



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:40 AM UTC

PDB ID : 3SFU / pdb_00003sfu
Title : crystal structure of murine norovirus RNA dependent RNA polymerase in complex with ribavirin
Authors : Kim, K.H.; Alam, I.
Deposited on : 2011-06-14
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

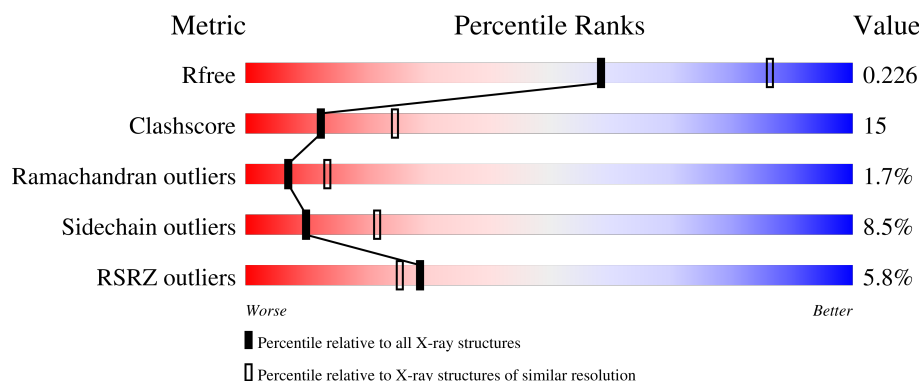
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	5% 70% 17% 5% 7%
1	B	517	6% 68% 21% 6% 6%
1	C	517	5% 66% 21% 5% 8%

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	RBV	C	601	-	-	X	-
3	SO4	B	606	-	-	X	-
3	SO4	C	613	-	-	X	-
5	GOL	A	617	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12321 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
			3828	2423	674	706	25			
1	B	487	Total	C	N	O	S	0	0	0
			3865	2444	680	716	25			
1	C	478	Total	C	N	O	S	0	0	0
			3800	2405	669	702	24			

There are 33 discrepancies between the modelled and reference sequences:

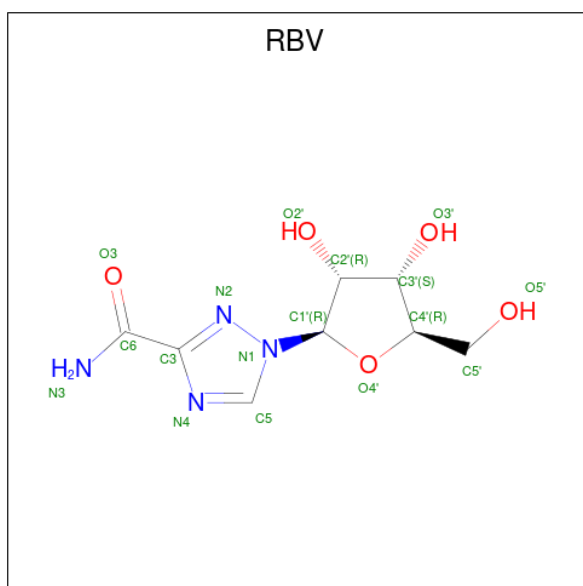
Chain	Residue	Modelled	Actual	Comment	Reference
A	510	ALA	-	expression tag	UNP Q80J95
A	511	ALA	-	expression tag	UNP Q80J95
A	512	ALA	-	expression tag	UNP Q80J95
A	513	LEU	-	expression tag	UNP Q80J95
A	514	GLU	-	expression tag	UNP Q80J95
A	515	HIS	-	expression tag	UNP Q80J95
A	516	HIS	-	expression tag	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)-1H-1,2,4-triazole-3-carboxamide (CCD ID: RBV) (formula: C₈H₁₂N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	8	4	5		
2	B	1	Total	C	N	O	0	0
			17	8	4	5		
2	C	1	Total	C	N	O	0	0
			17	8	4	5		

- 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		
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	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		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

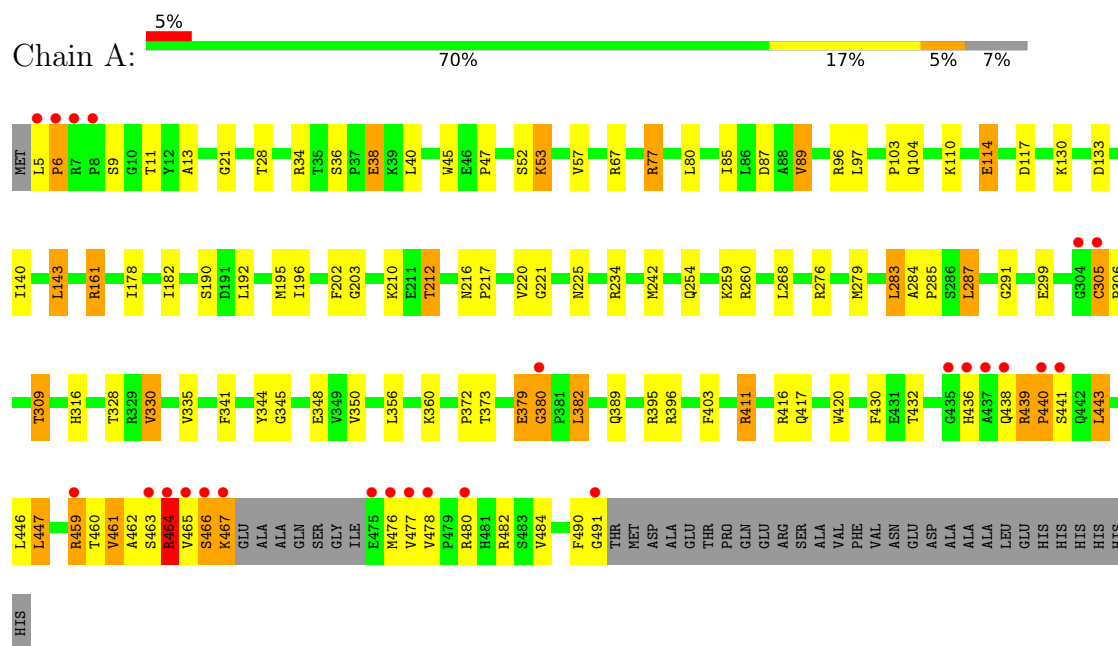
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	179	Total O 179 179	0	0
6	B	149	Total O 149 149	0	0
6	C	155	Total O 155 155	0	0

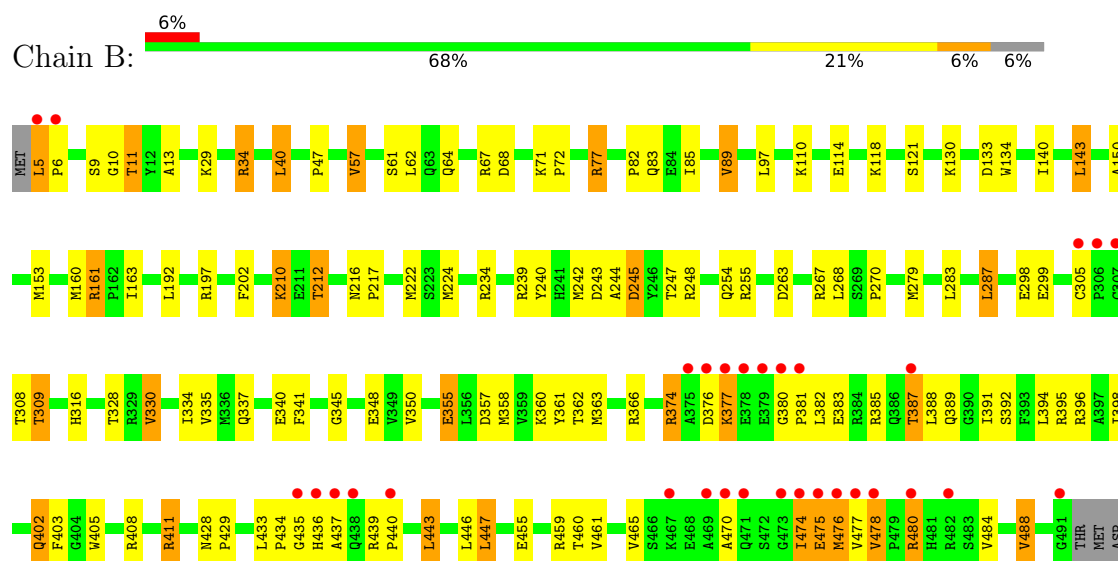
3 Residue-property plots [i](#)

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

• Molecule 1: RNA polymerase

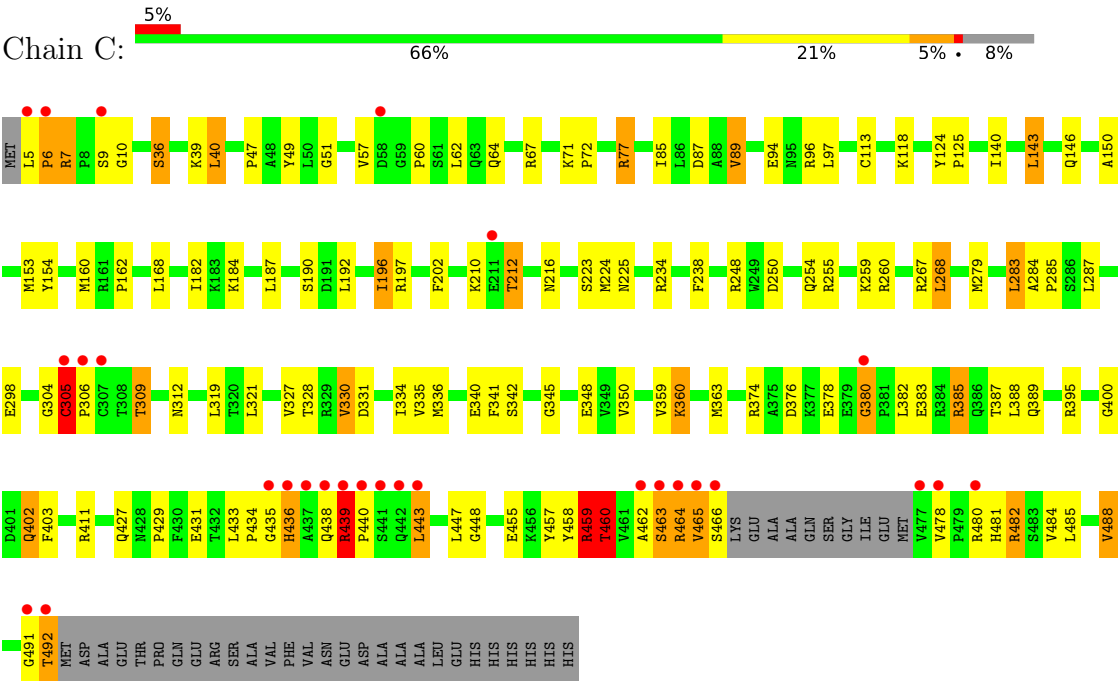


• Molecule 1: RNA polymerase



ALA
GLU
THR
PRO
GLN
GLU
ARG
SER
ALA
VAL
PHE
VAL
ASN
GLU
ASP
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS

● 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	119.95Å 196.08Å 109.21Å 90.00° 114.12° 90.00°	Depositor
Resolution (Å)	47.85 – 2.50 47.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.85-2.50) 95.6 (47.85-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.46	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.51Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.7.1_743	Depositor
R, R_{free}	0.181 , 0.229 0.184 , 0.226	Depositor DCC
R_{free} test set	2000 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12321	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, GOL, MG, RBV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/3923	0.81	0/5314
1	B	0.49	0/3961	0.82	5/5368 (0.1%)
1	C	0.49	0/3895	0.84	6/5280 (0.1%)
All	All	0.49	0/11779	0.82	11/15962 (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	C	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	CYS	CA-C-N	7.28	128.94	119.84
1	C	305	CYS	C-N-CA	7.28	128.94	119.84
1	B	478	VAL	N-CA-C	6.28	113.27	107.56
1	B	11	THR	N-CA-C	5.65	118.11	108.90
1	C	460	THR	N-CA-C	-5.62	98.83	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	459	ARG	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	3828	0	3790	120	1
1	B	3865	0	3822	116	0
1	C	3800	0	3757	122	0
2	A	17	0	12	4	0
2	B	17	0	12	4	0
2	C	17	0	12	10	0
3	A	40	0	0	1	0
3	B	35	0	0	4	0
3	C	60	0	0	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	60	0	80	12	0
5	B	54	0	72	5	0
5	C	42	0	56	9	0
6	A	179	0	0	5	0
6	B	149	0	0	4	0
6	C	155	0	0	4	0
All	All	12321	0	11613	360	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 15.

The worst 5 of 360 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:463:SER:HA	1:A:464:ARG:HB3	1.18	1.17
1:A:104:GLN:H	5:A:618:GOL:H32	1.02	1.15
1:B:150:ALA:HA	1:B:160:MET:HE1	1.30	1.11
1:B:436:HIS:H	1:B:437:ALA:HA	1.16	1.08
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.22	1.04

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:234:ARG:NH2	1:A:403:PHE:O[2_454]	2.02	0.18

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%)	455 (95%)	16 (3%)	6 (1%)	9	18
1	B	485/517 (94%)	456 (94%)	22 (4%)	7 (1%)	9	17
1	C	474/517 (92%)	444 (94%)	18 (4%)	12 (2%)	4	7
All	All	1436/1551 (93%)	1355 (94%)	56 (4%)	25 (2%)	7	13

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	PRO
1	B	475	GLU
1	C	6	PRO
1	C	305	CYS
1	C	436	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/440 (94%)	374 (91%)	38 (9%)	8	19
1	B	415/440 (94%)	381 (92%)	34 (8%)	10	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	409/440 (93%)	376 (92%)	33 (8%)	11	23
All	All	1236/1320 (94%)	1131 (92%)	105 (8%)	10	22

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	355	GLU
1	B	488	VAL
1	C	459	ARG
1	B	374	ARG
1	B	411	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	ASN
1	C	69	GLN
1	C	481	HIS
1	C	129	GLN
1	A	427	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
5	GOL	B	611	-	5,5,5	0.37	0	5,5,5	0.30	0
3	SO4	A	604	-	4,4,4	0.23	0	6,6,6	0.07	0
5	GOL	C	617	-	5,5,5	0.40	0	5,5,5	0.25	0
5	GOL	A	615	-	5,5,5	0.41	0	5,5,5	0.46	0
3	SO4	A	608	-	4,4,4	0.24	0	6,6,6	0.14	0
5	GOL	A	613	-	5,5,5	0.36	0	5,5,5	0.46	0
5	GOL	C	616	-	5,5,5	0.31	0	5,5,5	0.34	0
3	SO4	B	603	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	A	603	-	4,4,4	0.22	0	6,6,6	0.18	0
5	GOL	B	610	-	5,5,5	0.37	0	5,5,5	0.32	0
5	GOL	B	615	-	5,5,5	0.37	0	5,5,5	0.29	0
3	SO4	A	605	-	4,4,4	0.26	0	6,6,6	0.27	0
3	SO4	C	615	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.20	0
5	GOL	A	614	-	5,5,5	0.33	0	5,5,5	0.47	0
5	GOL	C	606	-	5,5,5	0.34	0	5,5,5	0.35	0
3	SO4	C	608	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	C	613	-	4,4,4	0.26	0	6,6,6	0.09	0
5	GOL	A	619	-	5,5,5	0.36	0	5,5,5	0.42	0
3	SO4	C	609	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	605	-	4,4,4	0.26	0	6,6,6	0.11	0
5	GOL	A	617	-	5,5,5	0.38	0	5,5,5	0.30	0
5	GOL	C	621	-	5,5,5	0.28	0	5,5,5	0.60	0
2	RBV	C	601	-	18,18,18	1.13	2 (11%)	25,26,26	2.32	7 (28%)
5	GOL	A	616	-	5,5,5	0.41	0	5,5,5	0.19	0
3	SO4	A	606	-	4,4,4	0.21	0	6,6,6	0.07	0
2	RBV	A	601	-	18,18,18	1.59	2 (11%)	25,26,26	2.30	7 (28%)
5	GOL	A	612	-	5,5,5	0.36	0	5,5,5	0.30	0
5	GOL	B	612	-	5,5,5	0.38	0	5,5,5	0.35	0
5	GOL	C	619	-	5,5,5	0.39	0	5,5,5	0.24	0
3	SO4	C	611	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	606	-	4,4,4	0.21	0	6,6,6	0.10	0
5	GOL	A	620	-	5,5,5	0.45	0	5,5,5	0.32	0
5	GOL	B	618	-	5,5,5	0.35	0	5,5,5	0.44	0
3	SO4	C	607	-	4,4,4	0.23	0	6,6,6	0.07	0
5	GOL	B	613	-	5,5,5	0.36	0	5,5,5	0.41	0
3	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RBV	B	601	-	18,18,18	1.35	2 (11%)	25,26,26	2.25	6 (24%)
3	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	B	608	-	4,4,4	0.24	0	6,6,6	0.13	0
5	GOL	A	611	-	5,5,5	0.41	0	5,5,5	0.17	0
3	SO4	C	612	-	4,4,4	0.23	0	6,6,6	0.10	0
5	GOL	A	618	-	5,5,5	0.38	0	5,5,5	0.31	0
5	GOL	C	618	-	5,5,5	0.37	0	5,5,5	0.59	0
5	GOL	C	620	-	5,5,5	0.51	0	5,5,5	0.39	0
3	SO4	A	609	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	B	607	-	4,4,4	0.28	0	6,6,6	0.19	0
5	GOL	B	617	-	5,5,5	0.43	0	5,5,5	0.25	0
3	SO4	A	607	-	4,4,4	0.26	0	6,6,6	0.13	0
5	GOL	B	614	-	5,5,5	0.37	0	5,5,5	0.34	0
3	SO4	C	603	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	604	-	4,4,4	0.27	0	6,6,6	0.16	0
3	SO4	C	614	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	C	610	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	C	605	-	4,4,4	0.23	0	6,6,6	0.07	0
5	GOL	B	616	-	5,5,5	0.41	0	5,5,5	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	611	-	-	2/4/4/4	-
5	GOL	C	617	-	-	2/4/4/4	-
5	GOL	A	615	-	-	2/4/4/4	-
5	GOL	A	613	-	-	2/4/4/4	-
5	GOL	C	616	-	-	0/4/4/4	-
5	GOL	B	610	-	-	4/4/4/4	-
5	GOL	B	615	-	-	2/4/4/4	-
5	GOL	A	614	-	-	2/4/4/4	-
5	GOL	C	606	-	-	2/4/4/4	-
5	GOL	A	619	-	-	0/4/4/4	-
5	GOL	A	617	-	-	2/4/4/4	-
5	GOL	C	621	-	-	4/4/4/4	-
2	RBV	C	601	-	-	7/10/26/26	0/2/2/2
5	GOL	A	616	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RBV	A	601	-	-	9/10/26/26	0/2/2/2
5	GOL	A	612	-	-	2/4/4/4	-
5	GOL	B	612	-	-	2/4/4/4	-
5	GOL	C	619	-	-	2/4/4/4	-
5	GOL	A	620	-	-	0/4/4/4	-
5	GOL	B	618	-	-	2/4/4/4	-
5	GOL	B	613	-	-	0/4/4/4	-
2	RBV	B	601	-	-	7/10/26/26	0/2/2/2
5	GOL	A	611	-	-	2/4/4/4	-
5	GOL	C	618	-	-	2/4/4/4	-
5	GOL	A	618	-	-	4/4/4/4	-
5	GOL	B	617	-	-	4/4/4/4	-
5	GOL	B	614	-	-	2/4/4/4	-
5	GOL	C	620	-	-	4/4/4/4	-
5	GOL	B	616	-	-	2/4/4/4	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	RBV	C6-C3	5.08	1.53	1.49
2	B	601	RBV	C6-C3	3.88	1.52	1.49
2	A	601	RBV	C6-N3	3.56	1.43	1.33
2	B	601	RBV	C6-N3	3.45	1.43	1.33
2	C	601	RBV	C6-N3	3.42	1.43	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	RBV	C6-C3-N2	6.57	127.69	121.98
2	B	601	RBV	N1-C5-N4	-6.26	107.39	110.53
2	A	601	RBV	N1-C5-N4	-6.20	107.42	110.53
2	A	601	RBV	N2-C3-N4	-5.03	107.63	114.90
2	B	601	RBV	N2-C3-N4	-4.93	107.78	114.90

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	RBV	C2'-C1'-N1-N2

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Mol	Chain	Res	Type	Atoms
2	B	601	RBV	N2-C3-C6-N3
2	B	601	RBV	N2-C3-C6-O3
2	B	601	RBV	N4-C3-C6-N3
2	B	601	RBV	N4-C3-C6-O3

There are no ring outliers.

24 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	615	GOL	1	0
3	A	608	SO4	1	0
5	C	616	GOL	1	0
3	C	615	SO4	1	0
5	A	614	GOL	1	0
5	C	606	GOL	1	0
3	C	613	SO4	2	0
5	A	619	GOL	2	0
3	C	609	SO4	1	0
5	A	617	GOL	4	0
5	C	621	GOL	1	0
2	C	601	RBV	10	0
2	A	601	RBV	4	0
5	B	612	GOL	1	0
3	B	606	SO4	2	0
5	A	620	GOL	1	0
5	B	618	GOL	1	0
2	B	601	RBV	4	0
3	B	608	SO4	1	0
5	A	618	GOL	3	0
5	C	618	GOL	3	0
5	C	620	GOL	3	0
3	B	607	SO4	1	0
5	B	614	GOL	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	25 (5%)	33 29	9, 25, 72, 161	1 (0%)
1	B	487/517 (94%)	-0.16	31 (6%)	25 22	15, 29, 77, 149	0
1	C	478/517 (92%)	-0.14	28 (5%)	28 24	14, 28, 75, 137	0
All	All	1445/1551 (93%)	-0.20	84 (5%)	29 25	9, 28, 74, 161	1 (0%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	LEU	6.7
1	C	492	THR	6.4
1	C	6	PRO	6.3
1	B	5	LEU	5.6
1	A	466	SER	5.5

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($\text{\AA}^2$)	Q<0.9
5	GOL	B	615	6/6	0.68	0.18	68,75,75,81	0
3	SO4	C	609	5/5	0.72	0.27	8,23,26,26	4
3	SO4	C	611	5/5	0.73	0.10	86,91,106,109	1
5	GOL	C	619	6/6	0.79	0.17	49,54,60,65	0
3	SO4	B	608	5/5	0.80	0.11	59,69,74,79	2
3	SO4	C	605	5/5	0.80	0.17	60,65,80,81	3
5	GOL	B	616	6/6	0.81	0.21	57,63,66,69	1
5	GOL	A	618	6/6	0.81	0.21	31,34,40,40	4
3	SO4	A	605	5/5	0.82	0.15	52,52,55,58	1
2	RBV	B	601	17/17	0.83	0.24	40,53,63,70	17
5	GOL	A	617	6/6	0.83	0.23	19,24,29,31	4
2	RBV	C	601	17/17	0.83	0.30	49,72,82,83	17
3	SO4	C	607	5/5	0.84	0.17	62,64,74,81	2
2	RBV	A	601	17/17	0.85	0.19	24,39,45,45	17
3	SO4	A	609	5/5	0.85	0.15	72,76,88,92	2
3	SO4	C	612	5/5	0.85	0.17	74,75,87,102	4
5	GOL	C	606	6/6	0.85	0.19	58,61,68,70	1
3	SO4	B	603	5/5	0.85	0.13	59,67,81,87	2
3	SO4	C	614	5/5	0.86	0.17	75,77,93,100	2
5	GOL	B	611	6/6	0.86	0.16	51,52,61,66	2
3	SO4	B	606	5/5	0.86	0.14	53,58,64,68	3
5	GOL	B	614	6/6	0.87	0.15	54,56,60,61	1
5	GOL	A	612	6/6	0.87	0.17	53,55,63,65	1
3	SO4	B	605	5/5	0.87	0.14	61,65,77,80	2
5	GOL	B	617	6/6	0.87	0.20	41,45,49,54	4
3	SO4	C	615	5/5	0.87	0.19	66,71,73,74	3
5	GOL	A	611	6/6	0.87	0.16	35,37,40,44	2
5	GOL	C	617	6/6	0.88	0.16	49,50,55,55	1
5	GOL	C	616	6/6	0.88	0.16	43,47,48,54	1
5	GOL	A	615	6/6	0.89	0.16	28,37,39,44	4
3	SO4	C	603	5/5	0.89	0.14	52,60,80,81	2
3	SO4	C	610	5/5	0.89	0.12	42,44,46,55	2
3	SO4	A	608	5/5	0.89	0.13	44,47,60,65	4
3	SO4	A	604	5/5	0.89	0.16	41,48,54,57	3
5	GOL	A	613	6/6	0.89	0.14	58,62,64,66	0
3	SO4	A	602	5/5	0.90	0.11	45,47,53,59	4
3	SO4	C	608	5/5	0.90	0.12	52,65,73,74	3
5	GOL	B	610	6/6	0.90	0.10	46,52,56,57	0
3	SO4	C	613	5/5	0.90	0.20	59,64,66,72	4
3	SO4	A	606	5/5	0.91	0.14	68,69,84,95	1
3	SO4	A	607	5/5	0.91	0.10	58,58,73,74	2
5	GOL	B	618	6/6	0.91	0.16	47,48,57,59	1
5	GOL	B	612	6/6	0.91	0.13	49,51,55,58	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	613	6/6	0.91	0.11	41,44,46,47	2
5	GOL	A	614	6/6	0.91	0.11	48,55,58,59	0
5	GOL	A	619	6/6	0.91	0.13	46,49,54,56	2
5	GOL	A	620	6/6	0.92	0.11	31,37,41,55	2
5	GOL	A	616	6/6	0.92	0.12	33,35,36,37	1
5	GOL	C	620	6/6	0.92	0.15	26,28,31,41	4
5	GOL	C	618	6/6	0.93	0.09	38,39,44,47	2
3	SO4	A	603	5/5	0.93	0.12	49,50,55,57	3
3	SO4	B	604	5/5	0.93	0.10	43,46,55,60	3
3	SO4	B	607	5/5	0.94	0.16	34,35,37,38	4
5	GOL	C	621	6/6	0.94	0.14	35,39,41,46	4
3	SO4	C	602	5/5	0.95	0.13	29,34,43,43	3
4	MG	B	609	1/1	0.96	0.08	45,45,45,45	0
3	SO4	B	602	5/5	0.97	0.09	40,47,51,54	3
4	MG	C	604	1/1	0.97	0.08	40,40,40,40	0
4	MG	A	610	1/1	0.99	0.04	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.