



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:55 PM GMT

PDB ID : 3SFG
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

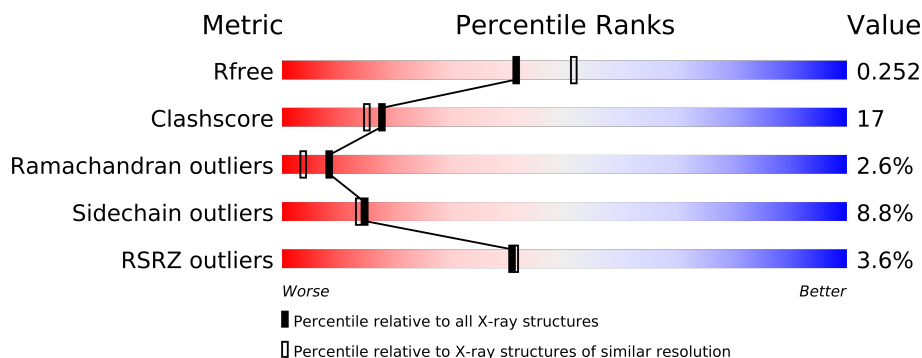
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	517	
1	B	517	
1	C	517	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	2TU	A	601	-	X
2	2TU	B	601	-	X
2	2TU	C	601	-	X
3	SO4	A	603	-	X
3	SO4	A	604	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	607	-	X
3	SO4	A	608	-	X
3	SO4	A	609	-	X
3	SO4	A	610	-	X
3	SO4	B	602	-	X
3	SO4	B	603	-	X
3	SO4	B	604	-	X
3	SO4	B	605	-	X
3	SO4	B	606	-	X
3	SO4	B	607	-	X
3	SO4	B	608	-	X
3	SO4	B	609	-	X
3	SO4	C	602	-	X
3	SO4	C	603	-	X
3	SO4	C	607	-	X
3	SO4	C	608	-	X
3	SO4	C	610	-	X
3	SO4	C	611	-	X
3	SO4	C	612	-	X
4	GOL	A	611	-	X
4	GOL	A	612	-	X
4	GOL	A	615	-	X
4	GOL	A	616	-	X
4	GOL	A	619	-	X
4	GOL	A	620	-	X
4	GOL	B	610	-	X
4	GOL	B	611	-	X
4	GOL	B	612	-	X
4	GOL	B	614	-	X
4	GOL	B	616	-	X
4	GOL	C	614	-	X
4	GOL	C	615	-	X
4	GOL	C	616	-	X
4	GOL	C	617	-	X
4	GOL	C	618	-	X
5	MG	B	617	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12359 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

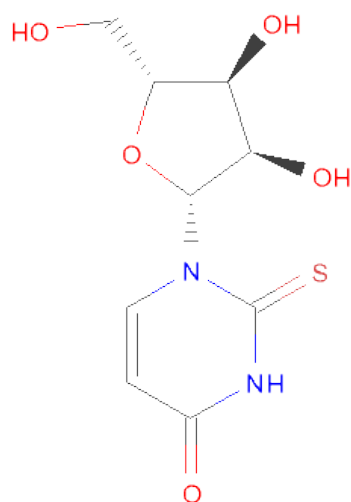
Chain	Residue	Modelled	Actual	Comment	Reference
A	510	ALA	-	EXPRESSION TAG	UNP Q80J95
A	511	ALA	-	EXPRESSION TAG	UNP Q80J95
A	512	ALA	-	EXPRESSION TAG	UNP Q80J95
A	513	LEU	-	EXPRESSION TAG	UNP Q80J95
A	514	GLU	-	EXPRESSION TAG	UNP Q80J95
A	515	HIS	-	EXPRESSION TAG	UNP Q80J95
A	516	HIS	-	EXPRESSION TAG	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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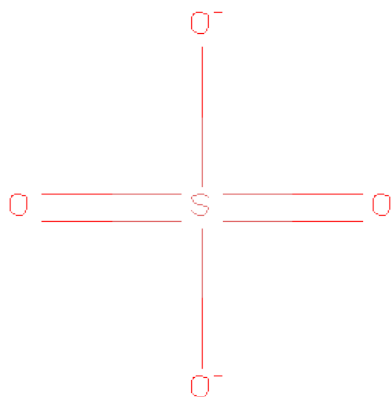
Chain	Residue	Modelled	Actual	Comment	Reference
C	511	ALA	-	EXPRESSION TAG	UNP Q80J95
C	512	ALA	-	EXPRESSION TAG	UNP Q80J95
C	513	LEU	-	EXPRESSION TAG	UNP Q80J95
C	514	GLU	-	EXPRESSION TAG	UNP Q80J95
C	515	HIS	-	EXPRESSION TAG	UNP Q80J95
C	516	HIS	-	EXPRESSION TAG	UNP Q80J95
C	517	HIS	-	EXPRESSION TAG	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 (three-letter code: 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 (three-letter code: SO4) (formula: O₄S).



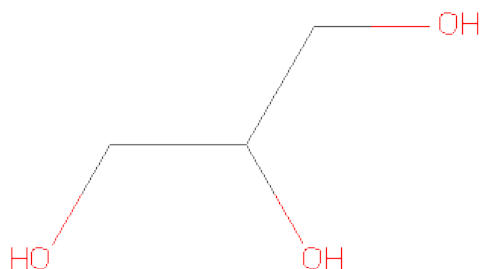
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	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 (three-letter code: GOL) (formula: C₃H₈O₃).



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	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 (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

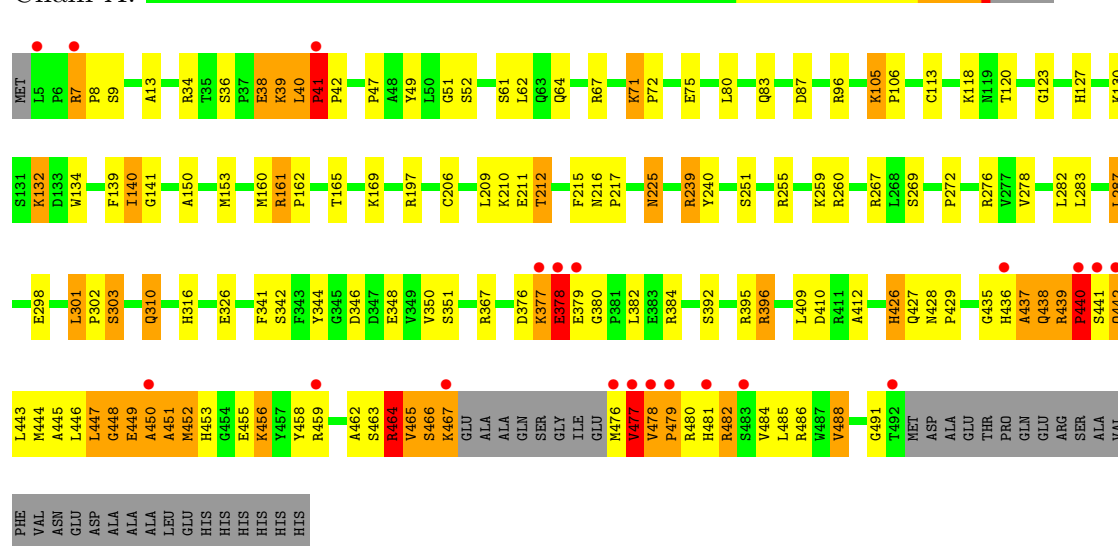
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	212	Total O 212 212	0	0
6	B	168	Total O 168 168	0	0
6	C	163	Total O 163 163	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

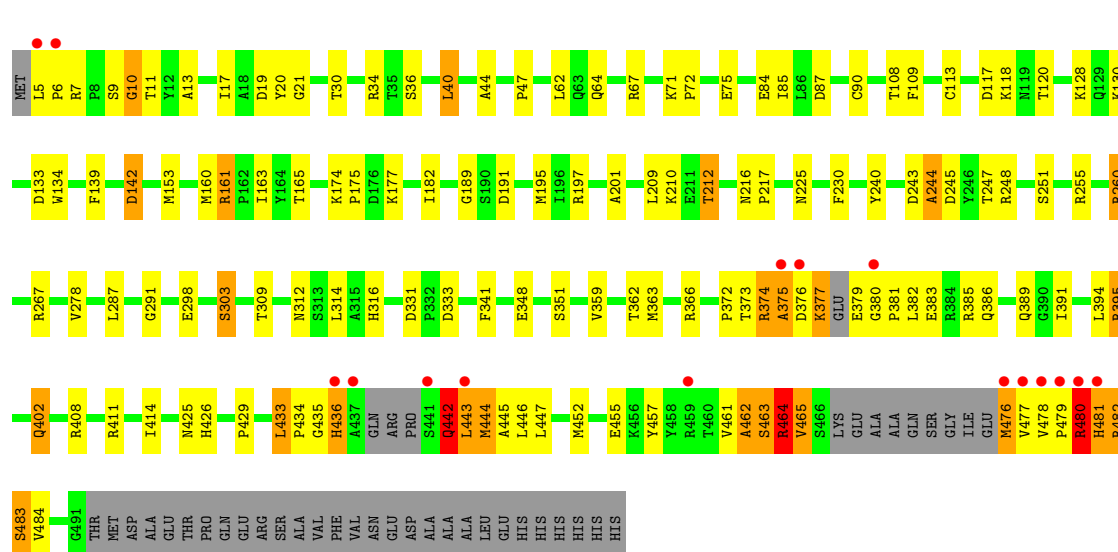
• Molecule 1: RNA polymerase

Chain A:



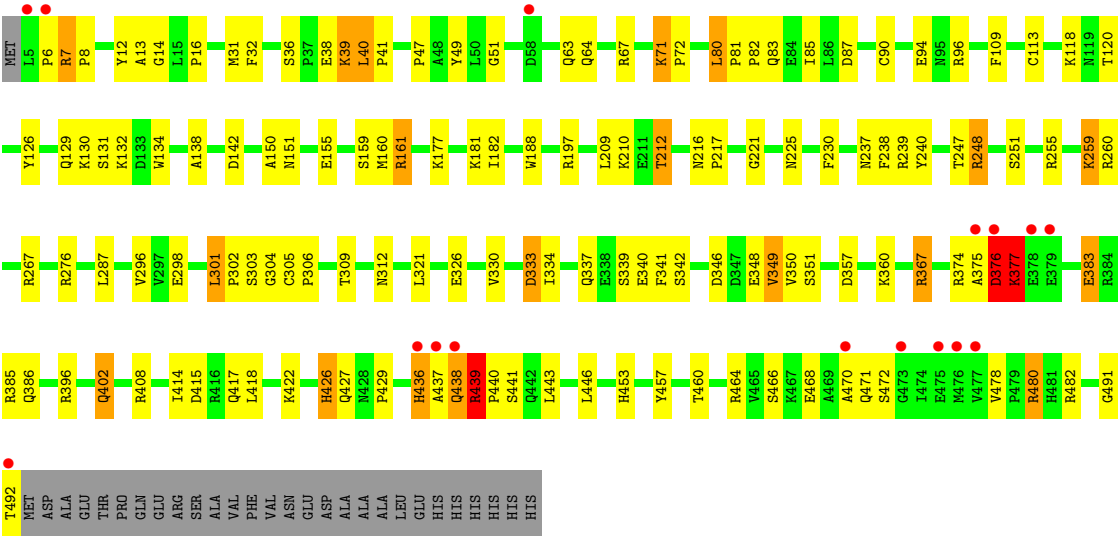
• Molecule 1: RNA polymerase

Chain B:



• Molecule 1: RNA polymerase

Chain C:



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	1.66 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.253 0.203 , 0.252	Depositor DCC
R_{free} test set	1988 reflections (1.75%)	DCC
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 113874 reflections	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 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2TU, GOL, MG, 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	0.49	0/3921	0.65	1/5313 (0.0%)
1	B	0.45	0/3866	0.58	0/5236
1	C	0.46	0/3968	0.57	0/5378
All	All	0.47	0/11755	0.60	1/15927 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	LEU	CA-CB-CG	6.14	129.42	115.30

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

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Mol	Chain	Res	Type	Group
1	A	450	ALA	Peptide
1	A	465	VAL	Peptide
1	B	442	GLN	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3826	0	3786	165	1
1	B	3774	0	3730	132	0
1	C	3872	0	3829	106	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	405	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (405) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:113:CYS:HG	4:A:617:GOL:HO3	1.13	0.91
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: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:B:153:MET:HB2	1:B:160:MET:HE1	1.59	0.83
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:HG3	1:A:161:ARG:HH11	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:A:150:ALA:HA	1:A:160:MET:HE1	1.67	0.77
1:B:165:THR:HB	4:B:614:GOL:H2	1.66	0.77
1:C:267:ARG:HH12	4:C:617:GOL:H2	1.49	0.77
1:C:32:PHE:O	1:C:426:HIS:HE1	1.68	0.77
1:C:375:ALA:O	1:C:376:ASP:HB2	1.85	0.76
1:B:109:PHE:H	4:B:616:GOL:H2	1.51	0.76
1:A:160:MET:HE2	1:A:197:ARG:HD3	1.68	0.75
1:A:451:ALA:O	1:A:453:HIS:N	2.18	0.75
1:B:462:ALA:HA	1:B:463:SER:C	2.05	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:ARG:NH1	4:A:613:GOL:O2	2.20	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:7:ARG:HA	1:A:8:PRO:C	2.08	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: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: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: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:443:LEU:C	1:B:445:ALA:H	1.94	0.69
1:B:433:LEU:HD22	1:B:434:PRO:HD2	1.74	0.69
1:A:456:LYS:CD	1:A:456:LYS:H	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:C:87:ASP:OD1	1:C:260:ARG:NH2	2.27	0.68
1:A:161:ARG:HD2	1:A:287:LEU:HD22	1.75	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:359:VAL:HG22	1:B:381:PRO:HG3	1.77	0.67
1:B:13:ALA:HB2	1:B:67:ARG:HG2	1.76	0.67
1:A:165:THR:HG21	4:A:619:GOL:H2	1.77	0.67
1:B:163:ILE:HG13	1:B:287:LEU:HD23	1.75	0.67
1:A:153:MET:HB2	1:A:160:MET:HE1	1.77	0.67
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:A:377:LYS:HG3	1:A:378:GLU:N	2.11	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:A:132:LYS:HZ2	1:A:132:LYS:HB3	1.61	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:377:LYS:HG3	1:A:378:GLU:H	1.61	0.65
1:A:96:ARG:HE	1:A:216:ASN:HD22	1.43	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:463:SER:N	1:B:464:ARG:HB3	2.14	0.61
1:A:303:SER:HB2	6:A:726:HOH:O	2.00	0.61
1:B:461:VAL:O	1:B:462:ALA:CB	2.49	0.61
1:A:132:LYS:NZ	1:A:132:LYS:HB3	2.16	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: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:C:427:GLN:H	4:C:618:GOL:H11	1.66	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:439:ARG:HB2	1:A:464:ARG:HH12	1.66	0.60
1:B:117:ASP:HB3	4:B:610:GOL:H32	1.83	0.59
1:A:217:PRO:HB3	1:A:341:PHE:HB2	1.85	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: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:B:160:MET:HE3	1:B:197:ARG:HD3	1.86	0.57
1:A:396:ARG:HE	1:A:409:LEU:HD13	1.68	0.57
1:C:160:MET:HE3	1:C:197:ARG:NE	2.19	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:426:HIS:CE1	1:A:428:ASN:O	2.58	0.57
1:A:367:ARG:HD3	6:A:714:HOH:O	2.04	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:C:402:GLN:H	1:C:402:GLN:CD	2.10	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:B:463:SER:HA	1:B:464:ARG:O	2.06	0.55
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: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:A:87:ASP:OD1	1:A:260:ARG:NH2	2.39	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:408:ARG:HG3	1:B:452:MET:HE3	1.90	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:C:49:TYR:CE2	1:C:51:GLY:HA2	2.42	0.54
1:B:243:ASP:HB3	1:B:391:ILE:HG23	1.89	0.54
1:A:463:SER:O	1:A:465:VAL:N	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:375:ALA:O	1:C:376:ASP:CB	2.53	0.54
1:A:482:ARG:CG	1:A:482:ARG:O	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:B:247:THR:HG23	1:B:373:THR:HG21	1.90	0.53
1:A:479:PRO:CD	1:A:480:ARG:HD2	2.39	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:87:ASP:OD1	1:B:260:ARG:NH2	2.41	0.53
1:A:212:THR:HG23	1:A:216:ASN:HB2	1.91	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:479:PRO:HD2	1:A:480:ARG:CD	2.39	0.52
1:A:341:PHE:CE1	1:A:350:VAL:HG13	2.44	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:C:96:ARG:HE	1:C:216:ASN:ND2	2.07	0.51
1:B:255:ARG:HG3	1:B:298:GLU:O	2.09	0.51
1:C:212:THR:HG23	1:C:212:THR:O	2.10	0.51
1:B:47:PRO:HG2	1:B:429:PRO:HB3	1.93	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: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:O	1:A:212:THR:HG23	2.11	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:C:31:MET:CE	1:C:422:LYS:HE2	2.42	0.50
1:A:153:MET:HB2	1:A:160:MET:CE	2.41	0.50
4:A:615:GOL:H12	6:A:897:HOH:O	2.10	0.50
1:B:402[A]:GLN:CD	1:B:402[A]:GLN:H	2.14	0.50
1:C:374:ARG:HH21	1:C:377:LYS:HD3	1.77	0.49
1:B:359:VAL:CG2	1:B:381:PRO:HG3	2.42	0.49
1:B:312:ASN:HD22	2:B:601:2TU:C5'	2.22	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:427:GLN:H	4:A:620:GOL:H2	1.75	0.49
1:B:303:SER:HB2	6:B:806:HOH:O	2.13	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:C:301:LEU:CD2	1:C:302:PRO:HD2	2.43	0.49
1:C:85:ILE:HD13	1:C:326:GLU:HG3	1.94	0.49
1:B:109:PHE:N	4:B:616:GOL:H2	2.25	0.48
1:C:374:ARG:HH21	1:C:377:LYS:CD	2.25	0.48
1:B:462:ALA:HA	1:B:463:SER:O	2.13	0.48
1:B:443:LEU:C	1:B:445:ALA:N	2.63	0.48
1:C:341:PHE:HE1	1:C:350:VAL:HG13	1.78	0.48
1:A:342:SER:O	1:A:348:GLU:HA	2.14	0.48
1:B:333:ASP:N	1:B:333:ASP:OD1	2.46	0.48
1:C:39:LYS:H	1:C:39:LYS:HE3	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: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: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:478:VAL:HB	1:A:479:PRO:CA	2.44	0.48
1:A:61:SER:OG	1:A:64:GLN:HG3	2.14	0.48
1:B:120:THR:OG1	1:B:130:LYS:NZ	2.47	0.48
1:A:105:LYS:HD2	1:A:106:PRO:HD2	1.95	0.48
1:B:411:ARG:NH1	1:B:457:TYR:HB2	2.29	0.48
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:C:63:GLN:O	1:C:67:ARG:HG3	2.13	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:C:439:ARG:N	1:C:440:PRO:CD	2.78	0.47
1:B:333:ASP:OD1	6:B:770:HOH:O	2.20	0.47
1:C:210:LYS:HG3	1:C:221:GLY:HA3	1.96	0.47
1:C:129:GLN:HG2	1:C:131:SER:OG	2.13	0.47
1:C:330:VAL:CG1	1:C:334:ILE:HB	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:150:ALA:HA	1:C:160:MET:HE2	1.97	0.47
4:A:613:GOL:O2	6:A:876:HOH:O	2.20	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
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:450:ALA:O	1:A:458:TYR:HA	2.15	0.47
1:A:448:GLY:H	1:A:451:ALA:CB	2.28	0.47
1:A:479:PRO:HD2	1:A:480:ARG:CG	2.45	0.47
1:C:470:ALA:C	1:C:472:SER:H	2.19	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:C:32:PHE:O	1:C:426:HIS:CE1	2.58	0.46
1:B:443:LEU:HD11	1:B:446:LEU:HD12	1.97	0.46
1:B:348:GLU:OE1	6:B:737:HOH:O	2.20	0.46
1:B:174:LYS:HB2	1:B:174:LYS:HE3	1.85	0.46
1:B:374:ARG:HA	1:B:377:LYS:HB3	1.97	0.46
1:B:165:THR:CG2	4:B:614:GOL:H2	2.46	0.46
1:C:478:VAL:HG12	1:C:478:VAL:O	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:444:MET:HB2	1:A:447:LEU:HD12	1.98	0.46
1:A:13:ALA:N	4:A:613:GOL:H2	2.18	0.46
1:B:10:GLY:HA2	1:B:17:ILE:H	1.81	0.46
1:A:382:LEU:HD13	6:A:763:HOH:O	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:120:THR:OG1	4:A:612:GOL:H2	2.16	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: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:A:379:GLU:HA	1:A:380:GLY:O	2.16	0.45
1:B:443:LEU:HD11	1:B:446:LEU:HB2	1.98	0.45
1:A:210:LYS:C	1:A:212:THR:H	2.20	0.45
1:B:375:ALA:HB1	1:B:380:GLY:CA	2.45	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:30:THR:O	1:B:425:ASN:HA	2.16	0.45
1:A:384:ARG:HD2	6:A:727:HOH:O	2.16	0.45
1:C:408:ARG:HD2	1:C:453:HIS:CD2	2.52	0.45
1:B:244:ALA:O	1:B:245:ASP:CB	2.64	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:B:153:MET:CB	1:B:160:MET:HE1	2.37	0.45
1:C:346:ASP:OD1	2:C:601:2TU:N3	2.50	0.45
1:A:240:TYR:O	1:A:351:SER:HA	2.17	0.45
1:B:113:CYS:SG	4:B:613:GOL:C3	3.05	0.44
1:A:72:PRO:HA	1:A:75:GLU:HG2	2.00	0.44
1:C:255:ARG:O	1:C:259:LYS:HD2	2.18	0.44
1:C:71:LYS:HB2	1:C:72:PRO:HD3	1.97	0.44
1:B:21:GLY:HA3	1:B:291:GLY:O	2.17	0.44
1:B:436:HIS:C	1:B:436:HIS:HD1	2.21	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:B:442:GLN:N	1:B:442:GLN:CD	2.70	0.44
1:C:151:ASN:O	1:C:155:GLU:HG3	2.17	0.44
1:C:374:ARG:NE	1:C:377:LYS:HE2	2.33	0.44
1:A:140:ILE:HG23	1:A:141:GLY:N	2.32	0.44
1:B:359:VAL:O	1:B:363:MET:HG2	2.18	0.44
1:B:244:ALA:O	1:B:245:ASP:HB3	2.18	0.44
1:C:240:TYR:O	1:C:351:SER:HA	2.18	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:201:ALA:HB2	1:B:278:VAL:HG21	1.98	0.44
1:C:312:ASN:HD22	2:C:601:2TU:C1'	2.25	0.43
1:A:160:MET:O	1:A:162:PRO:HD3	2.17	0.43
1:B:462:ALA:N	1:B:463:SER:OG	2.51	0.43
1:B:230:PHE:CD1	1:C:230:PHE:HB3	2.53	0.43
1:A:278:VAL:O	1:A:282:LEU:HG	2.17	0.43
1:C:357:ASP:CG	1:C:360:LYS:HG3	2.37	0.43
1:C:239:ARG:HH21	1:C:386:GLN:HE22	1.65	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:B:331:ASP:HB3	1:B:333:ASP:OD1	2.17	0.43
1:C:238:PHE:HE1	1:C:340:GLU:HG2	1.84	0.43
1:A:450:ALA:C	1:A:451:ALA:O	2.56	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:LYS:HE2	1:B:134:TRP:CE2	2.53	0.43
1:A:269:SER:O	1:A:272:PRO:HD3	2.17	0.43
1:C:160:MET:CE	1:C:197:ARG:HD3	2.49	0.43
1:B:442:GLN:H	1:B:442:GLN:CD	2.22	0.43
1:C:118:LYS:HE2	1:C:134:TRP:CE2	2.52	0.43
1:A:161:ARG:NH1	1:A:161:ARG:HG3	2.20	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:A:341:PHE:HE1	1:A:350:VAL:HG13	1.82	0.43
1:B:177:LYS:O	1:B:182:ILE:HA	2.19	0.43
1:A:301:LEU:HD23	1:A:302:PRO:HD2	2.01	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:A:445:ALA:O	1:A:449:GLU:HB2	2.18	0.43
1:B:118:LYS:HA	1:B:130:LYS:HB2	2.01	0.43
1:C:446:LEU:HA	1:C:446:LEU:HD23	1.84	0.43
1:A:225:ASN:HB2	4:A:614:GOL:H11	2.00	0.43
1:B:84:GLU:HG3	1:B:85:ILE:N	2.34	0.43
1:B:189:GLY:HA3	4:B:614:GOL:O1	2.19	0.42
1:C:402:GLN:N	1:C:402:GLN:OE1	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:B:455:GLU:HA	1:B:482:ARG:HD3	2.00	0.42
1:A:326:GLU:CD	1:A:367:ARG:HH22	2.23	0.42
1:A:130:LYS:NZ	4:A:612:GOL:H2	2.34	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:C:427:GLN:H	4:C:618:GOL:C1	2.32	0.42
1:A:211:GLU:CG	6:A:800:HOH:O	2.67	0.42
1:C:341:PHE:CD1	1:C:350:VAL:HG13	2.54	0.42
1:C:150:ALA:HA	1:C:160:MET:CE	2.48	0.42
1:B:153:MET:HB2	1:B:160:MET:CE	2.40	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:B:444:MET:SD	1:B:447:LEU:HD12	2.59	0.42
1:A:225:ASN:H	4:A:614:GOL:H2	1.84	0.42
1:C:16:PRO:HG2	1:C:296:VAL:HB	2.02	0.42
1:B:366:ARG:NH2	6:B:703:HOH:O	2.53	0.42
1:A:448:GLY:N	1:A:451:ALA:CB	2.83	0.42
1:C:439:ARG:HD3	1:C:468:GLU:OE2	2.20	0.42
1:B:314:LEU:HA	1:B:314:LEU:HD12	1.88	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:394:LEU:O	1:B:395:ARG:HB2	2.19	0.41
1:B:248:ARG:HG2	1:B:251:SER:OG	2.20	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:B:374:ARG:HE	1:B:374:ARG:HB3	1.40	0.41
1:A:217:PRO:CB	1:A:341:PHE:HB2	2.50	0.41
1:B:109:PHE:H	4:B:616:GOL:C1	2.33	0.41
1:C:427:GLN:CB	4:C:618:GOL:H11	2.47	0.41
1:A:169:LYS:HG3	3:A:609:SO4:O4	2.21	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:455:GLU:HG3	1:A:482:ARG:CD	2.51	0.41
1:A:260:ARG:NH1	3:A:608:SO4:O2	2.53	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:C:109:PHE:CZ	4:C:613:GOL:H31	2.56	0.40
1:A:316:HIS:CE1	1:A:348:GLU:HB3	2.56	0.40
1:A:49:TYR:CE2	1:A:51:GLY:HA2	2.56	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:A:259:LYS:HA	1:A:283:LEU:CD1	2.50	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	Distance(Å)	Clash(Å)
1:A:9:SER:O	4:A:613:GOL:O1[2_655]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	7	2
1	B	467/517 (90%)	434 (93%)	21 (4%)	12 (3%)	8	4
1	C	486/517 (94%)	458 (94%)	18 (4%)	10 (2%)	11	5
All	All	1430/1551 (92%)	1334 (93%)	59 (4%)	37 (3%)	8	4

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%)	373 (90%)	39 (10%)	12	11
1	B	406/440 (92%)	373 (92%)	33 (8%)	17	16
1	C	416/440 (94%)	378 (91%)	38 (9%)	14	13
All	All	1234/1320 (94%)	1124 (91%)	110 (9%)	14	13

All (110) 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	105	LYS
1	A	132	LYS
1	A	140	ILE
1	A	161	ARG
1	A	212	THR
1	A	225	ASN
1	A	239	ARG
1	A	267	ARG
1	A	287	LEU
1	A	301	LEU
1	A	303	SER
1	A	310	GLN
1	A	344	TYR
1	A	377	LYS

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Mol	Chain	Res	Type
1	A	378	GLU
1	A	392	SER
1	A	396	ARG
1	A	426	HIS
1	A	438	GLN
1	A	440	PRO
1	A	443	LEU
1	A	452	MET
1	A	456	LYS
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	7	ARG
1	B	11	THR
1	B	36	SER
1	B	40	LEU
1	B	64	GLN
1	B	128	LYS
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	374	ARG
1	B	377	LYS
1	B	379	GLU
1	B	383	GLU
1	B	385	ARG
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	426	HIS
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	C	36	SER
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	237	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	426	HIS
1	C	438	GLN

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Mol	Chain	Res	Type
1	C	439	ARG
1	C	441	SER
1	C	464	ARG
1	C	466	SER
1	C	480	ARG
1	C	492	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	442	GLN
1	C	426	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	2TU	A	601	-	18,18,18	0.88	1 (5%)	20,26,26	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	602	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	A	604	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	A	605	-	4,4,4	0.06	0	6,6,6	0.12	0
3	SO4	A	606	-	4,4,4	0.10	0	6,6,6	0.07	0
3	SO4	A	607	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	A	608	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	A	609	-	4,4,4	0.20	0	6,6,6	0.16	0
3	SO4	A	610	-	4,4,4	0.03	0	6,6,6	0.13	0
4	GOL	A	611	-	5,5,5	0.30	0	5,5,5	0.55	0
4	GOL	A	612	-	5,5,5	0.33	0	5,5,5	0.42	0
4	GOL	A	613	-	5,5,5	0.20	0	5,5,5	0.47	0
4	GOL	A	614	-	5,5,5	0.23	0	5,5,5	0.54	0
4	GOL	A	615	-	5,5,5	0.44	0	5,5,5	1.01	0
4	GOL	A	616	-	5,5,5	0.35	0	5,5,5	0.50	0
4	GOL	A	617	-	5,5,5	0.35	0	5,5,5	0.24	0
4	GOL	A	618	-	5,5,5	0.31	0	5,5,5	0.26	0
4	GOL	A	619	-	5,5,5	0.39	0	5,5,5	0.28	0
4	GOL	A	620	-	5,5,5	0.24	0	5,5,5	0.61	0
4	GOL	A	621	-	5,5,5	0.38	0	5,5,5	0.23	0
4	GOL	A	622	-	5,5,5	0.34	0	5,5,5	0.63	0
2	2TU	B	601	-	18,18,18	1.05	2 (11%)	20,26,26	0.79	0
3	SO4	B	602	-	4,4,4	0.21	0	6,6,6	0.17	0
3	SO4	B	603	-	4,4,4	0.16	0	6,6,6	0.06	0
3	SO4	B	604	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	B	605	-	4,4,4	0.08	0	6,6,6	0.07	0
3	SO4	B	606	-	4,4,4	0.09	0	6,6,6	0.20	0
3	SO4	B	607	-	4,4,4	0.28	0	6,6,6	0.28	0
3	SO4	B	608	-	4,4,4	0.11	0	6,6,6	0.10	0
3	SO4	B	609	-	4,4,4	0.06	0	6,6,6	0.14	0
4	GOL	B	610	-	5,5,5	0.40	0	5,5,5	0.43	0
4	GOL	B	611	-	5,5,5	0.40	0	5,5,5	0.70	0
4	GOL	B	612	-	5,5,5	0.44	0	5,5,5	0.32	0
4	GOL	B	613	-	5,5,5	0.27	0	5,5,5	0.63	0
4	GOL	B	614	-	5,5,5	0.26	0	5,5,5	0.59	0
4	GOL	B	615	-	5,5,5	0.30	0	5,5,5	0.57	0
4	GOL	B	616	-	5,5,5	0.27	0	5,5,5	0.76	0
2	2TU	C	601	-	18,18,18	0.97	1 (5%)	20,26,26	0.75	0
3	SO4	C	602	-	4,4,4	0.10	0	6,6,6	0.07	0
3	SO4	C	603	-	4,4,4	0.22	0	6,6,6	0.22	0
3	SO4	C	604	-	4,4,4	0.09	0	6,6,6	0.20	0
3	SO4	C	605	-	4,4,4	0.05	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	606	-	4,4,4	0.13	0	6,6,6	0.18	0
3	SO4	C	607	-	4,4,4	0.08	0	6,6,6	0.06	0
3	SO4	C	608	-	4,4,4	0.07	0	6,6,6	0.16	0
3	SO4	C	609	-	4,4,4	0.11	0	6,6,6	0.17	0
3	SO4	C	610	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	C	611	-	4,4,4	0.31	0	6,6,6	0.14	0
3	SO4	C	612	-	4,4,4	0.06	0	6,6,6	0.13	0
4	GOL	C	613	-	5,5,5	0.20	0	5,5,5	0.44	0
4	GOL	C	614	-	5,5,5	0.25	0	5,5,5	0.38	0
4	GOL	C	615	-	5,5,5	0.30	0	5,5,5	0.51	0
4	GOL	C	616	-	5,5,5	0.29	0	5,5,5	0.75	0
4	GOL	C	617	-	5,5,5	0.33	0	5,5,5	0.31	0
4	GOL	C	618	-	5,5,5	0.33	0	5,5,5	0.45	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
2	2TU	A	601	-	-	0/4/22/22	0/2/2/2
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
3	SO4	A	606	-	-	0/0/0/0	0/0/0/0
3	SO4	A	607	-	-	0/0/0/0	0/0/0/0
3	SO4	A	608	-	-	0/0/0/0	0/0/0/0
3	SO4	A	609	-	-	0/0/0/0	0/0/0/0
3	SO4	A	610	-	-	0/0/0/0	0/0/0/0
4	GOL	A	611	-	-	0/4/4/4	0/0/0/0
4	GOL	A	612	-	-	0/4/4/4	0/0/0/0
4	GOL	A	613	-	-	0/4/4/4	0/0/0/0
4	GOL	A	614	-	-	0/4/4/4	0/0/0/0
4	GOL	A	615	-	-	0/4/4/4	0/0/0/0
4	GOL	A	616	-	-	0/4/4/4	0/0/0/0
4	GOL	A	617	-	-	0/4/4/4	0/0/0/0
4	GOL	A	618	-	-	0/4/4/4	0/0/0/0
4	GOL	A	619	-	-	0/4/4/4	0/0/0/0
4	GOL	A	620	-	-	0/4/4/4	0/0/0/0
4	GOL	A	621	-	-	0/4/4/4	0/0/0/0
4	GOL	A	622	-	-	0/4/4/4	0/0/0/0
2	2TU	B	601	-	-	0/4/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
3	SO4	B	606	-	-	0/0/0/0	0/0/0/0
3	SO4	B	607	-	-	0/0/0/0	0/0/0/0
3	SO4	B	608	-	-	0/0/0/0	0/0/0/0
3	SO4	B	609	-	-	0/0/0/0	0/0/0/0
4	GOL	B	610	-	-	0/4/4/4	0/0/0/0
4	GOL	B	611	-	-	0/4/4/4	0/0/0/0
4	GOL	B	612	-	-	0/4/4/4	0/0/0/0
4	GOL	B	613	-	-	0/4/4/4	0/0/0/0
4	GOL	B	614	-	-	0/4/4/4	0/0/0/0
4	GOL	B	615	-	-	0/4/4/4	0/0/0/0
4	GOL	B	616	-	-	0/4/4/4	0/0/0/0
2	2TU	C	601	-	-	0/4/22/22	0/2/2/2
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0
3	SO4	C	605	-	-	0/0/0/0	0/0/0/0
3	SO4	C	606	-	-	0/0/0/0	0/0/0/0
3	SO4	C	607	-	-	0/0/0/0	0/0/0/0
3	SO4	C	608	-	-	0/0/0/0	0/0/0/0
3	SO4	C	609	-	-	0/0/0/0	0/0/0/0
3	SO4	C	610	-	-	0/0/0/0	0/0/0/0
3	SO4	C	611	-	-	0/0/0/0	0/0/0/0
3	SO4	C	612	-	-	0/0/0/0	0/0/0/0
4	GOL	C	613	-	-	0/4/4/4	0/0/0/0
4	GOL	C	614	-	-	0/4/4/4	0/0/0/0
4	GOL	C	615	-	-	0/4/4/4	0/0/0/0
4	GOL	C	616	-	-	0/4/4/4	0/0/0/0
4	GOL	C	617	-	-	0/4/4/4	0/0/0/0
4	GOL	C	618	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	2TU	C2-N1	3.27	1.41	1.37
2	C	601	2TU	C2-N1	2.62	1.40	1.37
2	B	601	2TU	C6-C5	2.35	1.39	1.36
2	A	601	2TU	C6-C5	2.09	1.39	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	2TU	C5-C6-N1	-2.17	118.76	121.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	-0.29	20 (4%) 35 35	15, 27, 66, 107	0
1	B	474/517 (91%)	-0.21	16 (3%) 43 43	19, 32, 66, 112	0
1	C	488/517 (94%)	-0.27	16 (3%) 44 45	18, 32, 66, 105	0
All	All	1442/1551 (92%)	-0.26	52 (3%) 41 41	15, 31, 66, 112	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	7.6
1	A	441	SER	7.4
1	B	479	PRO	6.8
1	C	437	ALA	6.7
1	B	476	MET	6.7
1	C	5	LEU	6.5
1	C	375	ALA	6.4
1	A	477	VAL	6.4
1	C	6	PRO	5.9
1	C	492	THR	5.6
1	B	375	ALA	5.4
1	A	41	PRO	5.4
1	C	376	ASP	5.0
1	A	478	VAL	4.8
1	A	440	PRO	4.4
1	C	438	GLN	4.2
1	C	475	GLU	4.2
1	B	480	ARG	4.1
1	B	441	SER	4.0
1	A	476	MET	4.0
1	A	436	HIS	3.9
1	B	437	ALA	3.9
1	C	473	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	481	HIS	3.7
1	B	376	ASP	3.6
1	A	442	GLN	3.5
1	A	479	PRO	3.4
1	B	477	VAL	3.3
1	A	5	LEU	3.3
1	A	7	ARG	3.2
1	A	378	GLU	3.2
1	B	459	ARG	3.0
1	B	380	GLY	3.0
1	B	436	HIS	2.9
1	C	58	ASP	2.9
1	C	477	VAL	2.9
1	A	467	LYS	2.8
1	C	378	GLU	2.8
1	A	379	GLU	2.8
1	B	6	PRO	2.7
1	A	459	ARG	2.7
1	B	443	LEU	2.6
1	B	478	VAL	2.6
1	C	470	ALA	2.4
1	A	450	ALA	2.3
1	C	476	MET	2.3
1	A	481	HIS	2.3
1	C	436	HIS	2.2
1	C	379	GLU	2.2
1	A	377	LYS	2.1
1	A	492	THR	2.1
1	A	483	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	C	610	5/5	0.30	18.61	37,52,74,77	0
4	GOL	A	619	6/6	0.31	18.32	29,35,45,50	0
3	SO4	A	609	5/5	0.30	15.81	34,50,66,70	0
3	SO4	A	608	5/5	0.28	13.89	46,52,59,76	0
4	GOL	B	614	6/6	0.34	13.58	28,35,42,43	0
3	SO4	C	603	5/5	0.14	10.54	37,38,56,63	0
2	2TU	C	601	17/17	0.29	10.25	28,34,41,46	17
3	SO4	C	612	5/5	0.23	8.53	56,59,72,74	0
4	GOL	A	612	6/6	0.19	7.93	29,35,40,42	0
4	GOL	A	616	6/6	0.21	7.85	36,47,56,58	0
2	2TU	A	601	17/17	0.25	7.23	27,38,42,43	17
3	SO4	B	602	5/5	0.17	6.64	42,47,60,66	0
3	SO4	C	608	5/5	0.35	6.52	61,76,86,89	0
2	2TU	B	601	17/17	0.26	6.24	33,42,47,47	17
4	GOL	B	610	6/6	0.22	5.63	44,48,51,53	0
4	GOL	A	611	6/6	0.14	5.21	34,37,45,47	0
4	GOL	C	618	6/6	0.22	5.17	42,48,53,54	0
3	SO4	C	611	5/5	0.22	5.12	43,51,62,80	0
5	MG	B	617	1/1	0.30	5.08	49,49,49,49	0
3	SO4	C	602	5/5	0.16	4.78	47,52,67,78	0
4	GOL	C	616	6/6	0.26	4.67	49,57,59,67	0
3	SO4	B	609	5/5	0.32	4.58	61,67,86,87	0
3	SO4	A	607	5/5	0.24	4.49	55,59,72,74	0
4	GOL	C	615	6/6	0.16	4.40	36,40,49,51	0
3	SO4	B	608	5/5	0.24	4.25	55,56,76,78	0
3	SO4	B	604	5/5	0.35	4.10	48,59,82,90	0
3	SO4	B	606	5/5	0.24	3.94	61,63,71,81	0
3	SO4	A	610	5/5	0.21	3.90	57,61,72,73	0
3	SO4	B	603	5/5	0.26	3.89	55,65,82,87	0
4	GOL	B	612	6/6	0.18	3.72	36,47,51,54	0
4	GOL	C	614	6/6	0.14	3.68	42,46,47,53	0
3	SO4	C	607	5/5	0.21	3.33	73,74,80,97	0
4	GOL	A	615	6/6	0.25	3.29	23,38,47,50	0
4	GOL	B	611	6/6	0.18	3.21	25,42,43,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	B	616	6/6	0.24	3.16	33,37,40,48	0
3	SO4	A	603	5/5	0.10	3.08	43,44,57,59	0
3	SO4	B	605	5/5	0.18	2.84	56,57,71,72	0
3	SO4	A	604	5/5	0.19	2.82	46,46,62,62	0
4	GOL	A	620	6/6	0.21	2.45	38,42,54,60	0
4	GOL	C	617	6/6	0.14	2.27	38,47,53,56	0
3	SO4	B	607	5/5	0.17	2.11	43,43,56,71	0
4	GOL	B	615	6/6	0.15	1.91	39,41,45,46	0
3	SO4	A	605	5/5	0.20	1.85	61,61,71,73	0
3	SO4	C	609	5/5	0.18	1.62	39,47,54,62	0
4	GOL	A	622	6/6	0.14	1.47	48,51,56,57	0
3	SO4	C	605	5/5	0.23	1.13	74,74,92,93	0
4	GOL	A	614	6/6	0.14	1.11	40,44,47,55	0
3	SO4	A	606	5/5	0.23	1.07	76,85,95,100	0
4	GOL	B	613	6/6	0.15	0.99	37,39,40,42	1
4	GOL	A	613	6/6	0.20	0.94	41,46,51,53	0
3	SO4	C	604	5/5	0.17	0.94	55,56,61,68	0
4	GOL	C	613	6/6	0.13	0.44	34,39,45,47	0
4	GOL	A	617	6/6	0.11	0.22	34,39,40,47	0
3	SO4	A	602	5/5	0.12	-0.01	45,53,61,74	0
4	GOL	A	621	6/6	0.12	-0.17	40,43,48,50	0
4	GOL	A	618	6/6	0.09	-0.33	28,32,33,33	1
3	SO4	C	606	5/5	0.11	-0.70	52,59,69,71	0
5	MG	C	619	1/1	0.06	-2.48	32,32,32,32	0
5	MG	A	623	1/1	0.05	-3.83	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.