



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:36 PM UTC

PDB ID : 3UQS / pdb_00003uqs
Title : Crystal structures of murine norovirus RNA-dependent RNA polymerase
Authors : Milani, M.; Mastrangelo, E.; Bolognesi, M.
Deposited on : 2011-11-21
Resolution : 2.00 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

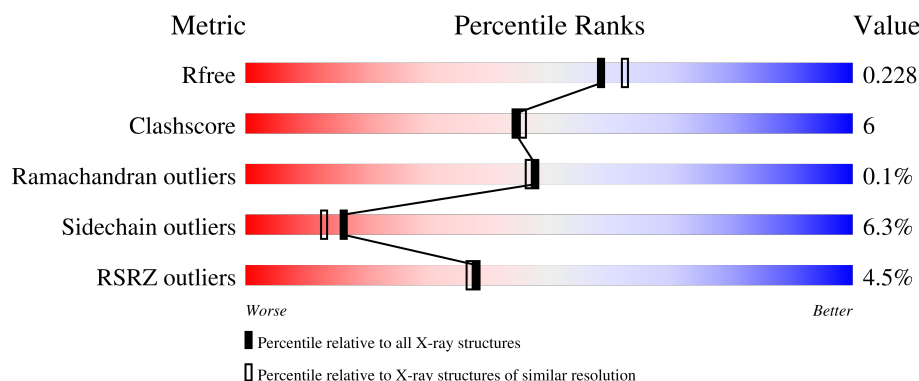
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	515	4% 78% 14% • 7%
1	B	515	5% 78% 13% • 6%
1	C	515	3% 78% 13% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12943 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	478	Total	C	N	O	S	0	5	0
			3828	2428	673	702	25			
1	B	482	Total	C	N	O	S	6	8	0
			3880	2458	685	710	27			
1	C	475	Total	C	N	O	S	0	6	0
			3815	2415	673	702	25			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	LEU	-	expression tag	UNP Q80J95
A	509	GLU	-	expression tag	UNP Q80J95
A	510	HIS	-	expression tag	UNP Q80J95
A	511	HIS	-	expression tag	UNP Q80J95
A	512	HIS	-	expression tag	UNP Q80J95
A	513	HIS	-	expression tag	UNP Q80J95
A	514	HIS	-	expression tag	UNP Q80J95
A	515	HIS	-	expression tag	UNP Q80J95
B	508	LEU	-	expression tag	UNP Q80J95
B	509	GLU	-	expression tag	UNP Q80J95
B	510	HIS	-	expression tag	UNP Q80J95
B	511	HIS	-	expression tag	UNP Q80J95
B	512	HIS	-	expression tag	UNP Q80J95
B	513	HIS	-	expression tag	UNP Q80J95
B	514	HIS	-	expression tag	UNP Q80J95
B	515	HIS	-	expression tag	UNP Q80J95
C	508	LEU	-	expression tag	UNP Q80J95
C	509	GLU	-	expression tag	UNP Q80J95
C	510	HIS	-	expression tag	UNP Q80J95
C	511	HIS	-	expression tag	UNP Q80J95
C	512	HIS	-	expression tag	UNP Q80J95
C	513	HIS	-	expression tag	UNP Q80J95
C	514	HIS	-	expression tag	UNP Q80J95

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Chain	Residue	Modelled	Actual	Comment	Reference
C	515	HIS	-	expression tag	UNP Q80J95

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

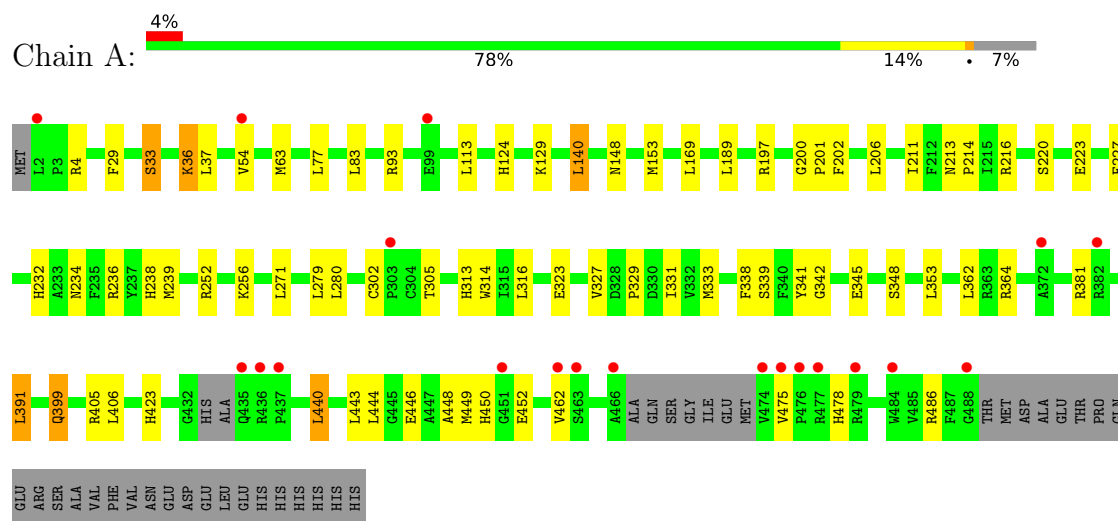
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	444	Total	O	0	0
			444	444		
3	B	450	Total	O	0	0
			450	450		
3	C	461	Total	O	0	0
			461	461		

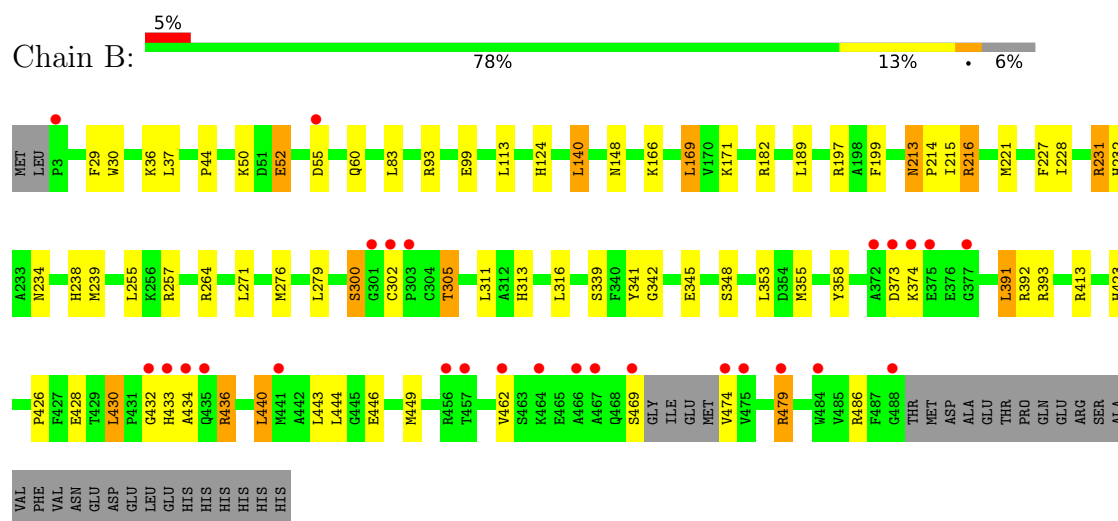
3 Residue-property plots [i](#)

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.

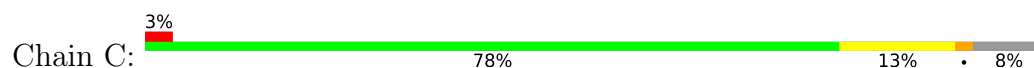
• Molecule 1: RNA-dependent RNA polymerase

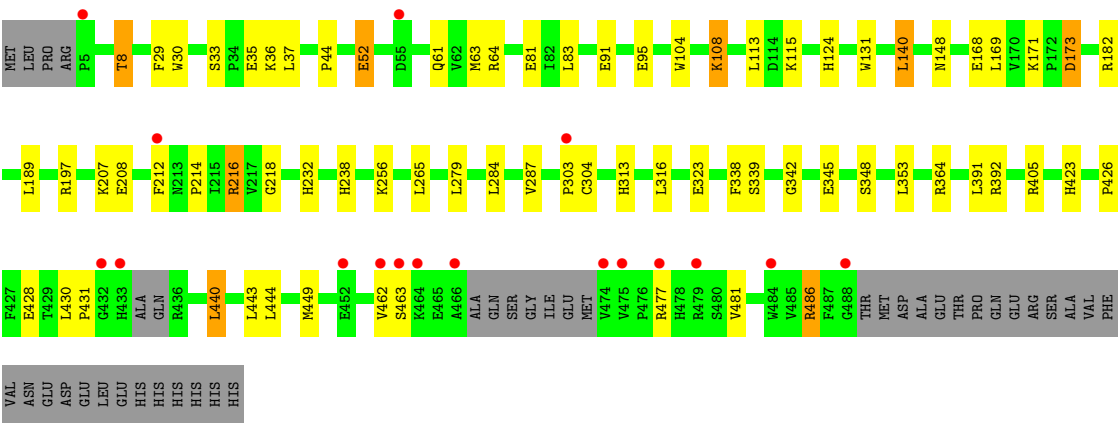


• Molecule 1: RNA-dependent RNA polymerase



• 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	120.67Å 196.33Å 109.15Å 90.00° 114.34° 90.00°	Depositor
Resolution (Å)	28.75 – 2.00 28.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.75-2.00) 99.6 (28.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.227 0.186 , 0.228	Depositor DCC
R_{free} test set	7807 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.9	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	0.95	EDS
Total number of atoms	12943	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: 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	0.68	0/3937	0.85	3/5331 (0.1%)
1	B	0.68	0/4000	0.84	2/5414 (0.0%)
1	C	0.70	0/3926	0.83	0/5314
All	All	0.69	0/11863	0.84	5/16059 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ASN	CA-C-N	5.58	125.41	119.28
1	B	213	ASN	C-N-CA	5.58	125.41	119.28
1	A	236	ARG	N-CA-C	5.50	117.08	111.14
1	A	4	ARG	CA-C-N	-5.30	115.12	120.21
1	A	4	ARG	C-N-CA	-5.30	115.12	120.21

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	3828	0	3803	47	0
1	B	3880	0	3865	55	0
1	C	3815	0	3790	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
3	A	444	0	0	6	0
3	B	450	0	0	5	0
3	C	461	0	0	9	0
All	All	12943	0	11458	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (137) 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:B:239:MET:CE	1:B:355:MET:HE1	1.93	0.98
1:A:148:ASN:HD21	1:A:197:ARG:NH1	1.62	0.97
1:A:148:ASN:ND2	1:A:197:ARG:HH11	1.65	0.94
1:B:239:MET:HE1	1:B:355:MET:HE1	1.51	0.93
1:C:148:ASN:HD21	1:C:197:ARG:HH11	1.12	0.92
1:B:479:ARG:HH11	1:B:479:ARG:HG3	1.39	0.85
1:B:148:ASN:HD21	1:B:197:ARG:HH11	1.30	0.77
1:C:168:GLU:OE2	1:C:182:ARG:HD3	1.85	0.77
1:B:216[B]:ARG:NH1	1:B:228:ILE:HG12	2.00	0.77
1:A:148:ASN:HD21	1:A:197:ARG:HH11	0.84	0.76
1:B:446:GLU:HA	1:B:449:MET:HE3	1.68	0.74
1:A:29:PHE:O	1:A:423:HIS:HE1	1.69	0.72
1:C:440:LEU:HG	1:C:462:VAL:HG13	1.71	0.72
1:B:486[A]:ARG:HH11	1:B:486[A]:ARG:HB3	1.54	0.72
1:B:239:MET:HE3	1:B:355:MET:HE1	1.72	0.70
1:A:238:HIS:HD2	1:A:348:SER:OG	1.76	0.68
1:A:314:TRP:HZ2	1:A:333[A]:MET:HE1	1.60	0.66
1:C:148:ASN:HD21	1:C:197:ARG:NH1	1.91	0.66
1:C:148:ASN:ND2	1:C:197:ARG:HH11	1.91	0.65
1:A:313:HIS:HD2	1:A:342:GLY:O	1.79	0.65
1:C:238:HIS:HD2	1:C:348:SER:OG	1.79	0.65
1:C:81:GLU:H	1:C:81:GLU:CD	2.05	0.65
1:B:486[A]:ARG:HB3	1:B:486[A]:ARG:NH1	2.11	0.65
1:A:232:HIS:HE1	1:A:339:SER:OG	1.82	0.62
1:A:440:LEU:HG	1:A:462:VAL:HG13	1.80	0.62
1:B:29:PHE:O	1:B:423:HIS:HE1	1.82	0.62
1:B:313:HIS:HE1	1:B:345:GLU:OE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:HIS:HE1	3:A:827:HOH:O	1.82	0.62
1:B:238:HIS:HD2	1:B:348:SER:OG	1.82	0.62
1:C:140:LEU:HG	1:C:189:LEU:HD22	1.81	0.61
1:B:232:HIS:HD2	1:B:348:SER:OG	1.84	0.60
1:A:406:LEU:O	1:A:450:HIS:HE1	1.85	0.60
1:C:95:GLU:HG3	1:C:265:LEU:HD21	1.84	0.59
1:B:479:ARG:HG3	1:B:479:ARG:NH1	2.06	0.58
1:A:36:LYS:H	1:A:36:LYS:HE2	1.68	0.58
1:C:303:PRO:HD2	3:C:550:HOH:O	2.03	0.58
1:A:211:ILE:HG21	1:A:227[A]:PHE:CD2	2.37	0.58
1:B:216[B]:ARG:HH11	1:B:228:ILE:HG12	1.67	0.58
1:A:405:ARG:HG3	1:A:449:MET:HE3	1.86	0.57
1:A:448:ALA:O	1:A:478:HIS:HE1	1.87	0.56
1:A:93:ARG:HE	1:A:213:ASN:HD22	1.52	0.56
1:B:232:HIS:HE1	1:B:339:SER:OG	1.88	0.56
1:B:313:HIS:HD2	1:B:342:GLY:O	1.89	0.56
1:C:104:TRP:CD1	1:C:108:LYS:HE2	2.40	0.55
1:A:399:GLN:NE2	1:A:399:GLN:H	2.03	0.55
1:C:323:GLU:OE2	1:C:364:ARG:NH2	2.31	0.55
3:A:811:HOH:O	1:B:231:ARG:HD2	2.06	0.54
1:A:29:PHE:O	1:A:423:HIS:CE1	2.58	0.54
1:A:227[B]:PHE:HD1	1:B:227[B]:PHE:HB3	1.73	0.54
1:C:232:HIS:HE1	1:C:339:SER:OG	1.91	0.54
1:B:436:ARG:HD3	1:B:440:LEU:HD13	1.89	0.53
1:C:256:LYS:HD2	3:C:860:HOH:O	2.07	0.53
1:A:227[B]:PHE:CD1	1:B:227[B]:PHE:HB3	2.42	0.53
1:B:44:PRO:HG2	1:B:426:PRO:HB3	1.91	0.53
1:C:29:PHE:O	1:C:423:HIS:HE1	1.90	0.53
1:A:232:HIS:HD2	1:A:348:SER:OG	1.92	0.53
1:C:214:PRO:HB3	1:C:338:PHE:HB2	1.90	0.53
1:B:124:HIS:HE1	3:B:854:HOH:O	1.92	0.53
1:A:486[A]:ARG:NH1	3:A:869:HOH:O	2.41	0.53
1:B:148:ASN:HD21	1:B:197:ARG:NH1	2.05	0.53
1:B:440:LEU:HG	1:B:462:VAL:HG13	1.91	0.52
1:A:314:TRP:CZ2	1:A:333[A]:MET:HE1	2.44	0.52
1:B:140:LEU:HG	1:B:189:LEU:HD22	1.91	0.52
1:A:329:PRO:O	1:A:333[A]:MET:HG3	2.10	0.52
1:C:8:THR:HG22	3:C:903:HOH:O	2.10	0.52
1:C:124:HIS:HE1	3:C:808:HOH:O	1.92	0.52
1:C:313:HIS:HD2	1:C:342:GLY:O	1.92	0.52
1:A:140:LEU:HG	1:A:189:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LYS:HD3	1:B:182[B]:ARG:HE	1.74	0.51
1:C:30:TRP:CD2	1:C:430:LEU:HD13	2.45	0.51
1:C:232:HIS:HD2	1:C:348:SER:OG	1.94	0.51
1:B:257:ARG:NH1	3:B:913:HOH:O	2.31	0.51
1:A:227[B]:PHE:CD1	1:B:227[B]:PHE:CG	2.99	0.50
1:C:61:GLN:NE2	1:C:64:ARG:HH21	2.08	0.50
1:B:214:PRO:O	1:B:216[A]:ARG:HD2	2.12	0.50
1:C:81:GLU:CD	1:C:81:GLU:N	2.69	0.50
1:A:341:TYR:CD1	1:A:391:LEU:HD11	2.47	0.50
1:C:313:HIS:HE1	1:C:345:GLU:OE2	1.95	0.49
1:A:302:CYS:O	1:A:305:THR:HB	2.13	0.49
1:B:148:ASN:ND2	1:B:197:ARG:HH11	2.05	0.48
1:A:129:LYS:HG2	3:A:699:HOH:O	2.12	0.48
1:B:30:TRP:CD2	1:B:430:LEU:HD13	2.49	0.48
1:A:234:ASN:OD1	1:B:234:ASN:ND2	2.44	0.47
1:B:341:TYR:CD1	1:B:391:LEU:HD11	2.49	0.47
1:A:446:GLU:HA	1:A:449:MET:HE2	1.97	0.47
1:A:399:GLN:H	1:A:399:GLN:CD	2.23	0.47
1:A:302:CYS:O	1:A:305:THR:CB	2.63	0.47
1:B:221:MET:HG2	1:B:393:ARG:HG3	1.97	0.46
1:B:433:HIS:ND1	1:B:469:SER:HA	2.30	0.46
1:A:256:LYS:HG3	1:A:280:LEU:HD13	1.97	0.46
1:A:327:VAL:CG1	1:A:331:ILE:HB	2.46	0.46
1:B:423:HIS:HD2	1:B:428:GLU:OE1	1.99	0.46
1:C:216[A]:ARG:NH1	1:C:339:SER:OG	2.49	0.45
1:A:33:SER:HB3	3:A:519:HOH:O	2.16	0.45
1:A:381:ARG:HD2	3:A:544:HOH:O	2.16	0.45
1:B:60:GLN:HG2	3:B:875:HOH:O	2.17	0.45
1:B:93:ARG:HE	1:B:213:ASN:ND2	2.15	0.45
1:B:239:MET:HE1	1:B:358:TYR:CE2	2.51	0.45
1:C:115:LYS:HE2	1:C:131:TRP:CD2	2.52	0.44
1:B:300:SER:HA	1:B:305:THR:HG21	1.98	0.44
1:B:391:LEU:O	1:B:392:ARG:HB2	2.17	0.44
1:B:239:MET:CE	1:B:358:TYR:CE2	3.01	0.44
1:C:52:GLU:H	1:C:52:GLU:HG2	1.42	0.44
1:B:264:ARG:HD3	3:B:753:HOH:O	2.17	0.44
1:B:302:CYS:O	1:B:305:THR:HB	2.18	0.43
1:A:153:MET:O	1:C:431:PRO:HG3	2.18	0.43
1:B:169:LEU:HD23	1:B:413:ARG:HG2	2.00	0.43
1:C:63:MET:HE3	1:C:287:VAL:HB	1.99	0.43
1:B:339:SER:O	1:B:345:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:SER:HB3	1:A:223:GLU:HG2	2.01	0.43
1:B:52:GLU:H	1:B:52:GLU:HG2	1.59	0.43
1:C:171:LYS:HE3	1:C:173[A]:ASP:OD1	2.19	0.43
1:C:486[A]:ARG:HD2	1:C:486[A]:ARG:HA	1.72	0.43
1:A:239:MET:HE1	1:A:353:LEU:CD1	2.49	0.42
1:A:323:GLU:OE1	1:A:364[B]:ARG:NH1	2.43	0.42
1:C:304:CYS:HB3	3:C:686:HOH:O	2.19	0.42
1:B:373:ASP:O	1:B:373:ASP:CG	2.62	0.42
1:B:432:GLY:C	1:B:434:ALA:H	2.28	0.42
1:C:392:ARG:NH1	3:C:676:HOH:O	2.52	0.42
1:A:232:HIS:CE1	1:A:339:SER:OG	2.68	0.42
1:B:313:HIS:CE1	1:B:345:GLU:OE2	2.66	0.42
1:B:199:PHE:CZ	1:B:276:MET:HE2	2.54	0.42
1:A:214:PRO:HB3	1:A:338:PHE:HB2	2.00	0.42
1:C:405:ARG:HG3	1:C:449:MET:HE3	2.01	0.42
1:A:313:HIS:HE1	1:A:345:GLU:OE2	2.03	0.41
1:B:215:ILE:HD11	1:B:311:LEU:HD13	2.03	0.41
1:A:202:PHE:CE1	1:A:206:LEU:HD22	2.56	0.41
1:C:423:HIS:HD2	1:C:428:GLU:OE1	2.03	0.41
1:B:60:GLN:NE2	3:B:530:HOH:O	2.54	0.41
1:C:208:GLU:HG3	3:C:689:HOH:O	2.20	0.41
1:C:238:HIS:HE1	3:C:911:HOH:O	2.02	0.41
1:C:207:LYS:HG3	1:C:218:GLY:HA3	2.02	0.40
1:C:44:PRO:HG2	1:C:426:PRO:HB3	2.01	0.40
1:C:303:PRO:HD2	3:C:910:HOH:O	2.20	0.40
1:A:200:GLY:N	1:A:201:PRO:CD	2.84	0.40
1:A:252:ARG:HB3	1:A:256:LYS:HE3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/515 (93%)	469 (98%)	8 (2%)	0	100	100
1	B	486/515 (94%)	476 (98%)	9 (2%)	1 (0%)	43	42
1	C	475/515 (92%)	467 (98%)	8 (2%)	0	100	100
All	All	1438/1545 (93%)	1412 (98%)	25 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	374	LYS

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	412/441 (93%)	389 (94%)	23 (6%)	19	16
1	B	419/441 (95%)	390 (93%)	29 (7%)	14	11
1	C	412/441 (93%)	382 (93%)	30 (7%)	13	9
All	All	1243/1323 (94%)	1161 (93%)	82 (7%)	16	12

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	36	LYS
1	A	37	LEU
1	A	54	VAL
1	A	63	MET
1	A	77	LEU
1	A	83	LEU
1	A	113	LEU
1	A	140	LEU
1	A	169	LEU
1	A	216[A]	ARG
1	A	216[B]	ARG

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	279	LEU
1	A	316	LEU
1	A	362	LEU
1	A	391	LEU
1	A	399	GLN
1	A	440	LEU
1	A	443	LEU
1	A	444	LEU
1	A	452	GLU
1	A	475	VAL
1	B	36	LYS
1	B	37	LEU
1	B	50	LYS
1	B	52	GLU
1	B	55	ASP
1	B	83	LEU
1	B	99	GLU
1	B	113	LEU
1	B	140	LEU
1	B	169	LEU
1	B	171	LYS
1	B	216[A]	ARG
1	B	216[B]	ARG
1	B	231	ARG
1	B	255	LEU
1	B	271	LEU
1	B	279	LEU
1	B	300	SER
1	B	305	THR
1	B	316	LEU
1	B	353	LEU
1	B	391	LEU
1	B	430	LEU
1	B	436	ARG
1	B	440	LEU
1	B	443	LEU
1	B	444	LEU
1	B	474	VAL
1	B	479	ARG
1	C	8	THR
1	C	33	SER

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Mol	Chain	Res	Type
1	C	35	GLU
1	C	36	LYS
1	C	37	LEU
1	C	52	GLU
1	C	83	LEU
1	C	91	GLU
1	C	108	LYS
1	C	113	LEU
1	C	140	LEU
1	C	169	LEU
1	C	173[A]	ASP
1	C	173[B]	ASP
1	C	212	PHE
1	C	216[A]	ARG
1	C	216[B]	ARG
1	C	279	LEU
1	C	284	LEU
1	C	316	LEU
1	C	353	LEU
1	C	391	LEU
1	C	440	LEU
1	C	443	LEU
1	C	444	LEU
1	C	463	SER
1	C	477	ARG
1	C	481	VAL
1	C	486[A]	ARG
1	C	486[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	61	GLN
1	A	124	HIS
1	A	148	ASN
1	A	213	ASN
1	A	222	ASN
1	A	232	HIS
1	A	238	HIS
1	A	251	GLN
1	A	313	HIS

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Mol	Chain	Res	Type
1	A	383	GLN
1	A	399	GLN
1	A	423	HIS
1	A	424	GLN
1	A	439	GLN
1	A	450	HIS
1	A	478	HIS
1	B	61	GLN
1	B	124	HIS
1	B	148	ASN
1	B	213	ASN
1	B	222	ASN
1	B	232	HIS
1	B	238	HIS
1	B	313	HIS
1	B	334	GLN
1	B	423	HIS
1	B	478	HIS
1	C	61	GLN
1	C	124	HIS
1	C	148	ASN
1	C	222	ASN
1	C	232	HIS
1	C	238	HIS
1	C	313	HIS
1	C	334	GLN
1	C	423	HIS
1	C	424	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	516	-	4,4,4	0.26	0	6,6,6	0.12	0
2	SO4	B	518	-	4,4,4	0.33	0	6,6,6	0.37	0
2	SO4	C	518	-	4,4,4	0.22	0	6,6,6	0.16	0
2	SO4	C	519	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	A	518	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	B	520	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	A	516	-	4,4,4	0.20	0	6,6,6	0.51	0
2	SO4	C	517	-	4,4,4	0.19	0	6,6,6	0.30	0
2	SO4	C	516	-	4,4,4	0.24	0	6,6,6	0.19	0
2	SO4	C	520	-	4,4,4	0.44	0	6,6,6	0.42	0
2	SO4	B	519	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	A	517	-	4,4,4	0.28	0	6,6,6	0.22	0
2	SO4	B	517	-	4,4,4	0.69	0	6,6,6	0.93	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	478/515 (92%)	-0.09	20 (4%)	40 39	11, 26, 56, 86	7 (1%)
1	B	482/515 (93%)	-0.10	27 (5%)	30 29	11, 26, 58, 81	8 (1%)
1	C	475/515 (92%)	-0.27	17 (3%)	46 45	10, 23, 53, 80	8 (1%)
All	All	1435/1545 (92%)	-0.15	64 (4%)	38 37	10, 25, 57, 86	23 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	VAL	4.9
1	A	474	VAL	4.9
1	C	474	VAL	4.6
1	B	433	HIS	4.6
1	A	466	ALA	4.3
1	C	432	GLY	4.1
1	B	375	GLU	4.1
1	C	475	VAL	4.0
1	C	433	HIS	4.0
1	B	469	SER	3.8
1	B	467	ALA	3.7
1	A	99	GLU	3.7
1	B	484	TRP	3.6
1	A	475	VAL	3.6
1	A	435	GLN	3.5
1	B	434	ALA	3.3
1	C	466	ALA	3.3
1	B	3	PRO	3.2
1	B	372	ALA	3.2
1	C	463	SER	3.1
1	A	303	PRO	3.0
1	B	374	LYS	3.0
1	B	464	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	2	LEU	3.0
1	A	479	ARG	2.9
1	C	484	TRP	2.9
1	B	303	PRO	2.8
1	B	55	ASP	2.8
1	B	432	GLY	2.8
1	A	451	GLY	2.7
1	B	373	ASP	2.7
1	C	212	PHE	2.6
1	C	55	ASP	2.6
1	B	466	ALA	2.6
1	A	488	GLY	2.5
1	C	303	PRO	2.5
1	A	477	ARG	2.4
1	C	462	VAL	2.4
1	C	477	ARG	2.4
1	B	488	GLY	2.4
1	B	435	GLN	2.4
1	A	372	ALA	2.4
1	A	437	PRO	2.4
1	A	484	TRP	2.4
1	B	377	GLY	2.3
1	A	436	ARG	2.3
1	B	475	VAL	2.3
1	C	5	PRO	2.3
1	C	464	LYS	2.3
1	B	462	VAL	2.3
1	B	479	ARG	2.3
1	C	479	ARG	2.2
1	B	457	THR	2.2
1	C	452	GLU	2.1
1	B	441	MET	2.1
1	A	54	VAL	2.1
1	A	462	VAL	2.1
1	B	301	GLY	2.1
1	B	302	CYS	2.0
1	A	382	ARG	2.0
1	B	456	ARG	2.0
1	A	476	PRO	2.0
1	A	463	SER	2.0
1	C	488	GLY	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($\text{\AA}^2$)	Q<0.9
2	SO4	C	520	5/5	0.73	0.21	52,52,62,63	0
2	SO4	B	516	5/5	0.74	0.15	100,102,102,102	0
2	SO4	B	517	5/5	0.82	0.12	76,77,78,79	0
2	SO4	B	519	5/5	0.87	0.12	73,76,77,80	0
2	SO4	C	519	5/5	0.88	0.13	75,79,80,81	0
2	SO4	A	518	5/5	0.89	0.11	63,63,68,68	0
2	SO4	B	518	5/5	0.90	0.20	42,51,59,62	0
2	SO4	A	517	5/5	0.90	0.10	65,66,69,72	0
2	SO4	A	516	5/5	0.92	0.19	45,45,53,57	0
2	SO4	C	518	5/5	0.93	0.09	61,62,66,66	0
2	SO4	C	517	5/5	0.94	0.14	47,48,57,58	0
2	SO4	B	520	5/5	0.96	0.06	54,56,59,60	0
2	SO4	C	516	5/5	0.96	0.08	50,52,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.