:C:67:ARG:HG3	2.13	0.47
1:C:94:GLU:OE2	1:C:267:ARG:HD2	2.13	0.47
1:C:457:TYR:O	1:C:460:THR:HB	2.14	0.47
1:A:451:ALA:N	1:A:458:TYR:HD2	1.96	0.47
1:C:188:TRP:O	1:C:304:GLY:HA3	2.14	0.47
1:B:333:ASP:OD1	6:B:770:HOH:O	2.20	0.47
1:C:129:GLN:HG2	1:C:131:SER:OG	2.13	0.47
1:C:210:LYS:HG3	1:C:221:GLY:HA3	1.96	0.47
1:C:330:VAL:CG1	1:C:334:ILE:HB	2.44	0.47
1:C:439:ARG:N	1:C:440:PRO:CD	2.78	0.47
1:A:466:SER:CB	1:A:467:LYS:CA	2.64	0.47
1:B:212:THR:HG23	1:B:216:ASN:HB2	1.97	0.47
1:A:326:GLU:CD	1:A:367:ARG:HH22	2.23	0.47
1:C:31:MET:CE	1:C:422:LYS:HE2	2.42	0.47
1:A:239:ARG:CD	1:A:240:TYR:CZ	2.97	0.47
1:A:255:ARG:O	1:A:259:LYS:HG3	2.14	0.47
4:A:613:GOL:O2	6:A:876:HOH:O	2.20	0.47
1:C:82:PRO:HG2	1:C:85:ILE:HD12	1.97	0.47
1:C:276:ARG:HD2	6:C:744:HOH:O	2.15	0.47
1:A:448:GLY:H	1:A:451:ALA:CB	2.28	0.47
1:A:450:ALA:O	1:A:458:TYR:HA	2.15	0.47
1:A:479:PRO:HD2	1:A:480:ARG:CG	2.45	0.47
1:B:480:ARG:HA	1:B:481:HIS:HA	1.71	0.47
1:C:161:ARG:HD3	6:C:707:HOH:O	2.15	0.47
1:B:442:GLN:CD	1:B:442:GLN:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HB2	1:B:174:LYS:HE3	1.85	0.46
1:B:348:GLU:OE1	6:B:737:HOH:O	2.20	0.46
1:B:443:LEU:HD11	1:B:446:LEU:HD12	1.97	0.46
1:C:32:PHE:O	1:C:426:HIS:CE1	2.58	0.46
1:B:165:THR:CG2	4:B:614:GOL:H2	2.46	0.46
1:B:374:ARG:HA	1:B:377:LYS:HB3	1.97	0.46
1:C:478:VAL:O	1:C:478:VAL:HG12	2.16	0.46
1:A:127:HIS:CE1	6:A:706:HOH:O	2.68	0.46
1:C:120:THR:OG1	1:C:130:LYS:NZ	2.48	0.46
1:C:439:ARG:O	1:C:443:LEU:HG	2.15	0.46
1:C:47:PRO:HG2	1:C:429:PRO:HB3	1.97	0.46
1:B:312:ASN:ND2	2:B:601:2TU:O5'	2.26	0.46
1:A:13:ALA:N	4:A:613:GOL:H2	2.18	0.46
1:A:382:LEU:HD13	6:A:763:HOH:O	2.16	0.46
1:A:444:MET:HB2	1:A:447:LEU:HD12	1.98	0.46
1:B:10:GLY:HA2	1:B:17:ILE:H	1.81	0.46
1:A:120:THR:OG1	4:A:612:GOL:H2	2.16	0.46
1:A:444:MET:O	1:A:444:MET:HG3	2.16	0.46
2:C:601:2TU:S2	2:C:601:2TU:O4'	2.74	0.46
1:A:458:TYR:CE1	1:A:482:ARG:HB2	2.51	0.46
1:A:71:LYS:N	1:A:72:PRO:CD	2.79	0.46
1:C:159:SER:H	4:C:615:GOL:H2	1.80	0.46
1:C:242:MET:HE1	1:C:356:LEU:CD2	2.46	0.46
1:A:379:GLU:HA	1:A:380:GLY:O	2.16	0.45
1:A:438:GLN:HG2	1:A:438:GLN:H	1.61	0.45
1:A:448:GLY:O	1:A:449:GLU:CB	2.61	0.45
1:B:443:LEU:HD11	1:B:446:LEU:HB2	1.98	0.45
1:B:375:ALA:HB1	1:B:380:GLY:CA	2.45	0.45
1:A:384:ARG:HD2	6:A:727:HOH:O	2.16	0.45
1:B:30:THR:O	1:B:425:ASN:HA	2.16	0.45
1:B:244:ALA:O	1:B:245:ASP:CB	2.64	0.45
1:C:408:ARG:HD2	1:C:453:HIS:CD2	2.52	0.45
1:B:191:ASP:O	1:B:195:MET:HG3	2.16	0.45
1:A:139:PHE:H	4:A:617:GOL:H31	1.82	0.45
1:B:109:PHE:CB	4:B:616:GOL:H11	2.37	0.45
1:B:109:PHE:CB	4:B:616:GOL:H32	2.39	0.45
1:A:240:TYR:O	1:A:351:SER:HA	2.17	0.45
1:C:346:ASP:OD1	2:C:601:2TU:N3	2.50	0.45
1:A:72:PRO:HA	1:A:75:GLU:HG2	2.00	0.44
1:B:21:GLY:HA3	1:B:291:GLY:O	2.17	0.44
1:B:113:CYS:SG	4:B:613:GOL:C3	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LYS:HB2	1:C:72:PRO:HD3	1.97	0.44
1:C:255:ARG:O	1:C:259:LYS:HD2	2.18	0.44
1:A:72:PRO:HB2	1:A:251:SER:HB2	1.99	0.44
1:B:376:ASP:HA	6:B:850:HOH:O	2.16	0.44
1:C:260:ARG:HH12	4:C:617:GOL:H32	1.82	0.44
1:A:402[A]:GLN:CD	1:A:402[A]:GLN:H	2.26	0.44
1:B:9:SER:O	1:B:10:GLY:C	2.59	0.44
1:C:151:ASN:O	1:C:155:GLU:HG3	2.17	0.44
1:B:374:ARG:O	1:B:375:ALA:C	2.60	0.44
1:C:374:ARG:NE	1:C:377:LYS:HE2	2.33	0.44
1:A:410:ASP:OD2	1:A:412:ALA:HB3	2.17	0.44
1:B:160:MET:HE3	1:B:197:ARG:CD	2.48	0.44
1:B:244:ALA:O	1:B:245:ASP:HB3	2.18	0.44
1:B:359:VAL:O	1:B:363:MET:HG2	2.18	0.44
1:C:240:TYR:O	1:C:351:SER:HA	2.18	0.44
1:B:201:ALA:HB2	1:B:278:VAL:HG21	1.98	0.44
1:A:160:MET:O	1:A:162:PRO:HD3	2.17	0.43
1:A:278:VAL:O	1:A:282:LEU:HG	2.17	0.43
1:B:230:PHE:CD1	1:C:230:PHE:HB3	2.53	0.43
1:B:441:SER:HB3	1:B:442:GLN:CD	2.43	0.43
1:B:462:ALA:N	1:B:463:SER:OG	2.51	0.43
1:C:312:ASN:HD22	2:C:601:2TU:C1'	2.25	0.43
1:A:118:LYS:HE2	1:A:134:TRP:CD2	2.53	0.43
1:A:276:ARG:NH2	6:A:787:HOH:O	2.43	0.43
1:C:239:ARG:HH21	1:C:386:GLN:HE22	1.65	0.43
1:B:331:ASP:HB3	1:B:333:ASP:OD1	2.17	0.43
1:C:222:MET:HE2	1:C:224:MET:HA	2.00	0.43
1:C:238:PHE:HE1	1:C:340:GLU:HG2	1.84	0.43
1:A:269:SER:O	1:A:272:PRO:HD3	2.17	0.43
1:B:118:LYS:HE2	1:B:134:TRP:CE2	2.53	0.43
1:C:118:LYS:HE2	1:C:134:TRP:CE2	2.52	0.43
1:C:438:GLN:C	1:C:440:PRO:HD3	2.43	0.43
1:A:161:ARG:HG3	1:A:161:ARG:NH1	2.20	0.43
1:A:301:LEU:HD23	1:A:302:PRO:HD2	2.01	0.43
1:A:341:PHE:HE1	1:A:350:VAL:HG13	1.82	0.43
1:A:479:PRO:CB	1:A:480:ARG:CA	2.96	0.43
1:B:163:ILE:CG1	1:B:287:LEU:HD23	2.47	0.43
1:B:177:LYS:O	1:B:182:ILE:HA	2.19	0.43
1:A:34:ARG:HD2	1:A:40:LEU:HD21	2.01	0.43
1:B:481:HIS:O	1:B:484:VAL:HG12	2.19	0.43
1:C:202:PHE:CZ	1:C:279:MET:HE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:HB2	4:A:614:GOL:H11	2.00	0.43
1:A:445:ALA:O	1:A:449:GLU:HB2	2.18	0.43
1:B:84:GLU:HG3	1:B:85:ILE:N	2.34	0.43
1:B:118:LYS:HA	1:B:130:LYS:HB2	2.01	0.43
1:C:446:LEU:HD23	1:C:446:LEU:HA	1.84	0.43
1:A:244:ALA:O	1:A:245:ASP:C	2.61	0.42
1:B:189:GLY:HA3	4:B:614:GOL:O1	2.19	0.42
1:C:150:ALA:HA	1:C:160:MET:CE	2.48	0.42
1:C:402:GLN:OE1	1:C:402:GLN:N	2.39	0.42
1:A:451:ALA:HA	1:A:482:ARG:HH21	1.84	0.42
1:B:109:PHE:H	4:B:616:GOL:H11	1.85	0.42
1:C:301:LEU:HD22	1:C:302:PRO:CD	2.49	0.42
1:A:130:LYS:NZ	4:A:612:GOL:H2	2.34	0.42
1:A:140:ILE:HG23	1:A:141:GLY:N	2.32	0.42
1:B:455:GLU:HA	1:B:482:ARG:HD3	2.00	0.42
1:C:480:ARG:CG	1:C:482:ARG:HG2	2.49	0.42
1:B:212:THR:HG23	1:B:212:THR:O	2.18	0.42
1:A:211:GLU:CG	6:A:800:HOH:O	2.67	0.42
1:C:427:GLN:H	4:C:618:GOL:C1	2.32	0.42
1:A:463:SER:C	1:A:465:VAL:N	2.77	0.42
1:C:341:PHE:CD1	1:C:350:VAL:HG13	2.54	0.42
1:B:130:LYS:NZ	4:B:610:GOL:H31	2.33	0.42
1:B:240:TYR:O	1:B:351:SER:HA	2.20	0.42
1:A:225:ASN:H	4:A:614:GOL:H2	1.84	0.42
1:A:439:ARG:C	1:A:440:PRO:O	2.63	0.42
1:B:366:ARG:NH2	6:B:703:HOH:O	2.53	0.42
1:B:444:MET:SD	1:B:447:LEU:HD12	2.59	0.42
1:C:16:PRO:HG2	1:C:296:VAL:HB	2.02	0.42
1:A:448:GLY:N	1:A:451:ALA:CB	2.83	0.42
1:B:314:LEU:HD12	1:B:314:LEU:HA	1.88	0.42
1:C:439:ARG:HD3	1:C:468:GLU:OE2	2.20	0.42
1:B:248:ARG:HG2	1:B:251:SER:OG	2.20	0.41
1:B:394:LEU:O	1:B:395:ARG:HB2	2.19	0.41
1:A:465:VAL:HG22	1:A:466:SER:N	2.30	0.41
1:C:209:LEU:O	1:C:212:THR:HG22	2.20	0.41
1:A:210:LYS:HB2	1:A:210:LYS:HE3	1.76	0.41
1:A:428:ASN:HA	1:A:429:PRO:HD2	1.96	0.41
1:C:161:ARG:HD2	1:C:287:LEU:HD22	2.02	0.41
1:A:217:PRO:CB	1:A:341:PHE:HB2	2.50	0.41
1:B:374:ARG:HE	1:B:374:ARG:HB3	1.40	0.41
1:A:169:LYS:HG3	3:A:609:SO4:O4	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PHE:H	4:B:616:GOL:C1	2.33	0.41
1:B:375:ALA:O	1:B:376:ASP:CG	2.64	0.41
1:C:427:GLN:CB	4:C:618:GOL:H11	2.47	0.41
1:B:62:LEU:HB2	4:B:611:GOL:H11	2.01	0.41
1:C:13:ALA:HA	1:C:14:GLY:HA2	1.71	0.41
1:A:260:ARG:NH1	3:A:608:SO4:O2	2.53	0.41
1:A:455:GLU:HG3	1:A:482:ARG:CD	2.51	0.41
1:B:464:ARG:NE	1:B:464:ARG:C	2.79	0.41
1:B:481:HIS:C	1:B:483:SER:HB3	2.45	0.41
1:C:160:MET:CE	1:C:197:ARG:HD3	2.49	0.41
1:B:9:SER:C	1:B:10:GLY:O	2.63	0.41
1:C:248:ARG:HB2	1:C:251:SER:OG	2.20	0.41
1:A:40:LEU:CB	1:A:41:PRO:HA	2.47	0.40
1:A:49:TYR:CE2	1:A:51:GLY:HA2	2.56	0.40
1:A:316:HIS:CE1	1:A:348:GLU:HB3	2.56	0.40
1:C:109:PHE:CZ	4:C:613:GOL:H31	2.56	0.40
1:A:259:LYS:HA	1:A:283:LEU:CD1	2.50	0.40
1:A:440:PRO:HB2	1:A:441:SER:HB2	1.88	0.40
1:C:6:PRO:HA	1:C:7:ARG:HA	1.72	0.40
1:C:160:MET:HE3	1:C:197:ARG:NE	2.36	0.40
1:B:34:ARG:CD	1:B:40:LEU:HD13	2.47	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:O	4:A:613:GOL:O1[2_655]	2.12	0.08

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	477/517 (92%)	442 (93%)	20 (4%)	15 (3%)	3	1
1	B	467/517 (90%)	434 (93%)	21 (4%)	12 (3%)	4	2
1	C	486/517 (94%)	458 (94%)	18 (4%)	10 (2%)	5	3
All	All	1430/1551 (92%)	1334 (93%)	59 (4%)	37 (3%)	4	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	GLU
1	A	436	HIS
1	A	440	PRO
1	A	442	GLN
1	A	449	GLU
1	A	451	ALA
1	A	464	ARG
1	B	6	PRO
1	B	10	GLY
1	B	462	ALA
1	B	480	ARG
1	C	376	ASP
1	C	439	ARG
1	A	437	ALA
1	A	477	VAL
1	B	244	ALA
1	B	375	ALA
1	C	12	TYR
1	C	306	PRO
1	C	377	LYS
1	C	438	GLN
1	C	491	GLY
1	A	448	GLY
1	A	452	MET
1	B	464	ARG
1	C	7	ARG
1	C	436	HIS
1	C	471	GLN
1	A	41	PRO
1	A	479	PRO
1	A	491	GLY
1	B	463	SER
1	B	483	SER
1	A	462	ALA

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Mol	Chain	Res	Type
1	B	443	LEU
1	B	465	VAL
1	B	444	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/440 (94%)	377 (92%)	35 (8%)	10	11
1	B	406/440 (92%)	370 (91%)	36 (9%)	9	10
1	C	416/440 (94%)	382 (92%)	34 (8%)	10	12
All	All	1234/1320 (94%)	1129 (92%)	105 (8%)	10	11

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	36	SER
1	A	38	GLU
1	A	39	LYS
1	A	71	LYS
1	A	80	LEU
1	A	132	LYS
1	A	140	ILE
1	A	161	ARG
1	A	212	THR
1	A	225	ASN
1	A	267	ARG
1	A	287	LEU
1	A	301	LEU
1	A	303	SER
1	A	310	GLN
1	A	377	LYS
1	A	378	GLU
1	A	379	GLU

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Mol	Chain	Res	Type
1	A	392	SER
1	A	396	ARG
1	A	438	GLN
1	A	440	PRO
1	A	443	LEU
1	A	452	MET
1	A	464	ARG
1	A	466	SER
1	A	467	LYS
1	A	476	MET
1	A	477	VAL
1	A	478	VAL
1	A	481	HIS
1	A	482	ARG
1	A	485	LEU
1	A	488	VAL
1	B	5	LEU
1	B	11	THR
1	B	36	SER
1	B	39	LYS
1	B	40	LEU
1	B	64	GLN
1	B	128	LYS
1	B	140	ILE
1	B	142	ASP
1	B	161	ARG
1	B	210	LYS
1	B	212	THR
1	B	225	ASN
1	B	260	ARG
1	B	303	SER
1	B	308	THR
1	B	314	LEU
1	B	367	ARG
1	B	374	ARG
1	B	377	LYS
1	B	379	GLU
1	B	383	GLU
1	B	389	GLN
1	B	395	ARG
1	B	402[A]	GLN
1	B	402[B]	GLN

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Mol	Chain	Res	Type
1	B	433	LEU
1	B	436	HIS
1	B	442	GLN
1	B	464	ARG
1	B	476	MET
1	B	480	ARG
1	B	481	HIS
1	B	482	ARG
1	B	483	SER
1	B	488	VAL
1	C	38	GLU
1	C	39	LYS
1	C	40	LEU
1	C	64	GLN
1	C	71	LYS
1	C	80	LEU
1	C	83	GLN
1	C	132	LYS
1	C	161	ARG
1	C	181	LYS
1	C	212	THR
1	C	225	ASN
1	C	248	ARG
1	C	259	LYS
1	C	298	GLU
1	C	301	LEU
1	C	303	SER
1	C	305	CYS
1	C	321	LEU
1	C	333	ASP
1	C	339	SER
1	C	349	VAL
1	C	367	ARG
1	C	376	ASP
1	C	377	LYS
1	C	383	GLU
1	C	396	ARG
1	C	402	GLN
1	C	438	GLN
1	C	439	ARG
1	C	441	SER
1	C	464	ARG

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Mol	Chain	Res	Type
1	C	466	SER
1	C	492	THR

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

Mol	Chain	Res	Type
1	A	69	GLN
1	A	95	ASN
1	A	253	GLN
1	A	438	GLN
1	B	216	ASN
1	B	237	ASN
1	B	253	GLN
1	B	427	GLN
1	B	428	ASN
1	B	442	GLN
1	C	386	GLN
1	C	426	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 59 ligands modelled in this entry, 3 are monoatomic - leaving 56 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	GOL	B	616	-	5,5,5	0.37	0	5,5,5	0.66	0
4	GOL	C	616	-	5,5,5	0.40	0	5,5,5	0.68	0
4	GOL	A	620	-	5,5,5	0.30	0	5,5,5	0.68	0
4	GOL	A	621	-	5,5,5	0.43	0	5,5,5	0.27	0
3	SO4	A	602	-	4,4,4	0.30	0	6,6,6	0.18	0
4	GOL	B	614	-	5,5,5	0.37	0	5,5,5	0.54	0
3	SO4	A	605	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	A	604	-	4,4,4	0.33	0	6,6,6	0.09	0
4	GOL	B	615	-	5,5,5	0.37	0	5,5,5	0.69	0
4	GOL	A	618	-	5,5,5	0.37	0	5,5,5	0.27	0
3	SO4	C	610	-	4,4,4	0.35	0	6,6,6	0.15	0
3	SO4	A	609	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	C	605	-	4,4,4	0.26	0	6,6,6	0.09	0
4	GOL	C	618	-	5,5,5	0.42	0	5,5,5	0.53	0
2	2TU	A	601	-	17,18,18	1.25	1 (5%)	22,26,26	1.71	3 (13%)
3	SO4	A	607	-	4,4,4	0.31	0	6,6,6	0.16	0
3	SO4	C	602	-	4,4,4	0.31	0	6,6,6	0.07	0
4	GOL	B	610	-	5,5,5	0.48	0	5,5,5	0.42	0
3	SO4	C	604	-	4,4,4	0.28	0	6,6,6	0.18	0
4	GOL	A	617	-	5,5,5	0.42	0	5,5,5	0.27	0
3	SO4	B	608	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	B	609	-	4,4,4	0.28	0	6,6,6	0.19	0
4	GOL	A	614	-	5,5,5	0.27	0	5,5,5	0.67	0
3	SO4	A	606	-	4,4,4	0.27	0	6,6,6	0.09	0
4	GOL	A	619	-	5,5,5	0.49	0	5,5,5	0.27	0
3	SO4	C	611	-	4,4,4	0.38	0	6,6,6	0.20	0
4	GOL	A	613	-	5,5,5	0.28	0	5,5,5	0.64	0
3	SO4	C	608	-	4,4,4	0.30	0	6,6,6	0.10	0
2	2TU	B	601	-	17,18,18	1.06	2 (11%)	22,26,26	1.65	3 (13%)
4	GOL	B	611	-	5,5,5	0.49	0	5,5,5	0.76	0
3	SO4	B	606	-	4,4,4	0.30	0	6,6,6	0.12	0
4	GOL	A	612	-	5,5,5	0.42	0	5,5,5	0.37	0
4	GOL	C	617	-	5,5,5	0.38	0	5,5,5	0.22	0
3	SO4	C	609	-	4,4,4	0.25	0	6,6,6	0.20	0
2	2TU	C	601	-	17,18,18	1.30	2 (11%)	22,26,26	1.66	3 (13%)
3	SO4	B	604	-	4,4,4	0.33	0	6,6,6	0.17	0
3	SO4	B	605	-	4,4,4	0.29	0	6,6,6	0.05	0
4	GOL	A	611	-	5,5,5	0.39	0	5,5,5	0.57	0
4	GOL	B	612	-	5,5,5	0.47	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	613	-	5,5,5	0.30	0	5,5,5	0.74	0
4	GOL	C	614	-	5,5,5	0.36	0	5,5,5	0.42	0
3	SO4	A	608	-	4,4,4	0.44	0	6,6,6	0.12	0
3	SO4	C	603	-	4,4,4	0.37	0	6,6,6	0.20	0
3	SO4	B	602	-	4,4,4	0.36	0	6,6,6	0.14	0
3	SO4	C	606	-	4,4,4	0.33	0	6,6,6	0.14	0
4	GOL	A	616	-	5,5,5	0.39	0	5,5,5	0.63	0
3	SO4	B	607	-	4,4,4	0.33	0	6,6,6	0.41	0
4	GOL	A	622	-	5,5,5	0.45	0	5,5,5	0.53	0
4	GOL	C	613	-	5,5,5	0.24	0	5,5,5	0.51	0
4	GOL	A	615	-	5,5,5	0.42	0	5,5,5	1.25	1 (20%)
3	SO4	A	610	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	C	607	-	4,4,4	0.31	0	6,6,6	0.07	0
3	SO4	A	603	-	4,4,4	0.31	0	6,6,6	0.18	0
3	SO4	C	612	-	4,4,4	0.28	0	6,6,6	0.15	0
3	SO4	B	603	-	4,4,4	0.34	0	6,6,6	0.06	0
4	GOL	C	615	-	5,5,5	0.33	0	5,5,5	0.66	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	GOL	B	616	-	-	0/4/4/4	-
4	GOL	C	616	-	-	4/4/4/4	-
4	GOL	A	620	-	-	2/4/4/4	-
4	GOL	A	621	-	-	4/4/4/4	-
4	GOL	B	614	-	-	0/4/4/4	-
4	GOL	B	615	-	-	2/4/4/4	-
4	GOL	A	618	-	-	2/4/4/4	-
4	GOL	C	618	-	-	4/4/4/4	-
2	2TU	A	601	-	-	4/6/22/22	0/2/2/2
4	GOL	B	610	-	-	4/4/4/4	-
4	GOL	A	617	-	-	2/4/4/4	-
4	GOL	A	614	-	-	2/4/4/4	-
4	GOL	A	619	-	-	2/4/4/4	-
4	GOL	A	613	-	-	2/4/4/4	-
2	2TU	B	601	-	-	4/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	611	-	-	2/4/4/4	-
4	GOL	A	612	-	-	2/4/4/4	-
4	GOL	C	617	-	-	2/4/4/4	-
4	GOL	A	611	-	-	3/4/4/4	-
2	2TU	C	601	-	-	6/6/22/22	0/2/2/2
4	GOL	B	612	-	-	4/4/4/4	-
4	GOL	B	613	-	-	2/4/4/4	-
4	GOL	C	614	-	-	4/4/4/4	-
4	GOL	A	616	-	-	4/4/4/4	-
4	GOL	A	622	-	-	4/4/4/4	-
4	GOL	C	613	-	-	2/4/4/4	-
4	GOL	A	615	-	-	2/4/4/4	-
4	GOL	C	615	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	2TU	C2-S2	3.78	1.74	1.67
2	A	601	2TU	C2-S2	3.67	1.73	1.67
2	B	601	2TU	C2-S2	2.24	1.71	1.67
2	C	601	2TU	C5-C4	-2.10	1.39	1.43
2	B	601	2TU	C6-C5	2.04	1.39	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	2TU	C2-N3-C4	-5.68	120.34	127.33
2	A	601	2TU	C2-N3-C4	-5.64	120.38	127.33
2	C	601	2TU	C2-N3-C4	-5.26	120.86	127.33
2	C	601	2TU	C5-C4-N3	3.89	120.25	114.80
2	A	601	2TU	C5-C4-N3	3.81	120.14	114.80
2	B	601	2TU	C5-C4-N3	3.70	119.98	114.80
2	C	601	2TU	O4-C4-C5	-3.25	119.55	125.16
2	A	601	2TU	O4-C4-C5	-3.00	120.00	125.16
2	B	601	2TU	O4-C4-C5	-2.91	120.15	125.16
4	A	615	GOL	C3-C2-C1	-2.19	103.78	111.80

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	2TU	C2'-C1'-N1-C2
2	C	601	2TU	C2'-C1'-N1-C6
4	A	611	GOL	O1-C1-C2-C3
4	A	612	GOL	O1-C1-C2-O2
4	A	612	GOL	O1-C1-C2-C3
4	A	613	GOL	O1-C1-C2-C3
4	A	616	GOL	O1-C1-C2-C3
4	A	618	GOL	O1-C1-C2-C3
4	A	619	GOL	O1-C1-C2-C3
4	A	620	GOL	O1-C1-C2-C3
4	A	622	GOL	O1-C1-C2-C3
4	B	610	GOL	O1-C1-C2-C3
4	B	610	GOL	C1-C2-C3-O3
4	B	610	GOL	O2-C2-C3-O3
4	B	611	GOL	C1-C2-C3-O3
4	B	611	GOL	O2-C2-C3-O3
4	B	612	GOL	O1-C1-C2-C3
4	B	613	GOL	O1-C1-C2-C3
4	C	614	GOL	O1-C1-C2-O2
4	C	614	GOL	O1-C1-C2-C3
4	C	615	GOL	O1-C1-C2-O2
4	C	615	GOL	O1-C1-C2-C3
4	C	616	GOL	O1-C1-C2-O2
2	B	601	2TU	O4'-C4'-C5'-O5'
2	B	601	2TU	O4'-C1'-N1-C2
4	A	614	GOL	O1-C1-C2-O2
4	A	616	GOL	O1-C1-C2-O2
4	A	619	GOL	O1-C1-C2-O2
4	A	622	GOL	O2-C2-C3-O3
4	C	617	GOL	O2-C2-C3-O3
2	C	601	2TU	O4'-C4'-C5'-O5'
2	B	601	2TU	C3'-C4'-C5'-O5'
4	A	614	GOL	O1-C1-C2-C3
4	A	615	GOL	O1-C1-C2-C3
4	A	616	GOL	C1-C2-C3-O3
4	A	617	GOL	O1-C1-C2-C3
4	A	621	GOL	O1-C1-C2-C3
4	A	621	GOL	C1-C2-C3-O3
4	A	622	GOL	C1-C2-C3-O3
4	B	612	GOL	C1-C2-C3-O3
4	B	615	GOL	O1-C1-C2-C3
4	C	613	GOL	O1-C1-C2-C3
4	C	614	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	616	GOL	O1-C1-C2-C3
4	C	616	GOL	C1-C2-C3-O3
4	C	617	GOL	C1-C2-C3-O3
4	C	618	GOL	C1-C2-C3-O3
4	A	611	GOL	O1-C1-C2-O2
4	A	613	GOL	O1-C1-C2-O2
4	A	615	GOL	O1-C1-C2-O2
4	A	618	GOL	O1-C1-C2-O2
4	A	621	GOL	O1-C1-C2-O2
4	A	622	GOL	O1-C1-C2-O2
4	B	610	GOL	O1-C1-C2-O2
4	B	612	GOL	O1-C1-C2-O2
4	C	616	GOL	O2-C2-C3-O3
2	C	601	2TU	O4'-C1'-N1-C2
2	A	601	2TU	C2'-C1'-N1-C6
4	A	616	GOL	O2-C2-C3-O3
4	A	620	GOL	O1-C1-C2-O2
4	B	613	GOL	O1-C1-C2-O2
4	C	614	GOL	O2-C2-C3-O3
4	C	618	GOL	O2-C2-C3-O3
2	B	601	2TU	O4'-C1'-N1-C6
2	C	601	2TU	O4'-C1'-N1-C6
4	A	617	GOL	O1-C1-C2-O2
4	B	612	GOL	O2-C2-C3-O3
4	C	613	GOL	O1-C1-C2-O2
2	C	601	2TU	C3'-C4'-C5'-O5'
4	C	618	GOL	O1-C1-C2-O2
2	A	601	2TU	O4'-C1'-N1-C6
4	A	611	GOL	O2-C2-C3-O3
2	A	601	2TU	C2'-C1'-N1-C2
4	A	621	GOL	O2-C2-C3-O3
2	A	601	2TU	O4'-C1'-N1-C2
4	B	615	GOL	O1-C1-C2-O2
4	C	615	GOL	O2-C2-C3-O3
4	C	618	GOL	O1-C1-C2-C3

There are no ring outliers.

27 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	616	GOL	11	0
4	C	616	GOL	1	0

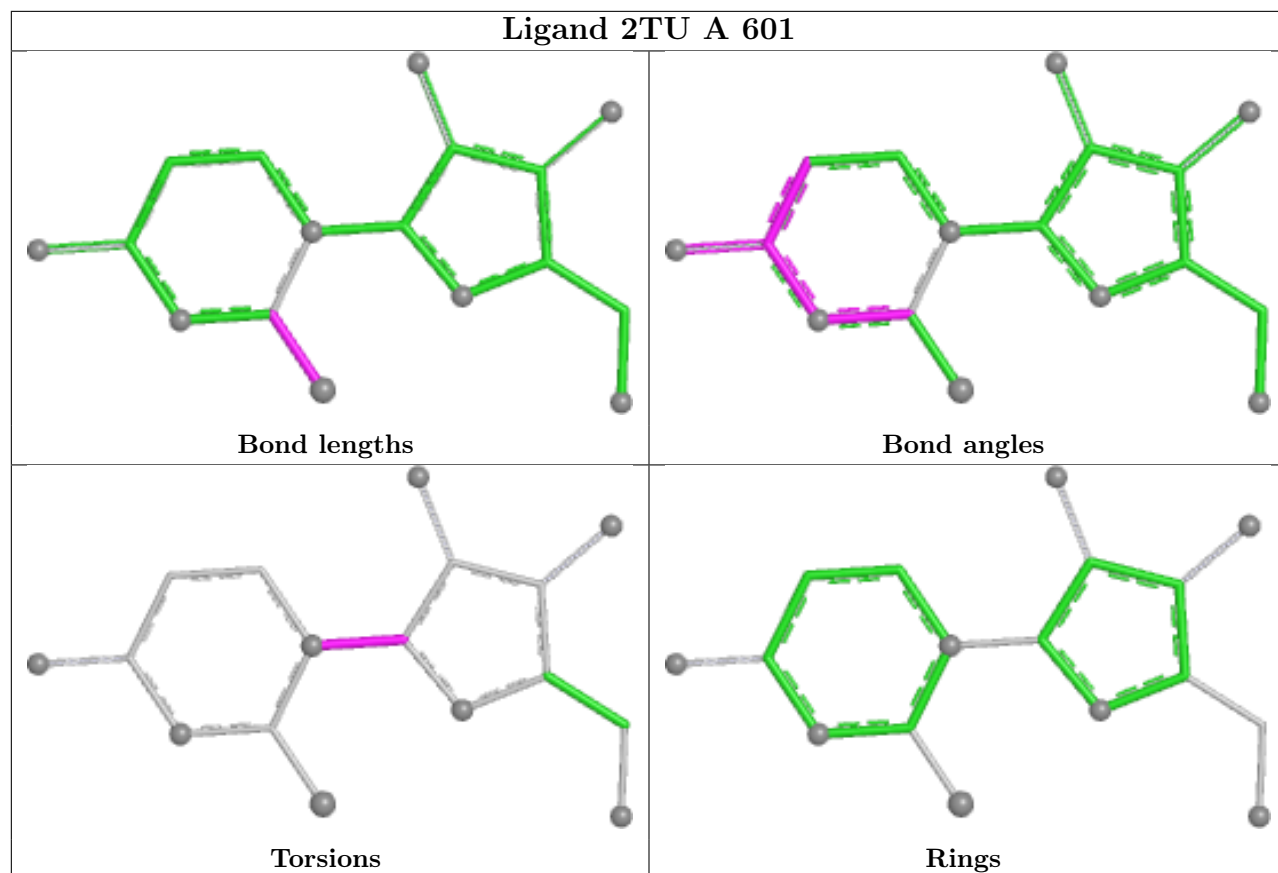
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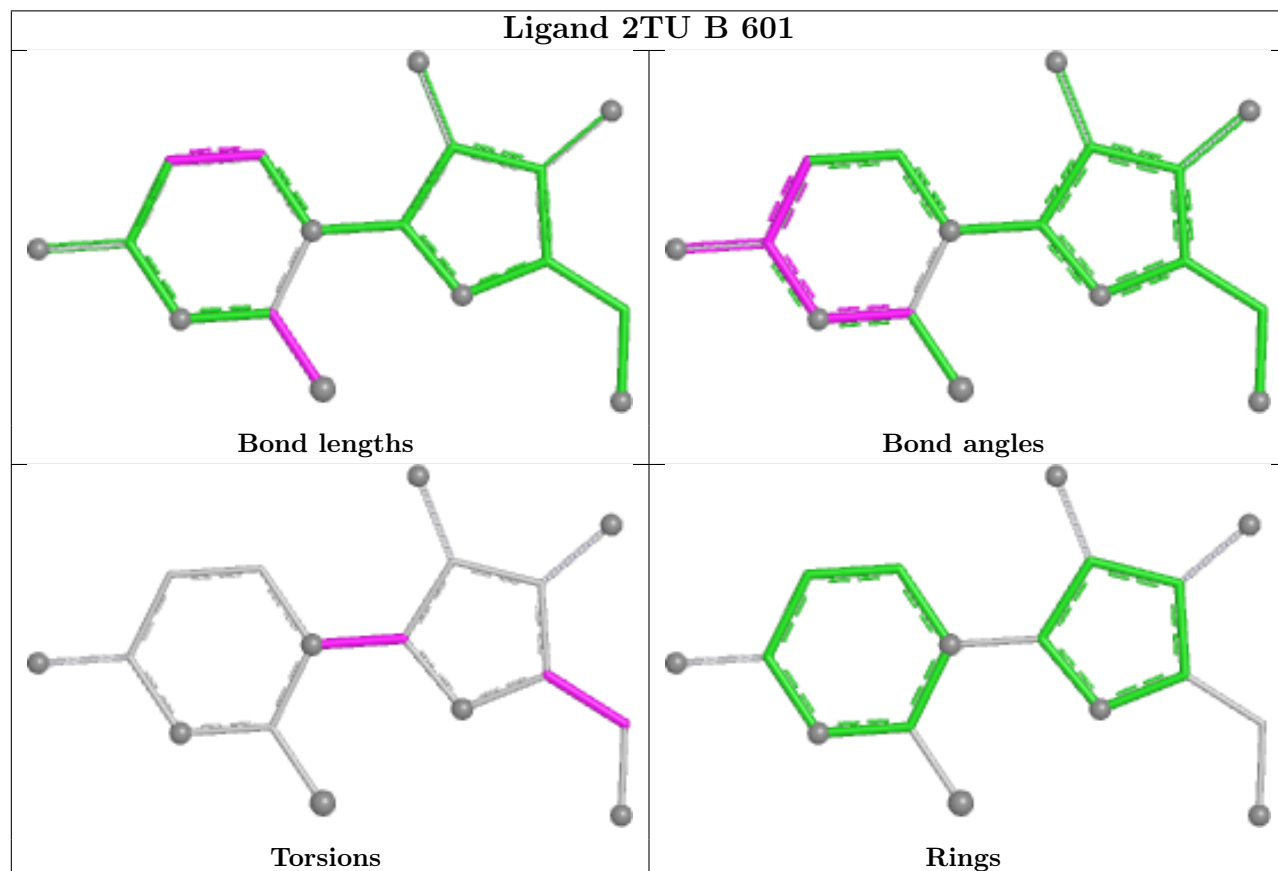
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	620	GOL	1	0
4	B	614	GOL	4	0
3	A	609	SO4	1	0
4	C	618	GOL	4	0
2	A	601	2TU	1	0
3	A	607	SO4	1	0
4	B	610	GOL	2	0
3	C	604	SO4	1	0
4	A	617	GOL	3	0
3	B	609	SO4	1	0
4	A	614	GOL	2	0
3	A	606	SO4	1	0
4	A	619	GOL	2	0
4	A	613	GOL	4	1
2	B	601	2TU	3	0
4	B	611	GOL	1	0
4	A	612	GOL	2	0
4	C	617	GOL	4	0
2	C	601	2TU	7	0
4	B	613	GOL	2	0
3	A	608	SO4	1	0
3	B	607	SO4	3	0
4	C	613	GOL	4	0
4	A	615	GOL	5	0
4	C	615	GOL	1	0

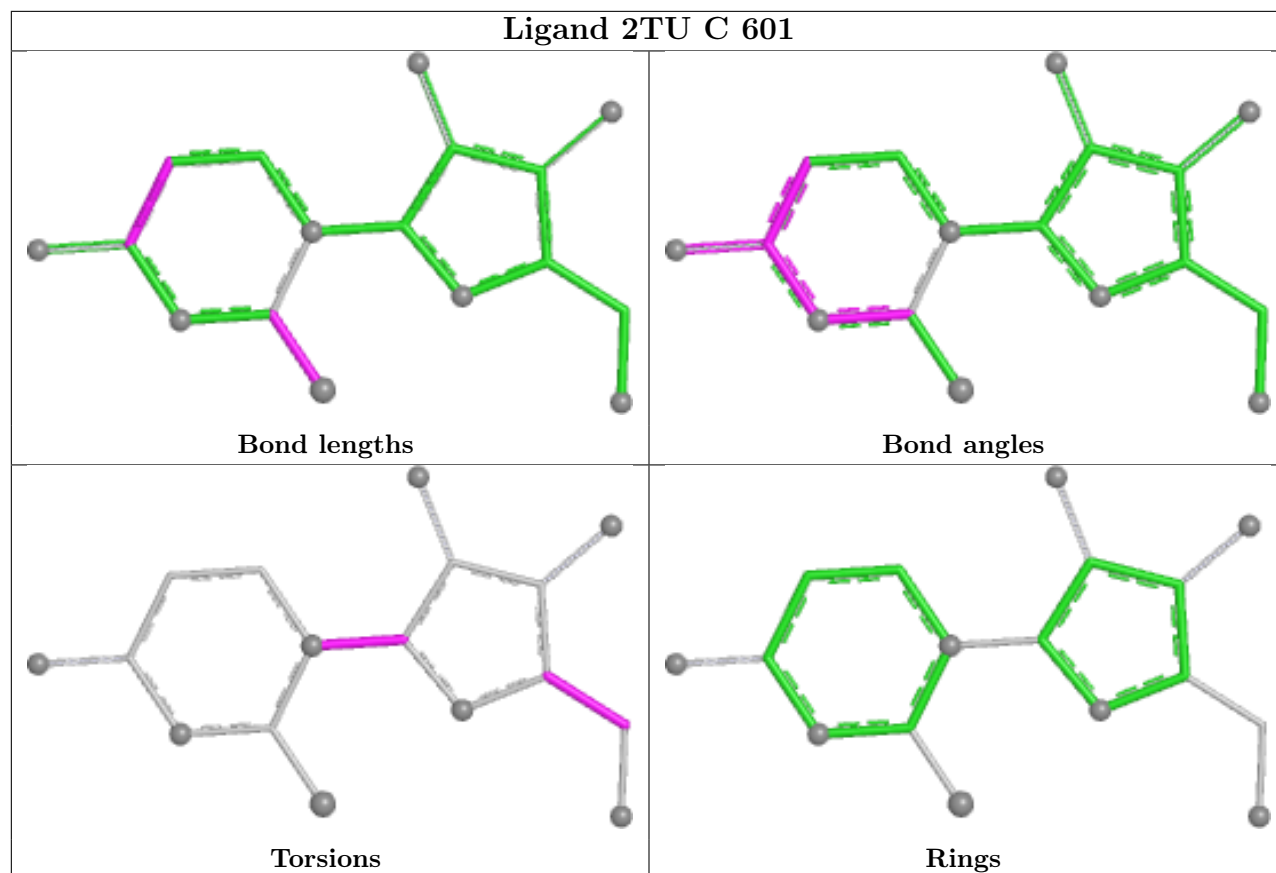
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 2TU A 601



Ligand 2TU B 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	480/517 (92%)	-0.15	32 (6%)	24 21	14, 27, 66, 107	1 (0%)
1	B	474/517 (91%)	-0.03	28 (5%)	28 25	16, 32, 66, 112	1 (0%)
1	C	488/517 (94%)	-0.10	16 (3%)	49 46	18, 32, 66, 105	0
All	All	1442/1551 (92%)	-0.09	76 (5%)	32 29	14, 31, 66, 112	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	LEU	7.3
1	C	6	PRO	7.3
1	B	437	ALA	7.2
1	B	477	VAL	6.9
1	C	375	ALA	6.7
1	A	5	LEU	6.7
1	B	466	SER	6.7
1	A	41	PRO	6.5
1	C	437	ALA	6.0
1	B	5	LEU	5.7
1	A	465	VAL	5.3
1	B	479	PRO	5.3
1	A	477	VAL	4.9
1	B	375	ALA	4.8
1	B	380	GLY	4.8
1	A	441	SER	4.7
1	C	376	ASP	4.6
1	A	450	ALA	4.6
1	A	478	VAL	4.3
1	C	474	ILE	4.3
1	A	440	PRO	4.2
1	B	465	VAL	4.2
1	B	480	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	443	LEU	4.1
1	A	492	THR	4.1
1	C	477	VAL	4.0
1	B	377	LYS	4.0
1	A	476	MET	4.0
1	A	483	SER	3.9
1	A	467	LYS	3.9
1	C	492	THR	3.9
1	B	478	VAL	3.9
1	A	479	PRO	3.8
1	A	443	LEU	3.7
1	C	473	GLY	3.7
1	C	476	MET	3.7
1	B	476	MET	3.6
1	B	441	SER	3.6
1	B	436	HIS	3.6
1	A	451	ALA	3.6
1	C	438	GLN	3.6
1	A	437	ALA	3.6
1	A	436	HIS	3.5
1	B	10	GLY	3.5
1	B	376	ASP	3.3
1	B	481	HIS	3.3
1	A	6	PRO	3.3
1	B	6	PRO	3.3
1	A	466	SER	3.2
1	A	463	SER	3.2
1	A	7	ARG	3.2
1	C	435	GLY	3.2
1	A	448	GLY	3.0
1	B	462	ALA	3.0
1	C	436	HIS	2.8
1	C	306	PRO	2.8
1	A	378	GLU	2.7
1	C	475	GLU	2.7
1	A	481	HIS	2.6
1	A	462	ALA	2.6
1	B	463	SER	2.5
1	B	244	ALA	2.5
1	C	440	PRO	2.5
1	A	435	GLY	2.5
1	A	8	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLU	2.4
1	A	442	GLN	2.4
1	A	377	LYS	2.3
1	B	464	ARG	2.3
1	B	306	PRO	2.2
1	A	446	LEU	2.2
1	B	442	GLN	2.2
1	B	487	TRP	2.1
1	B	374	ARG	2.1
1	B	459	ARG	2.1
1	A	491	GLY	2.1

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 oligosaccharides 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, 95th 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	SO4	C	608	5/5	0.63	0.15	61,76,86,89	0
3	SO4	C	607	5/5	0.66	0.12	73,74,80,97	0
3	SO4	A	606	5/5	0.70	0.11	76,85,95,100	0
2	2TU	A	601	17/17	0.77	0.20	27,38,42,43	17
3	SO4	C	605	5/5	0.78	0.11	74,74,92,93	0
2	2TU	C	601	17/17	0.79	0.22	28,34,41,46	17
4	GOL	A	620	6/6	0.79	0.18	38,42,54,60	0
4	GOL	A	622	6/6	0.79	0.15	48,51,56,57	0
4	GOL	C	614	6/6	0.79	0.15	42,46,47,53	0
4	GOL	C	616	6/6	0.79	0.17	49,57,59,67	0
4	GOL	C	617	6/6	0.79	0.14	38,47,53,56	0
3	SO4	A	608	5/5	0.81	0.23	46,52,59,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2TU	B	601	17/17	0.81	0.21	33,42,47,47	17
4	GOL	B	613	6/6	0.81	0.15	37,39,40,42	1
4	GOL	B	610	6/6	0.83	0.17	44,48,51,53	0
3	SO4	A	607	5/5	0.84	0.19	55,59,72,74	0
3	SO4	C	610	5/5	0.84	0.27	37,52,74,77	0
3	SO4	B	607	5/5	0.84	0.18	43,43,56,71	0
3	SO4	B	609	5/5	0.86	0.10	61,67,86,87	0
4	GOL	B	614	6/6	0.86	0.25	28,35,42,43	0
4	GOL	B	615	6/6	0.86	0.15	39,41,45,46	0
3	SO4	B	604	5/5	0.86	0.27	48,59,82,90	0
3	SO4	B	606	5/5	0.86	0.21	61,63,71,81	0
3	SO4	B	603	5/5	0.86	0.17	55,65,82,87	0
4	GOL	A	616	6/6	0.87	0.16	36,47,56,58	0
3	SO4	C	611	5/5	0.87	0.26	43,51,62,80	0
3	SO4	C	606	5/5	0.88	0.15	52,59,69,71	0
3	SO4	A	602	5/5	0.88	0.15	45,53,61,74	0
3	SO4	A	609	5/5	0.88	0.30	34,50,66,70	0
4	GOL	C	615	6/6	0.88	0.12	36,40,49,51	0
4	GOL	B	612	6/6	0.88	0.15	36,47,51,54	0
4	GOL	A	619	6/6	0.88	0.19	29,35,45,50	0
4	GOL	A	613	6/6	0.89	0.17	41,46,51,53	0
4	GOL	A	615	6/6	0.89	0.17	23,38,47,50	0
4	GOL	A	612	6/6	0.89	0.14	29,35,40,42	0
4	GOL	C	618	6/6	0.89	0.13	42,48,53,54	0
4	GOL	B	616	6/6	0.90	0.19	33,37,40,48	0
4	GOL	A	621	6/6	0.90	0.12	40,43,48,50	0
3	SO4	C	604	5/5	0.91	0.14	55,56,61,68	0
3	SO4	C	612	5/5	0.91	0.19	56,59,72,74	0
4	GOL	A	617	6/6	0.91	0.11	34,39,40,47	0
4	GOL	A	611	6/6	0.91	0.10	34,37,45,47	0
3	SO4	A	610	5/5	0.91	0.17	57,61,72,73	0
3	SO4	C	602	5/5	0.91	0.18	47,52,67,78	0
3	SO4	B	608	5/5	0.92	0.19	55,56,76,78	0
4	GOL	A	614	6/6	0.92	0.09	40,44,47,55	0
3	SO4	B	602	5/5	0.93	0.17	42,47,60,66	0
3	SO4	A	605	5/5	0.93	0.11	61,61,71,73	0
4	GOL	C	613	6/6	0.93	0.14	34,39,45,47	0
4	GOL	B	611	6/6	0.93	0.13	25,42,43,51	0
4	GOL	A	618	6/6	0.94	0.09	28,32,33,33	1
3	SO4	B	605	5/5	0.94	0.14	56,57,71,72	0
3	SO4	C	609	5/5	0.94	0.20	39,47,54,62	0
5	MG	B	617	1/1	0.94	0.22	49,49,49,49	0

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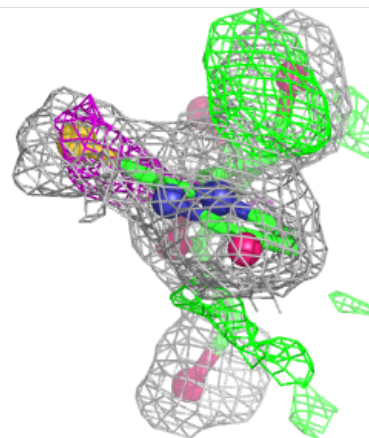
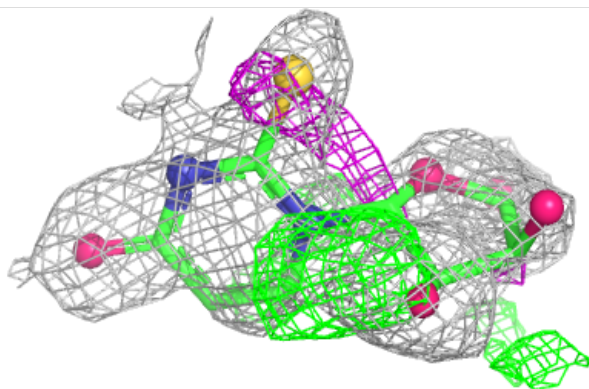
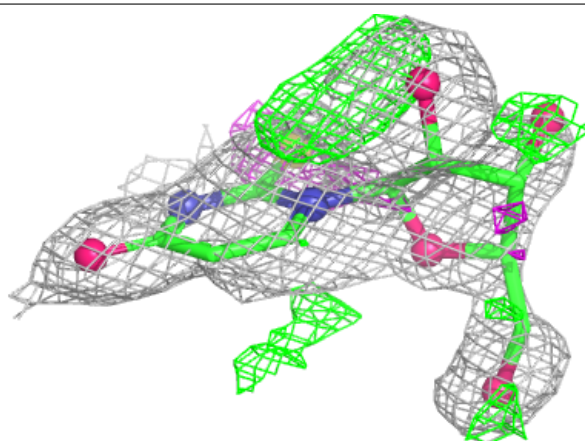
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	604	5/5	0.95	0.15	46,46,62,62	0
3	SO4	C	603	5/5	0.96	0.12	37,38,56,63	0
3	SO4	A	603	5/5	0.96	0.11	43,44,57,59	0
5	MG	A	623	1/1	0.98	0.07	29,29,29,29	0
5	MG	C	619	1/1	0.99	0.10	32,32,32,32	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.

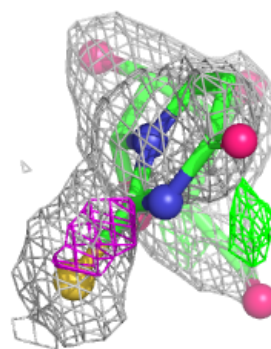
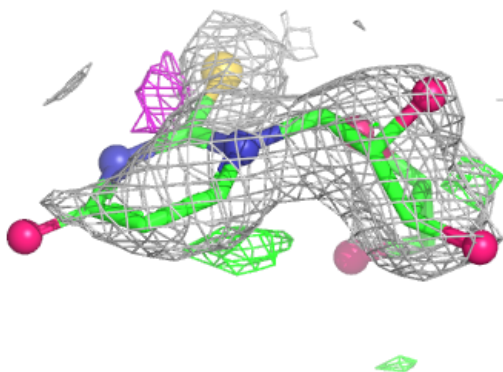
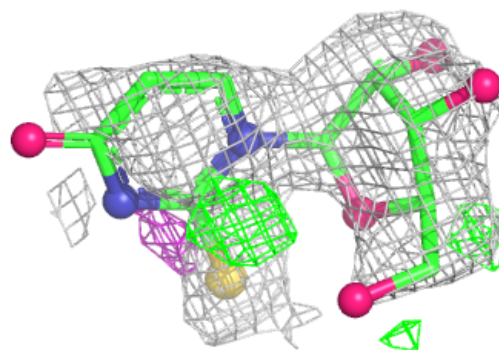
Electron density around 2TU A 601:

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

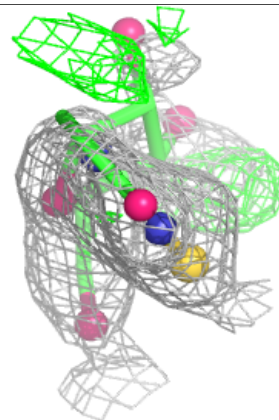
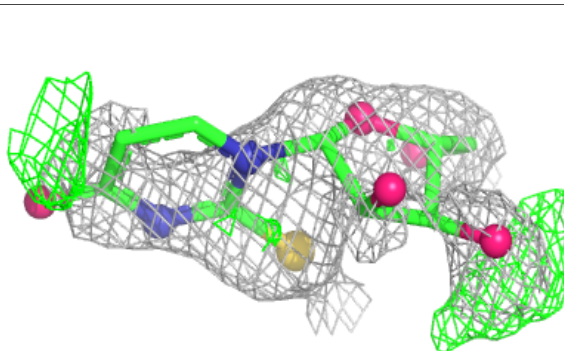
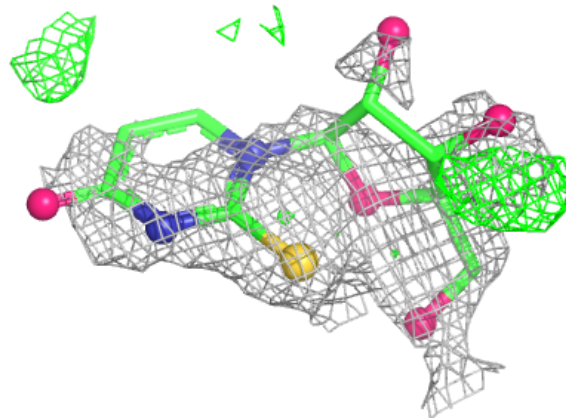


Electron density around 2TU C 601:

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

**Electron density around 2TU B 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.