



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:36 PM UTC

PDB ID : 3NAI / pdb_00003nai
Title : Crystal structures and functional analysis of murine norovirus RNA-dependent RNA polymerase
Authors : Kim, K.H.; Lee, J.H.; Alam, I.; Park, Y.; Kang, S.
Deposited on : 2010-06-02
Resolution : 2.56 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
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

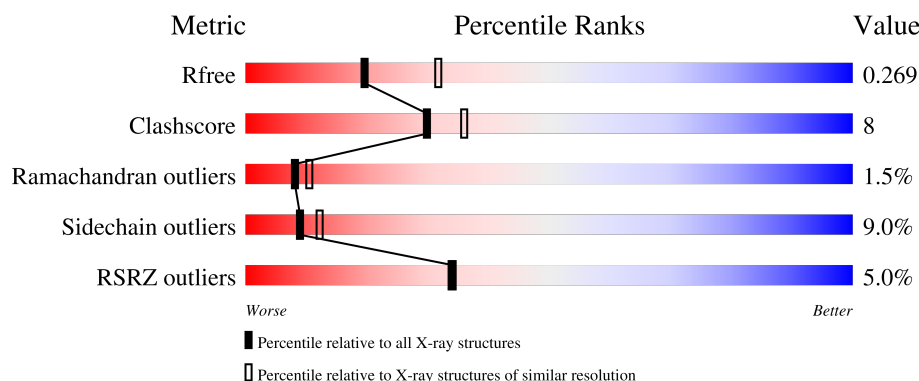
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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% 71% 20% • 6%
1	B	517	5% 73% 19% • 6%
1	C	517	4% 71% 19% • 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
3	URF	A	521	-	X	-	-
3	URF	B	521	-	X	-	-
3	URF	C	521	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12037 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 dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3857	2437	679	716	25			
1	B	486	Total	C	N	O	S	0	0	0
			3857	2437	679	716	25			
1	C	486	Total	C	N	O	S	0	0	0
			3857	2437	679	716	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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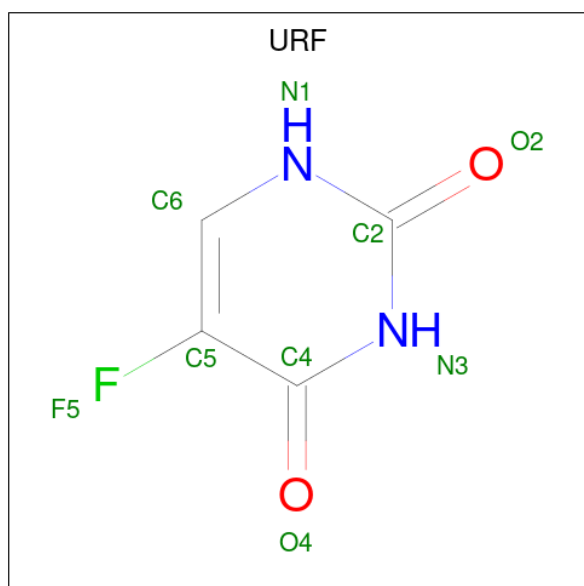
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Chain	Residue	Modelled	Actual	Comment	Reference
C	511	ALA	-	expression tag	UNP Q80J95
C	512	ALA	-	expression tag	UNP Q80J95
C	513	LEU	-	expression tag	UNP Q80J95
C	514	GLU	-	expression tag	UNP Q80J95
C	515	HIS	-	expression tag	UNP Q80J95
C	516	HIS	-	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 5-FLUOROURACIL (CCD ID: URF) (formula: C₄H₃FN₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O 9 4 1 2 2	0	0

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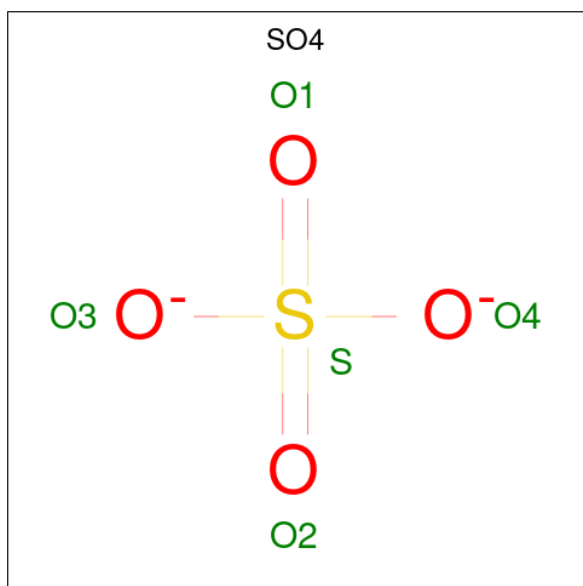
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
3	C	1	Total	C	F	N	O	0	0
			9	4	1	2	2		

- Molecule 4 is MANGANESE (III) ION (CCD ID: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	B	2	Total	Mn	0	0
			2	2		
4	C	2	Total	Mn	0	0
			2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



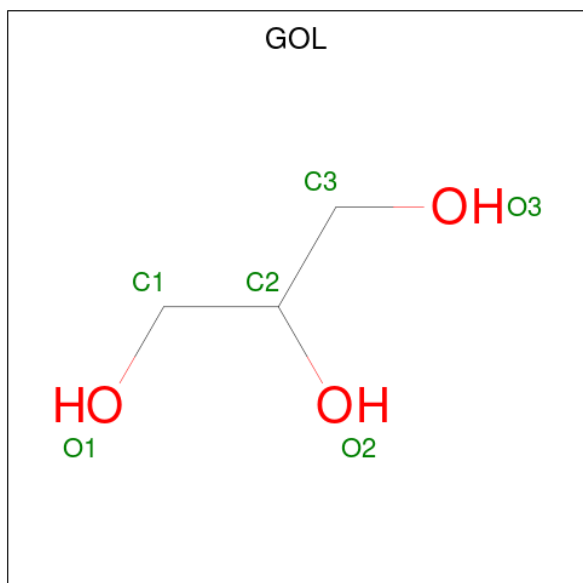
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

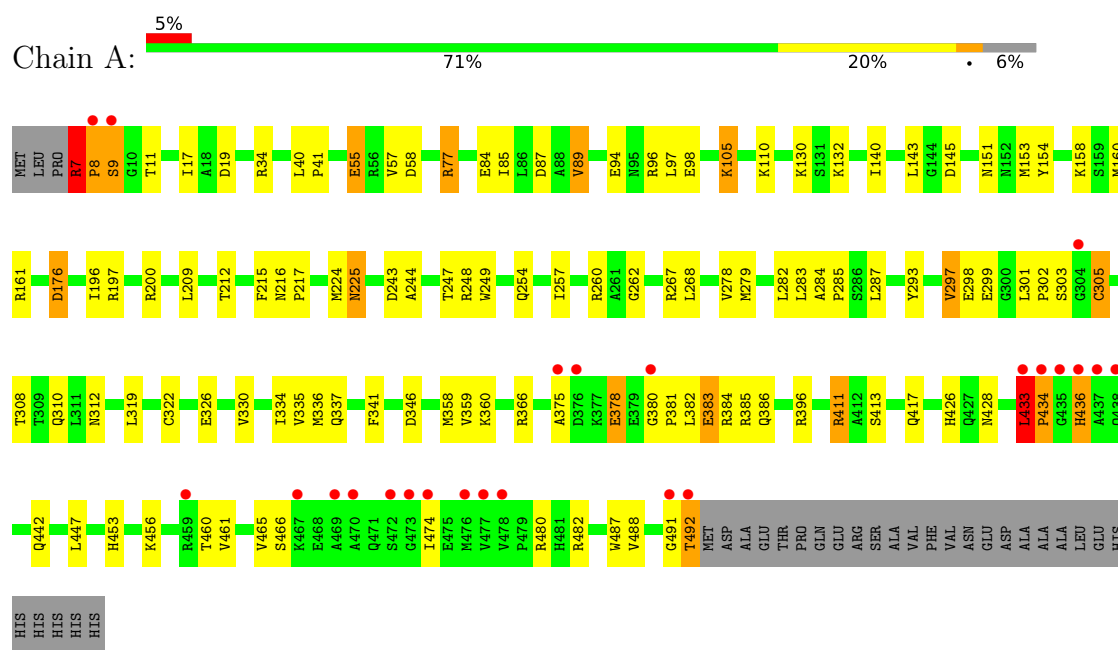
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	130	Total	O	0	0
			130	130		
7	B	106	Total	O	0	0
			106	106		
7	C	112	Total	O	0	0
			112	112		

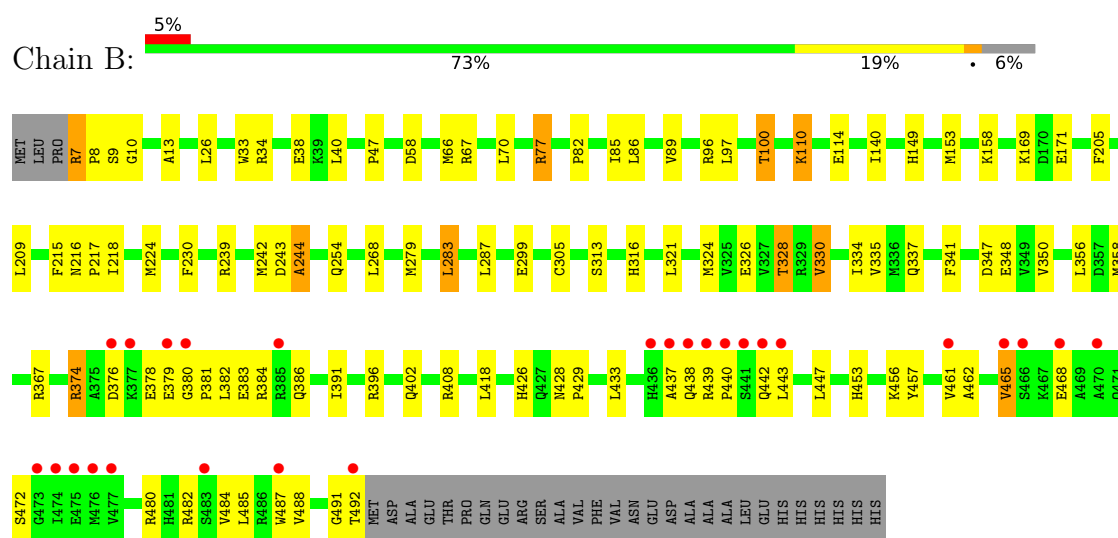
3 Residue-property plots [i](#)

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.

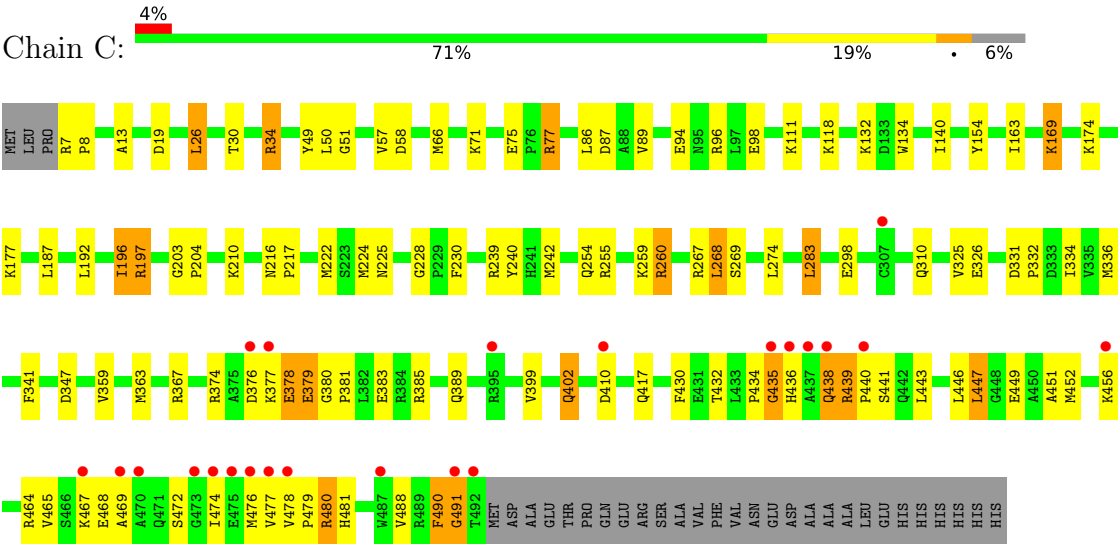
• Molecule 1: RNA dependent RNA polymerase



• Molecule 1: RNA dependent RNA polymerase



• Molecule 1: RNA dependent 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	121.25Å 196.56Å 109.60Å 90.00° 114.81° 90.00°	Depositor
Resolution (Å)	39.53 – 2.56 39.53 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.53-2.56) 98.7 (39.53-2.56)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.268 0.203 , 0.269	Depositor DCC
R_{free} test set	3738 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12037	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN3, URF, 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	0.59	0/3952	0.91	3/5355 (0.1%)
1	B	0.59	0/3952	0.88	0/5355
1	C	0.59	0/3952	0.87	4/5355 (0.1%)
All	All	0.59	0/11856	0.89	7/16065 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ARG	CA-C-N	5.41	126.60	119.84
1	A	7	ARG	C-N-CA	5.41	126.60	119.84
1	A	297	VAL	CB-CA-C	5.32	117.76	111.32
1	C	380	GLY	CA-C-N	5.10	126.22	119.84
1	C	380	GLY	C-N-CA	5.10	126.22	119.84
1	C	269	SER	CA-C-N	5.00	125.03	119.32
1	C	269	SER	C-N-CA	5.00	125.03	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3857	0	3812	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3857	0	3812	65	0
1	C	3857	0	3812	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	9	0	3	1	0
3	B	9	0	3	0	0
3	C	9	0	3	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	30	0	0	1	0
5	B	25	0	0	0	0
5	C	15	0	0	0	0
6	A	6	0	8	3	0
6	C	6	0	8	1	0
7	A	130	0	0	10	0
7	B	106	0	0	5	0
7	C	112	0	0	7	0
All	All	12037	0	11461	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (196) 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:305:CYS:HB2	7:A:561:HOH:O	1.40	1.21
1:B:328:THR:HG23	1:B:330:VAL:HG13	1.36	1.04
1:A:366:ARG:HD3	7:A:583:HOH:O	1.63	0.96
1:B:100:THR:CG2	1:B:216:ASN:HD21	1.84	0.90
1:A:487:TRP:HB2	7:A:606:HOH:O	1.70	0.90
1:B:100:THR:HG21	1:B:216:ASN:HD21	1.40	0.83
1:B:149:HIS:NE2	1:B:153:MET:HE2	1.93	0.83
1:A:7:ARG:HH11	1:A:7:ARG:HA	1.44	0.82
1:A:209:LEU:O	1:A:212:THR:HG22	1.81	0.80
1:A:151:ASN:HD21	1:A:200:ARG:HH11	1.31	0.78
1:B:358:MET:HE3	1:B:384:ARG:HB3	1.67	0.77
1:A:434:PRO:HD3	7:A:654:HOH:O	1.85	0.77
1:B:239:ARG:HD3	7:B:609:HOH:O	1.82	0.77
1:C:379:GLU:HG3	7:C:621:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:MET:HG2	1:A:396:ARG:HD2	1.69	0.74
1:C:464:ARG:HD2	7:C:592:HOH:O	1.87	0.73
1:C:436:HIS:HE1	1:C:439:ARG:HB2	1.54	0.72
1:C:87:ASP:OD1	1:C:260:ARG:NH2	2.23	0.72
1:B:149:HIS:HE2	1:B:153:MET:HE2	1.56	0.70
1:A:257:ILE:HD13	1:A:319:LEU:HD21	1.73	0.70
1:B:149:HIS:CE1	1:B:153:MET:HE2	2.27	0.69
1:C:439:ARG:H	1:C:440:PRO:HD3	1.59	0.67
1:B:13:ALA:HB2	1:B:67:ARG:HG2	1.76	0.66
1:A:358:MET:HE3	1:A:384:ARG:HB3	1.77	0.66
1:C:379:GLU:OE2	1:C:379:GLU:HA	1.97	0.65
1:A:433:LEU:HB2	1:A:434:PRO:HD2	1.78	0.64
1:A:380:GLY:HA2	1:A:381:PRO:O	1.97	0.64
1:B:82:PRO:HG2	1:B:85:ILE:HD12	1.81	0.62
1:B:328:THR:CG2	1:B:330:VAL:HG13	2.21	0.62
1:B:100:THR:HG21	1:B:216:ASN:ND2	2.14	0.62
1:A:346:ASP:CG	3:A:521:URF:HN3	2.07	0.61
1:C:98:GLU:HG3	1:C:268:LEU:HD11	1.83	0.61
1:C:439:ARG:N	1:C:440:PRO:CD	2.63	0.61
1:B:100:THR:HG23	1:B:216:ASN:HD21	1.62	0.60
1:C:225:ASN:HD21	1:C:488:VAL:HG22	1.66	0.60
1:B:243:ASP:HB3	1:B:391:ILE:HG23	1.82	0.60
1:C:94:GLU:OE2	1:C:267:ARG:HD2	2.02	0.60
1:B:356:LEU:HD23	1:B:358:MET:HE1	1.84	0.59
1:A:40:LEU:HD12	1:A:41:PRO:HD2	1.84	0.59
1:C:326:GLU:CD	1:C:367:ARG:HH22	2.11	0.58
1:C:443:LEU:HD11	1:C:469:ALA:HB3	1.84	0.58
1:B:324:MET:O	1:B:328:THR:HB	2.04	0.58
1:A:491:GLY:HA2	1:A:492:THR:HG23	1.86	0.57
1:A:243:ASP:HB3	1:A:375:ALA:HB2	1.87	0.57
1:A:383:GLU:HG2	1:A:385:ARG:NH1	2.20	0.56
1:B:7:ARG:N	1:B:8:PRO:CD	2.69	0.56
1:A:58:ASP:HB3	7:A:570:HOH:O	2.06	0.56
1:A:96:ARG:HE	1:A:216:ASN:ND2	2.04	0.56
1:A:417:GLN:HE21	1:A:442:GLN:NE2	2.04	0.56
1:A:85:ILE:O	1:A:89:VAL:HG13	2.06	0.55
1:A:433:LEU:HB2	1:A:434:PRO:CD	2.37	0.55
1:B:169:LYS:HD3	1:B:171:GLU:CD	2.32	0.55
1:C:374:ARG:HH21	1:C:377:LYS:HB2	1.72	0.55
1:A:417:GLN:HE21	1:A:442:GLN:HE21	1.54	0.55
1:C:439:ARG:N	1:C:440:PRO:HD3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LYS:HG3	1:B:457:TYR:H	1.73	0.54
1:B:437:ALA:C	1:B:439:ARG:H	2.14	0.54
1:A:105:LYS:H	1:A:105:LYS:NZ	2.05	0.54
1:C:13:ALA:H	6:C:2:GOL:H2	1.72	0.53
1:C:436:HIS:CE1	1:C:439:ARG:HB2	2.40	0.53
1:B:169:LYS:HD3	1:B:171:GLU:OE1	2.08	0.53
1:A:110:LYS:HD2	7:A:621:HOH:O	2.08	0.53
1:A:212:THR:HG23	1:A:216:ASN:HB2	1.91	0.53
1:A:491:GLY:HA3	1:A:492:THR:C	2.34	0.53
3:C:521:URF:N1	7:C:636:HOH:O	2.34	0.53
1:A:456:LYS:O	1:A:460:THR:HG23	2.09	0.52
1:A:151:ASN:ND2	1:A:200:ARG:HH11	2.03	0.52
1:B:443:LEU:HG	1:B:465:VAL:CG2	2.40	0.52
1:C:203:GLY:N	1:C:204:PRO:HD2	2.25	0.52
1:C:225:ASN:ND2	1:C:488:VAL:HG22	2.24	0.52
1:C:8:PRO:HD2	1:C:19:ASP:HA	1.92	0.52
1:B:97:LEU:HA	1:B:100:THR:HG22	1.92	0.52
1:B:34:ARG:NH1	1:B:40:LEU:HD13	2.25	0.52
1:C:383:GLU:CG	1:C:385:ARG:HH12	2.23	0.52
1:B:205:PHE:CE2	1:B:209:LEU:HD22	2.45	0.51
1:A:217:PRO:HB3	1:A:341:PHE:HB2	1.91	0.51
1:A:154:TYR:HB2	1:A:197:ARG:HG3	1.93	0.51
1:A:153:MET:HG3	1:A:160:MET:SD	2.51	0.51
1:C:383:GLU:HG2	1:C:385:ARG:HH12	1.76	0.51
1:B:330:VAL:HG22	1:B:335:VAL:HG22	1.92	0.51
1:C:118:LYS:HE2	1:C:134:TRP:CD2	2.45	0.51
1:B:426:HIS:CE1	1:B:428:ASN:O	2.65	0.50
1:A:94:GLU:OE2	1:A:267:ARG:HD2	2.12	0.50
1:C:169:LYS:HG2	1:C:187:LEU:HD11	1.93	0.50
1:B:386:GLN:NE2	7:B:609:HOH:O	2.41	0.50
1:C:439:ARG:H	1:C:440:PRO:CD	2.21	0.50
1:C:34:ARG:HG3	1:C:430:PHE:HA	1.94	0.50
1:C:255:ARG:HG3	1:C:298:GLU:O	2.12	0.50
1:A:249:TRP:HE1	1:A:312:ASN:ND2	2.10	0.50
1:A:334:ILE:HA	1:A:337:GLN:HG2	1.93	0.50
1:B:243:ASP:O	1:B:244:ALA:C	2.54	0.50
1:C:436:HIS:CE1	1:C:439:ARG:HD3	2.47	0.50
1:B:224:MET:HE3	1:B:396:ARG:HD3	1.94	0.50
1:A:7:ARG:CG	6:A:528:GOL:O3	2.60	0.49
1:C:49:TYR:CE2	1:C:51:GLY:HA2	2.47	0.49
1:B:408:ARG:HD3	1:B:453:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLN:HE22	1:C:399:VAL:HG13	1.78	0.49
1:A:247:THR:HG22	1:A:248:ARG:HG3	1.94	0.49
1:A:8:PRO:HG2	1:A:17:ILE:O	2.13	0.49
1:B:217:PRO:HB3	1:B:341:PHE:HB2	1.95	0.49
1:B:316:HIS:CE1	1:B:348:GLU:HB3	2.47	0.49
1:C:363:MET:HG3	7:C:603:HOH:O	2.12	0.49
1:A:278:VAL:O	1:A:282:LEU:HG	2.12	0.49
1:A:249:TRP:HE1	1:A:312:ASN:HD21	1.59	0.49
1:A:284:ALA:O	1:A:285:PRO:C	2.56	0.48
1:A:209:LEU:HD23	1:A:310:GLN:HG2	1.96	0.48
1:B:77:ARG:HG3	1:B:254:GLN:HG2	1.95	0.48
1:B:230:PHE:O	1:B:230:PHE:HD1	1.97	0.48
1:A:433:LEU:H	1:A:433:LEU:HD23	1.79	0.47
1:C:174:LYS:HG2	1:C:177:LYS:HD2	1.95	0.47
1:A:303:SER:HA	1:A:308:THR:HG21	1.95	0.47
1:B:487:TRP:HE1	1:B:492:THR:HB	1.79	0.47
1:C:224:MET:O	1:C:228:GLY:HA3	2.15	0.47
1:B:341:PHE:HE1	1:B:350:VAL:HG13	1.79	0.47
1:C:259:LYS:HA	1:C:283:LEU:HD23	1.96	0.47
1:C:239:ARG:HD2	1:C:240:TYR:CZ	2.49	0.47
1:C:310:GLN:HG2	7:C:569:HOH:O	2.14	0.47
1:A:9:SER:CB	6:A:528:GOL:H32	2.45	0.47
1:B:218:ILE:HG12	1:B:313:SER:HB3	1.97	0.47
1:B:10:GLY:HA2	7:B:588:HOH:O	2.13	0.47
1:A:77:ARG:HG3	1:A:254:GLN:HG2	1.97	0.47
1:C:197:ARG:NH1	7:C:570:HOH:O	2.48	0.46
1:A:96:ARG:HE	1:A:216:ASN:HD21	1.62	0.46
1:B:47:PRO:HG2	1:B:429:PRO:HB3	1.97	0.46
1:C:480:ARG:NH1	7:C:550:HOH:O	2.48	0.46
1:B:462:ALA:O	1:B:465:VAL:HG12	2.15	0.46
1:C:217:PRO:HB3	1:C:341:PHE:HB2	1.98	0.46
1:B:341:PHE:CE1	1:B:350:VAL:HG13	2.51	0.46
1:B:356:LEU:HD23	1:B:358:MET:CE	2.45	0.46
1:B:337:GLN:HG3	1:C:402:GLN:HG3	1.97	0.46
7:B:563:HOH:O	1:C:402:GLN:HB3	2.16	0.46
1:C:478:VAL:HA	1:C:479:PRO:HD3	1.76	0.46
1:B:77:ARG:HD2	1:B:299:GLU:OE1	2.15	0.45
1:A:426:HIS:CE1	1:A:428:ASN:O	2.69	0.45
1:C:26:LEU:HD11	1:C:66:MET:HE1	1.99	0.45
1:B:33:TRP:CE3	1:B:433:LEU:HB3	2.51	0.45
1:A:9:SER:OG	6:A:528:GOL:H12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:LEU:HD13	1:C:465:VAL:HG21	1.98	0.45
1:A:96:ARG:NH2	1:A:215:PHE:O	2.50	0.45
1:A:176:ASP:HB2	7:A:572:HOH:O	2.17	0.45
1:A:411:ARG:HD2	1:A:453:HIS:CE1	2.53	0.44
1:B:437:ALA:C	1:B:439:ARG:N	2.75	0.44
1:C:383:GLU:HG2	1:C:385:ARG:NH1	2.32	0.44
1:A:153:MET:HE3	1:A:158:LYS:HB3	1.98	0.44
1:A:436:HIS:HB2	7:A:619:HOH:O	2.17	0.44
1:A:225:ASN:HD21	1:A:488:VAL:HG13	1.82	0.44
1:B:96:ARG:NH2	1:B:215:PHE:O	2.50	0.44
1:B:456:LYS:CG	1:B:457:TYR:H	2.30	0.44
1:B:480:ARG:HH22	1:B:482:ARG:HG3	1.82	0.44
1:C:30:THR:HB	1:C:50:LEU:HD21	1.98	0.44
1:C:449:GLU:HA	1:C:452:MET:HE3	2.00	0.44
1:B:328:THR:HG22	1:B:330:VAL:H	1.82	0.44
1:B:461:VAL:O	1:B:465:VAL:HB	2.18	0.43
1:C:96:ARG:HE	1:C:216:ASN:HD22	1.66	0.43
1:A:8:PRO:HG3	1:A:19:ASP:HA	2.00	0.43
1:C:417:GLN:HB2	1:C:446:LEU:HD21	2.00	0.43
1:B:456:LYS:HG3	1:B:457:TYR:N	2.32	0.43
1:A:87:ASP:OD1	1:A:260:ARG:NH2	2.44	0.43
1:A:456:LYS:HG3	7:A:567:HOH:O	2.17	0.43
1:B:326:GLU:OE1	1:B:367:ARG:NH1	2.42	0.43
1:B:66:MET:HG2	1:B:66:MET:O	2.18	0.43
1:A:480:ARG:HD3	1:A:482:ARG:HG2	2.00	0.42
1:B:328:THR:CG2	1:B:330:VAL:H	2.32	0.42
1:C:490:PHE:HB2	1:C:491:GLY:H	1.73	0.42
1:A:301:LEU:HA	1:A:302:PRO:HD3	1.90	0.42
1:B:110:LYS:O	1:B:114:GLU:HB2	2.20	0.42
1:B:374:ARG:NH2	1:B:383:GLU:OE1	2.52	0.42
1:A:262:GLY:HA2	1:A:279:MET:HE3	2.01	0.42
1:B:485:LEU:HA	1:B:488:VAL:HG12	2.01	0.42
1:C:374:ARG:HG2	1:C:377:LYS:H	1.84	0.42
1:A:130:LYS:NZ	5:A:3:SO4:O3	2.53	0.42
1:A:480:ARG:HH11	1:A:482:ARG:H	1.66	0.42
1:B:77:ARG:CG	1:B:254:GLN:HG2	2.49	0.42
1:C:132:LYS:HE2	1:C:132:LYS:HB3	1.92	0.42
1:C:77:ARG:HG2	1:C:254:GLN:HG2	2.02	0.42
1:A:55:GLU:HG2	7:A:633:HOH:O	2.19	0.42
1:B:287:LEU:HD12	1:B:287:LEU:HA	1.93	0.42
1:B:380:GLY:HA2	1:B:381:PRO:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:VAL:HG21	1:C:332:PRO:HG3	2.01	0.41
1:A:17:ILE:HG23	1:A:293:TYR:HB3	2.03	0.41
1:A:322:CYS:O	1:A:326:GLU:HB2	2.20	0.41
1:A:383:GLU:HG2	1:A:385:ARG:HH12	1.86	0.41
1:C:154:TYR:HB2	1:C:197:ARG:HG3	2.03	0.41
1:C:222:MET:HE2	1:C:224:MET:HA	2.03	0.41
1:B:89:VAL:HG13	1:B:321:LEU:HD23	2.03	0.41
1:C:230:PHE:O	1:C:230:PHE:HD1	2.03	0.41
1:C:7:ARG:HA	1:C:8:PRO:HA	1.86	0.40
1:B:279:MET:SD	1:B:283:LEU:HD22	2.61	0.40
1:B:472:SER:HB3	7:B:602:HOH:O	2.19	0.40
1:C:331:ASP:HB2	1:C:334:ILE:HD12	2.03	0.40
1:C:192:LEU:O	1:C:196:ILE:HG23	2.21	0.40
1:C:434:PRO:O	1:C:435:GLY:C	2.64	0.40
1:C:451:ALA:O	1:C:481:HIS:HE1	2.04	0.40
1:A:77:ARG:CG	1:A:254:GLN:HG2	2.51	0.40
1:A:77:ARG:HD2	1:A:299:GLU:CD	2.47	0.40
1:C:374:ARG:HE	1:C:377:LYS:H	1.70	0.40

There are no symmetry-related clashes.

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	484/517 (94%)	460 (95%)	18 (4%)	6 (1%)	10	14
1	B	484/517 (94%)	465 (96%)	13 (3%)	6 (1%)	10	14
1	C	484/517 (94%)	454 (94%)	20 (4%)	10 (2%)	5	6
All	All	1452/1551 (94%)	1379 (95%)	51 (4%)	22 (2%)	8	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	244	ALA
1	B	440	PRO
1	B	438	GLN
1	C	376	ASP
1	C	438	GLN
1	C	491	GLY
1	A	378	GLU
1	B	244	ALA
1	B	376	ASP
1	C	435	GLY
1	C	439	ARG
1	C	472	SER
1	B	491	GLY
1	C	381	PRO
1	A	9	SER
1	A	434	PRO
1	B	379	GLU
1	C	378	GLU
1	C	468	GLU
1	C	402	GLN
1	A	433	LEU

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	414/440 (94%)	370 (89%)	44 (11%)	6	8
1	B	414/440 (94%)	384 (93%)	30 (7%)	13	18
1	C	414/440 (94%)	376 (91%)	38 (9%)	8	11
All	All	1242/1320 (94%)	1130 (91%)	112 (9%)	9	12

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG

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Mol	Chain	Res	Type
1	A	11	THR
1	A	34	ARG
1	A	55	GLU
1	A	57	VAL
1	A	77	ARG
1	A	84	GLU
1	A	89	VAL
1	A	97	LEU
1	A	98	GLU
1	A	105	LYS
1	A	132	LYS
1	A	140	ILE
1	A	143	LEU
1	A	145	ASP
1	A	161	ARG
1	A	176	ASP
1	A	196	ILE
1	A	225	ASN
1	A	268	LEU
1	A	283	LEU
1	A	287	LEU
1	A	297	VAL
1	A	298	GLU
1	A	305	CYS
1	A	330	VAL
1	A	335	VAL
1	A	336	MET
1	A	359	VAL
1	A	360	LYS
1	A	378	GLU
1	A	382	LEU
1	A	383	GLU
1	A	386	GLN
1	A	411	ARG
1	A	413	SER
1	A	433	LEU
1	A	436	HIS
1	A	447	LEU
1	A	461	VAL
1	A	465	VAL
1	A	466	SER
1	A	474	ILE

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Mol	Chain	Res	Type
1	A	492	THR
1	B	7	ARG
1	B	9	SER
1	B	26	LEU
1	B	38	GLU
1	B	58	ASP
1	B	70	LEU
1	B	77	ARG
1	B	86	LEU
1	B	100	THR
1	B	110	LYS
1	B	140	ILE
1	B	158	LYS
1	B	242	MET
1	B	268	LEU
1	B	283	LEU
1	B	305	CYS
1	B	328	THR
1	B	330	VAL
1	B	334	ILE
1	B	347	ASP
1	B	374	ARG
1	B	378	GLU
1	B	382	LEU
1	B	402	GLN
1	B	418	LEU
1	B	442	GLN
1	B	447	LEU
1	B	465	VAL
1	B	468	GLU
1	B	484	VAL
1	C	26	LEU
1	C	34	ARG
1	C	57	VAL
1	C	58	ASP
1	C	71	LYS
1	C	75	GLU
1	C	77	ARG
1	C	86	LEU
1	C	89	VAL
1	C	111	LYS
1	C	140	ILE

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Mol	Chain	Res	Type
1	C	163	ILE
1	C	169	LYS
1	C	196	ILE
1	C	197	ARG
1	C	210	LYS
1	C	242	MET
1	C	260	ARG
1	C	268	LEU
1	C	274	LEU
1	C	283	LEU
1	C	336	MET
1	C	347	ASP
1	C	359	VAL
1	C	378	GLU
1	C	379	GLU
1	C	410	ASP
1	C	432	THR
1	C	438	GLN
1	C	441	SER
1	C	447	LEU
1	C	456	LYS
1	C	467	LYS
1	C	474	ILE
1	C	476	MET
1	C	477	VAL
1	C	480	ARG
1	C	490	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	151	ASN
1	A	152	ASN
1	A	216	ASN
1	A	225	ASN
1	A	312	ASN
1	A	417	GLN
1	A	426	HIS
1	A	427	GLN
1	A	438	GLN
1	A	442	GLN

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Mol	Chain	Res	Type
1	A	481	HIS
1	B	129	GLN
1	B	216	ASN
1	B	237	ASN
1	B	253	GLN
1	B	254	GLN
1	B	337	GLN
1	B	427	GLN
1	B	428	ASN
1	B	442	GLN
1	C	63	GLN
1	C	64	GLN
1	C	104	GLN
1	C	216	ASN
1	C	225	ASN
1	C	253	GLN
1	C	425	ASN
1	C	436	HIS
1	C	442	GLN
1	C	471	GLN
1	C	481	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 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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	SO4	B	526	-	4,4,4	0.22	0	6,6,6	0.13	0
5	SO4	A	2	-	4,4,4	0.25	0	6,6,6	0.17	0
5	SO4	B	524	-	4,4,4	0.24	0	6,6,6	0.20	0
5	SO4	C	526	-	4,4,4	0.23	0	6,6,6	0.24	0
5	SO4	A	3	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	A	525	-	4,4,4	0.29	0	6,6,6	0.14	0
5	SO4	B	525	-	4,4,4	0.22	0	6,6,6	0.26	0
5	SO4	B	528	-	4,4,4	0.22	0	6,6,6	0.25	0
5	SO4	B	527	-	4,4,4	0.23	0	6,6,6	0.12	0
3	URF	A	521	2	9,9,9	2.98	4 (44%)	12,12,12	3.95	8 (66%)
5	SO4	A	524	-	4,4,4	0.24	0	6,6,6	0.34	0
6	GOL	C	2	-	5,5,5	0.35	0	5,5,5	0.25	0
3	URF	B	521	2	9,9,9	2.99	3 (33%)	12,12,12	4.13	8 (66%)
5	SO4	A	527	-	4,4,4	0.26	0	6,6,6	0.14	0
3	URF	C	521	-	9,9,9	2.80	4 (44%)	12,12,12	4.37	7 (58%)
6	GOL	A	528	-	5,5,5	0.42	0	5,5,5	0.42	0
5	SO4	C	525	-	4,4,4	0.25	0	6,6,6	0.21	0
5	SO4	C	524	-	4,4,4	0.21	0	6,6,6	0.26	0
5	SO4	A	526	-	4,4,4	0.25	0	6,6,6	0.31	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
6	GOL	A	528	-	-	2/4/4/4	-
6	GOL	C	2	-	-	2/4/4/4	-
3	URF	B	521	2	-	-	0/1/1/1
3	URF	A	521	2	-	-	0/1/1/1
3	URF	C	521	-	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	521	URF	C6-C5	7.02	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	521	URF	C6-C5	6.97	1.39	1.33
3	C	521	URF	C6-C5	6.16	1.39	1.33
3	B	521	URF	C4-C5	4.22	1.49	1.44
3	C	521	URF	C4-C5	4.16	1.49	1.44
3	A	521	URF	C4-C5	3.70	1.49	1.44
3	A	521	URF	C4-N3	-2.93	1.33	1.38
3	C	521	URF	C4-N3	-2.68	1.33	1.38
3	B	521	URF	C4-N3	-2.64	1.33	1.38
3	A	521	URF	C2-N3	-2.30	1.33	1.37
3	C	521	URF	C2-N3	-2.08	1.34	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	521	URF	N1-C2-N3	7.15	122.72	115.17
3	C	521	URF	C5-C4-N3	7.04	119.07	112.64
3	C	521	URF	F5-C5-C4	6.75	122.39	116.47
3	A	521	URF	N1-C2-N3	6.61	122.14	115.17
3	C	521	URF	N1-C2-N3	6.49	122.02	115.17
3	A	521	URF	C5-C4-N3	6.31	118.41	112.64
3	B	521	URF	C5-C4-N3	6.17	118.29	112.64
3	B	521	URF	F5-C5-C4	6.09	121.81	116.47
3	A	521	URF	C6-C5-C4	-5.46	117.41	122.11
3	C	521	URF	C6-C5-C4	-5.38	117.48	122.11
3	B	521	URF	C6-C5-C4	-5.13	117.70	122.11
3	A	521	URF	F5-C5-C4	5.11	120.95	116.47
3	C	521	URF	O4-C4-C5	-4.61	121.77	125.69
3	C	521	URF	C4-N3-C2	-4.53	120.13	126.37
3	A	521	URF	O4-C4-C5	-4.50	121.86	125.69
3	B	521	URF	C4-N3-C2	-4.22	120.56	126.37
3	B	521	URF	O4-C4-C5	-3.98	122.30	125.69
3	A	521	URF	C4-N3-C2	-3.77	121.18	126.37
3	C	521	URF	O2-C2-N1	-3.56	119.12	122.79
3	B	521	URF	O2-C2-N1	-2.86	119.84	122.79
3	B	521	URF	O2-C2-N3	-2.49	117.43	121.86
3	A	521	URF	O2-C2-N3	-2.45	117.51	121.86
3	A	521	URF	O2-C2-N1	-2.37	120.34	122.79

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	528	GOL	O1-C1-C2-C3
6	C	2	GOL	O1-C1-C2-C3
6	A	528	GOL	O1-C1-C2-O2
6	C	2	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3	SO4	1	0
3	A	521	URF	1	0
6	C	2	GOL	1	0
3	C	521	URF	1	0
6	A	528	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

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	486/517 (94%)	-0.09	24 (4%)	35 35	12, 24, 57, 76	2 (0%)
1	B	486/517 (94%)	0.02	26 (5%)	32 32	15, 28, 62, 78	1 (0%)
1	C	486/517 (94%)	0.06	23 (4%)	36 37	17, 29, 63, 81	1 (0%)
All	All	1458/1551 (94%)	-0.00	73 (5%)	34 34	12, 28, 61, 81	4 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	474	ILE	7.7
1	A	8	PRO	7.0
1	C	474	ILE	5.8
1	B	474	ILE	5.4
1	C	477	VAL	5.3
1	C	492	THR	5.3
1	A	473	GLY	5.2
1	C	469	ALA	5.1
1	A	437	ALA	4.9
1	A	477	VAL	4.9
1	A	492	THR	4.8
1	C	437	ALA	4.7
1	B	492	THR	4.4
1	C	476	MET	4.4
1	A	380	GLY	4.2
1	C	438	GLN	4.2
1	B	477	VAL	4.2
1	B	436	HIS	3.9
1	B	440	PRO	3.9
1	A	376	ASP	3.8
1	A	476	MET	3.8
1	C	377	LYS	3.7
1	B	438	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	376	ASP	3.6
1	A	435	GLY	3.6
1	B	473	GLY	3.5
1	B	476	MET	3.5
1	A	436	HIS	3.3
1	C	491	GLY	3.3
1	A	438	GLN	3.3
1	C	473	GLY	3.3
1	B	377	LYS	3.2
1	B	487	TRP	3.1
1	C	487	TRP	3.1
1	B	470	ALA	3.0
1	C	475	GLU	3.0
1	B	441	SER	2.8
1	C	410	ASP	2.8
1	C	470	ALA	2.8
1	A	434	PRO	2.7
1	B	475	GLU	2.7
1	B	437	ALA	2.7
1	A	491	GLY	2.7
1	C	478	VAL	2.7
1	B	380	GLY	2.6
1	A	433	LEU	2.6
1	A	472	SER	2.5
1	B	443	LEU	2.5
1	A	375	ALA	2.5
1	A	470	ALA	2.4
1	C	467	LYS	2.4
1	B	483	SER	2.4
1	B	442	GLN	2.4
1	A	467	LYS	2.3
1	B	379	GLU	2.3
1	C	307	CYS	2.3
1	B	376	ASP	2.3
1	B	465	VAL	2.2
1	C	435	GLY	2.2
1	A	9	SER	2.2
1	A	478	VAL	2.2
1	C	395	ARG	2.2
1	A	469	ALA	2.1
1	B	385	ARG	2.1
1	B	439	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	466	SER	2.1
1	C	440	PRO	2.1
1	A	459	ARG	2.1
1	C	436	HIS	2.1
1	C	456	LYS	2.1
1	A	304	GLY	2.1
1	B	468	GLU	2.1
1	B	461	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	URF	B	521	9/9	0.58	0.27	56,56,57,58	9
5	SO4	A	527	5/5	0.78	0.16	104,104,104,104	0
3	URF	C	521	9/9	0.79	0.17	71,71,72,72	0
6	GOL	A	528	6/6	0.85	0.12	37,39,39,40	0
3	URF	A	521	9/9	0.86	0.16	70,71,71,72	0
5	SO4	C	525	5/5	0.86	0.16	70,70,71,71	0
5	SO4	A	2	5/5	0.86	0.14	80,80,80,80	0
6	GOL	C	2	6/6	0.87	0.15	53,54,55,55	0
5	SO4	B	528	5/5	0.88	0.26	87,87,87,88	0
5	SO4	C	526	5/5	0.90	0.19	77,77,78,78	0
5	SO4	A	3	5/5	0.91	0.15	75,76,76,76	0
5	SO4	B	525	5/5	0.91	0.15	52,52,53,53	0
5	SO4	B	527	5/5	0.91	0.20	86,86,86,86	0
5	SO4	A	526	5/5	0.91	0.23	69,70,70,70	0
5	SO4	B	526	5/5	0.93	0.14	70,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	3	1/1	0.94	0.11	48,48,48,48	0
5	SO4	A	525	5/5	0.94	0.14	52,53,53,53	0
5	SO4	B	524	5/5	0.96	0.08	46,46,47,47	0
5	SO4	C	524	5/5	0.96	0.07	46,46,47,47	0
2	MG	B	2	1/1	0.98	0.06	33,33,33,33	0
4	MN3	C	523	1/1	0.98	0.05	55,55,55,55	0
5	SO4	A	524	5/5	0.98	0.07	40,40,40,41	0
4	MN3	A	522	1/1	0.99	0.03	47,47,47,47	0
4	MN3	A	523	1/1	0.99	0.03	40,40,40,40	0
4	MN3	C	522	1/1	0.99	0.03	46,46,46,46	0
2	MG	A	1	1/1	0.99	0.04	26,26,26,26	0
4	MN3	B	522	1/1	1.00	0.01	42,42,42,42	0
4	MN3	B	523	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.