



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:46 PM GMT

PDB ID : 3UQS  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

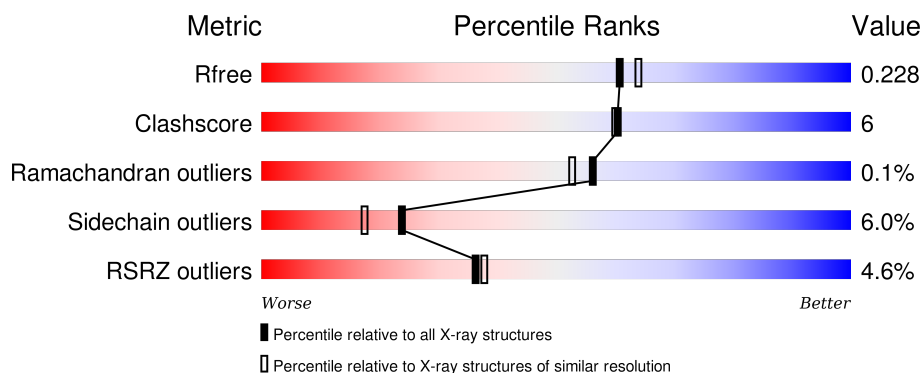
# 1 Overall quality at a glance

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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% 79% 13% • 4%
1	B	515	 4% 80% 11% • 6%
1	C	515	 4% 79% 12% • 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	SO4	B	517	-	-	-	X
2	SO4	C	520	-	-	-	X

## 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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

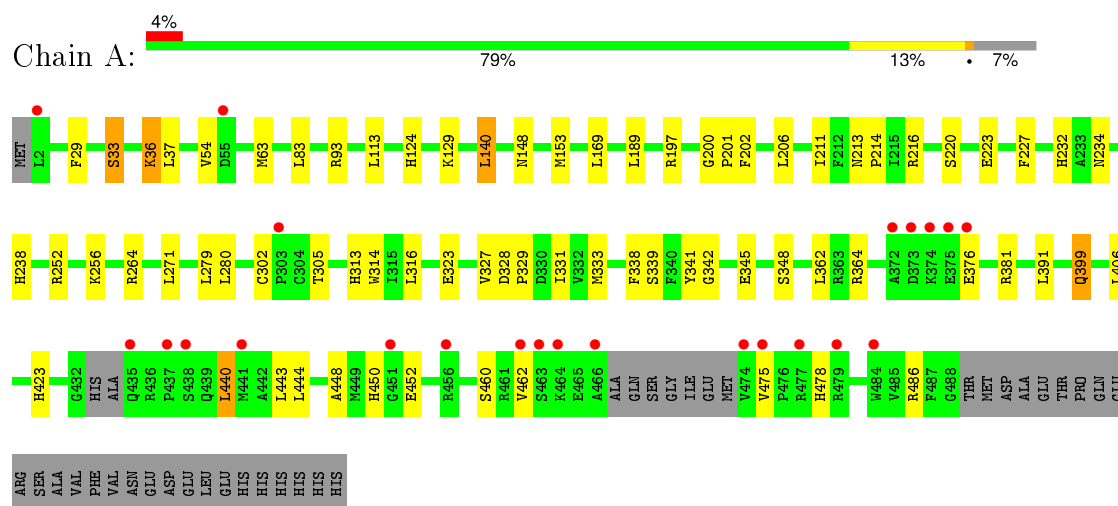
- Molecule 3 is water.

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		

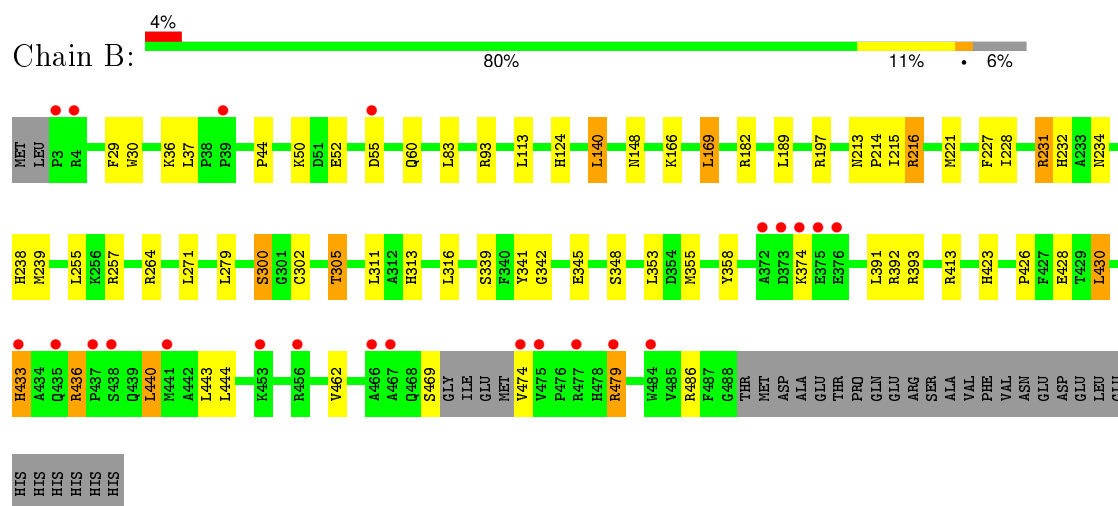
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

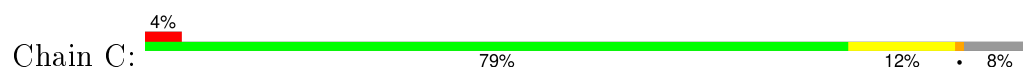
#### • Molecule 1: RNA-dependent RNA polymerase

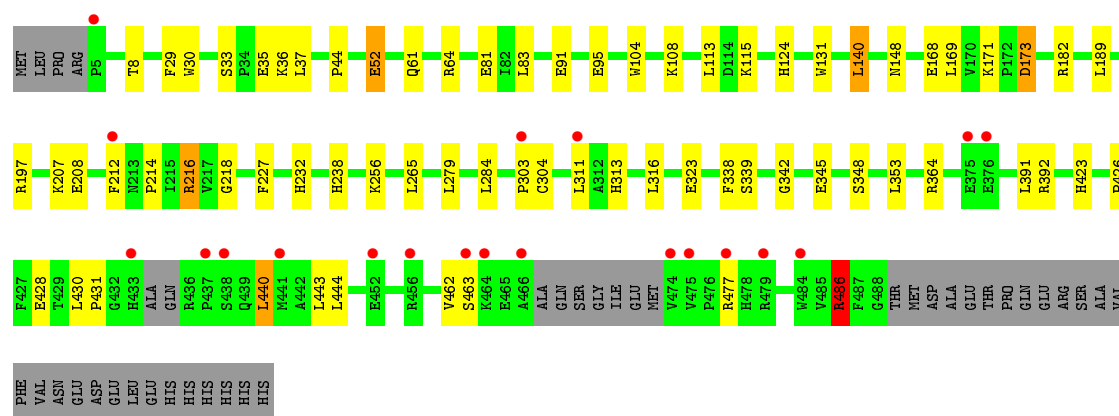


#### • Molecule 1: RNA-dependent RNA polymerase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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) 99.7 (28.75-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 154866 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	0/3937	0.66	0/5331
1	B	0.56	0/4000	0.67	0/5414
1	C	0.59	0/3926	0.69	3/5314 (0.1%)
All	All	0.57	0/11863	0.67	3/16059 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	486[A]	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	486[B]	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	311	LEU	CA-CB-CG	5.61	128.20	115.30

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	43	0
1	B	3880	0	3865	53	0
1	C	3815	0	3790	38	0
2	A	15	0	0	0	0
2	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	129	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 (129) 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: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:C:148:ASN:HD21	1:C:197:ARG:HH11	1.12	0.92
1:B:479:ARG:HG3	1:B:479:ARG:HH11	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:C:440:LEU:HG	1:C:462:VAL:HG13	1.71	0.72
1:A:29:PHE:O	1:A:423:HIS:HE1	1.69	0.72
1:B:486[A]:ARG:HH11	1:B:486[A]:ARG:HB3	1.54	0.72
1:A:238:HIS:HD2	1:A:348:SER:OG	1.76	0.68
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:B:486[A]:ARG:NH1	1:B:486[A]:ARG:HB3	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
1:B:238:HIS:HD2	1:B:348:SER:OG	1.82	0.62
1:A:124:HIS:HE1	3:A:827:HOH:O	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:C:81:GLU:CD	1:C:81:GLU:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:PRO:HD2	3:C:550:HOH:O	2.03	0.58
1:A:36:LYS:HE2	1:A:36:LYS:H	1.68	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:B:239:MET:HE1	1:B:355: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
1:B:239:MET:HE3	1:B:355:MET:HE1	1.89	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:B:148:ASN:HD21	1:B:197:ARG:NH1	2.05	0.53
1:A:486[A]:ARG:NH1	3:A:869:HOH:O	2.41	0.53
1:B:440:LEU:HG	1:B:462:VAL:HG13	1.91	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:B:239:MET:CE	1:B:355:MET:CE	2.88	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
1:B:166:LYS:HD3	1:B:182[B]:ARG:HE	1.74	0.51
1:C:232:HIS:HD2	1:C:348:SER:OG	1.94	0.51
1:C:30:TRP:CD2	1:C:430:LEU:HD13	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PRO:O	1:B:216[A]:ARG:HD2	2.12	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:B:239:MET:HE1	1:B:355:MET:CE	2.43	0.48
1:B:239:MET:CE	1:B:355:MET:HE1	2.43	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: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:314:TRP:HE1	1:A:333[A]:MET:HE3	1.80	0.46
1:A:256:LYS:HG3	1:A:280:LEU:HD13	1.97	0.46
1:B:423:HIS:HD2	1:B:428:GLU:OE1	1.99	0.46
1:A:327:VAL:CG1	1:A:331:ILE:HB	2.46	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:C:81:GLU:CD	1:C:81:GLU:N	2.69	0.45
1:C:115:LYS:HE2	1:C:131:TRP:CD2	2.52	0.44
1:B:391:LEU:O	1:B:392:ARG:HB2	2.17	0.44
1:B:300:SER:HA	1:B:305:THR:HG21	1.98	0.44
1:B:239:MET:CE	1:B:358:TYR:CE2	3.01	0.44
1:C:52:GLU:HG2	1:C:52:GLU:H	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:B:239:MET:HE1	1:B:358:TYR:CE2	2.53	0.43
1:B:339:SER:O	1:B:345:GLU:HA	2.18	0.43
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:HA	1:C:486[A]:ARG:HD2	1.72	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:214:PRO:HB3	1:A:338:PHE:HB2	2.00	0.42
1:A:399:GLN:H	1:A:399:GLN:CD	2.23	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:C:423:HIS:HD2	1:C:428:GLU:OE1	2.03	0.41
1:A:202:PHE:CE1	1:A:206:LEU:HD22	2.56	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:303:PRO:HD2	3:C:910:HOH:O	2.20	0.40
1:C:44:PRO:HG2	1:C:426:PRO:HB3	2.01	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

### 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	477/515 (93%)	469 (98%)	8 (2%)	0	100	100
1	B	486/515 (94%)	476 (98%)	9 (2%)	1 (0%)	52	48
1	C	475/515 (92%)	467 (98%)	8 (2%)	0	100	100
All	All	1438/1545 (93%)	1412 (98%)	25 (2%)	1 (0%)	56	53

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%)	387 (94%)	25 (6%)	23	17
1	B	419/441 (95%)	393 (94%)	26 (6%)	23	16
1	C	412/441 (93%)	384 (93%)	28 (7%)	20	13
All	All	1243/1323 (94%)	1164 (94%)	79 (6%)	24	15

All (79) 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	83	LEU
1	A	113	LEU
1	A	140	LEU
1	A	169	LEU
1	A	216[A]	ARG
1	A	216[B]	ARG
1	A	264	ARG
1	A	271	LEU
1	A	279	LEU
1	A	316	LEU
1	A	328	ASP
1	A	362	LEU
1	A	376	GLU
1	A	399	GLN
1	A	440	LEU
1	A	443	LEU
1	A	444	LEU

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Mol	Chain	Res	Type
1	A	452	GLU
1	A	460	SER
1	A	475	VAL
1	B	36	LYS
1	B	37	LEU
1	B	50	LYS
1	B	55	ASP
1	B	83	LEU
1	B	113	LEU
1	B	140	LEU
1	B	169	LEU
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	430	LEU
1	B	433	HIS
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	33	SER
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	113	LEU
1	C	140	LEU
1	C	169	LEU
1	C	173[A]	ASP
1	C	173[B]	ASP
1	C	212	PHE

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Mol	Chain	Res	Type
1	C	216[A]	ARG
1	C	216[B]	ARG
1	C	227	PHE
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	486[A]	ARG
1	C	486[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	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
1	A	334	GLN
1	A	383	GLN
1	A	399	GLN
1	A	423	HIS
1	A	439	GLN
1	A	450	HIS
1	A	478	HIS
1	B	66	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

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Mol	Chain	Res	Type
1	B	251	GLN
1	B	313	HIS
1	B	334	GLN
1	B	423	HIS
1	B	478	HIS
1	C	60	GLN
1	C	61	GLN
1	C	66	GLN
1	C	124	HIS
1	C	148	ASN
1	C	222	ASN
1	C	232	HIS
1	C	238	HIS
1	C	251	GLN
1	C	313	HIS
1	C	334	GLN
1	C	423	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 carbohydrates 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	A	516	-	4,4,4	0.30	0	6,6,6	0.48	0
2	SO4	A	517	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	A	518	-	4,4,4	0.27	0	6,6,6	0.20	0
2	SO4	B	516	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	B	517	-	4,4,4	1.62	0	6,6,6	0.58	0
2	SO4	B	518	-	4,4,4	0.43	0	6,6,6	0.31	0
2	SO4	B	519	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	B	520	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	C	516	-	4,4,4	0.33	0	6,6,6	0.22	0
2	SO4	C	517	-	4,4,4	0.24	0	6,6,6	0.40	0
2	SO4	C	518	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	C	519	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	C	520	-	4,4,4	0.38	0	6,6,6	0.27	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	SO4	A	516	-	-	0/0/0/0	0/0/0/0
2	SO4	A	517	-	-	0/0/0/0	0/0/0/0
2	SO4	A	518	-	-	0/0/0/0	0/0/0/0
2	SO4	B	516	-	-	0/0/0/0	0/0/0/0
2	SO4	B	517	-	-	0/0/0/0	0/0/0/0
2	SO4	B	518	-	-	0/0/0/0	0/0/0/0
2	SO4	B	519	-	-	0/0/0/0	0/0/0/0
2	SO4	B	520	-	-	0/0/0/0	0/0/0/0
2	SO4	C	516	-	-	0/0/0/0	0/0/0/0
2	SO4	C	517	-	-	0/0/0/0	0/0/0/0
2	SO4	C	518	-	-	0/0/0/0	0/0/0/0
2	SO4	C	519	-	-	0/0/0/0	0/0/0/0
2	SO4	C	520	-	-	0/0/0/0	0/0/0/0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	478/515 (92%)	-0.18	23 (4%)	34 36	15, 26, 56, 86	2 (0%)
1	B	482/515 (93%)	-0.20	23 (4%)	34 36	15, 26, 58, 81	1 (0%)
1	C	475/515 (92%)	-0.25	20 (4%)	40 41	12, 23, 53, 80	2 (0%)
All	All	1435/1545 (92%)	-0.21	66 (4%)	36 38	12, 25, 57, 86	5 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	ALA	7.1
1	A	474	VAL	7.0
1	C	474	VAL	5.7
1	A	463	SER	5.2
1	A	475	VAL	5.0
1	B	433	HIS	4.9
1	A	376	GLU	4.6
1	A	477	ARG	4.5
1	B	474	VAL	4.5
1	A	466	ALA	4.3
1	C	433	HIS	4.1
1	B	375	GLU	4.1
1	B	373	ASP	3.8
1	C	477	ARG	3.8
1	B	484	TRP	3.7
1	A	372	ALA	3.7
1	B	475	VAL	3.7
1	A	375	GLU	3.4
1	A	2	LEU	3.4
1	C	463	SER	3.4
1	B	456	ARG	3.4
1	B	374	LYS	3.4
1	A	438	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	373	ASP	3.4
1	B	477	ARG	3.3
1	C	464	LYS	3.3
1	C	466	ALA	3.1
1	C	456	ARG	3.1
1	B	39	PRO	3.1
1	C	438	SER	3.0
1	B	438	SER	3.0
1	A	441	MET	2.9
1	C	375	GLU	2.9
1	B	435	GLN	2.9
1	C	452	GLU	2.9
1	B	372	ALA	2.8
1	A	456	ARG	2.8
1	C	475	VAL	2.8
1	A	435	GLN	2.8
1	A	464	LYS	2.8
1	B	453	LYS	2.7
1	C	441	MET	2.7
1	A	437	PRO	2.7
1	B	376	GLU	2.7
1	B	437	PRO	2.6
1	C	484	TRP	2.5
1	B	55	ASP	2.5
1	B	441	MET	2.5
1	A	374	LYS	2.5
1	C	5	PRO	2.5
1	C	376	GLU	2.4
1	B	4	ARG	2.4
1	C	437	PRO	2.4
1	B	466	ALA	2.4
1	C	479	ARG	2.3
1	B	479	ARG	2.3
1	B	3	PRO	2.2
1	A	303	PRO	2.2
1	A	55	ASP	2.2
1	A	451	GLY	2.1
1	A	462	VAL	2.1
1	A	484	TRP	2.1
1	C	311	LEU	2.1
1	A	479	ARG	2.1
1	C	212	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	303	PRO	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	C	520	5/5	0.88	0.30	8.80	52,52,62,63	0
2	SO4	B	517	5/5	0.94	0.27	5.76	76,77,78,79	0
2	SO4	A	516	5/5	0.96	0.18	1.85	45,45,53,57	0
2	SO4	B	518	5/5	0.95	0.17	1.33	42,51,59,62	0
2	SO4	C	517	5/5	0.97	0.14	1.21	47,48,57,58	0
2	SO4	B	520	5/5	0.99	0.10	-0.03	54,56,59,60	0
2	SO4	C	518	5/5	0.97	0.10	-0.06	61,62,66,66	0
2	SO4	C	516	5/5	0.98	0.08	-0.36	50,52,55,56	0
2	SO4	A	518	5/5	0.96	0.13	-	63,63,68,68	0
2	SO4	A	517	5/5	0.93	0.14	-	65,66,69,72	0
2	SO4	B	519	5/5	0.94	0.15	-	73,76,77,80	0
2	SO4	B	516	5/5	0.78	0.20	-	100,102,102,102	0
2	SO4	C	519	5/5	0.91	0.18	-	75,79,80,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.