



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:19 pm BST

PDB ID : 3QID  
Title : Crystal structures and functional analysis of murine norovirus RNA-dependent RNA polymerase  
Authors : Kim, K.H.; Intekhab, A.; Lee, J.H.  
Deposited on : 2011-01-27  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

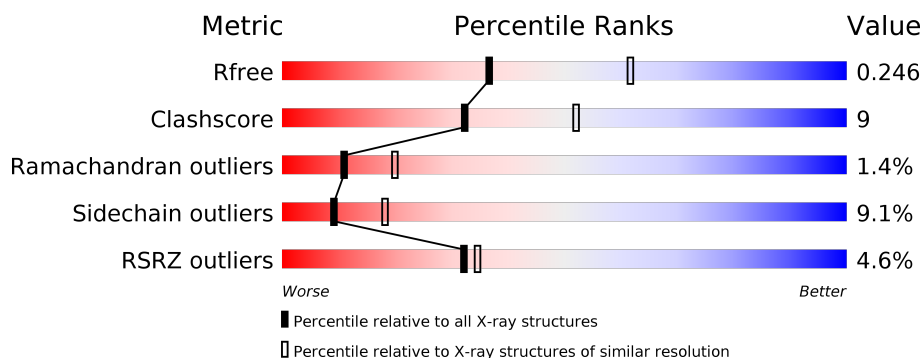
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	517	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	C	517	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12360 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	492	Total	C	N	O	S	0	0	0
			3901	2463	685	727	26			
1	B	492	Total	C	N	O	S	0	0	0
			3901	2463	685	727	26			
1	C	492	Total	C	N	O	S	0	0	0
			3901	2463	685	727	26			

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



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

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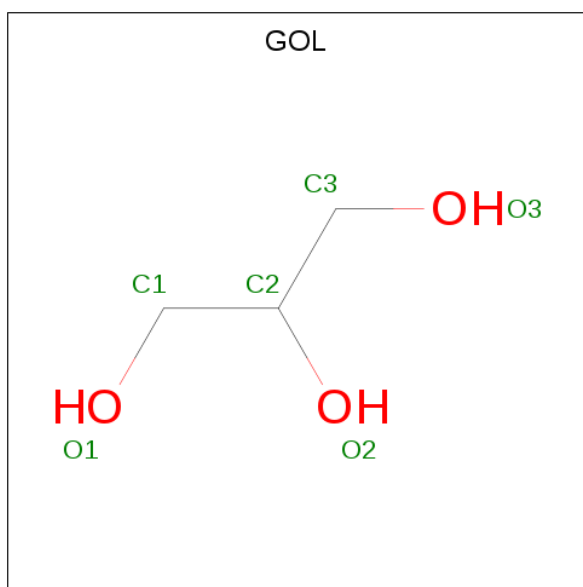
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MANGANESE (III) ION (three-letter code: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

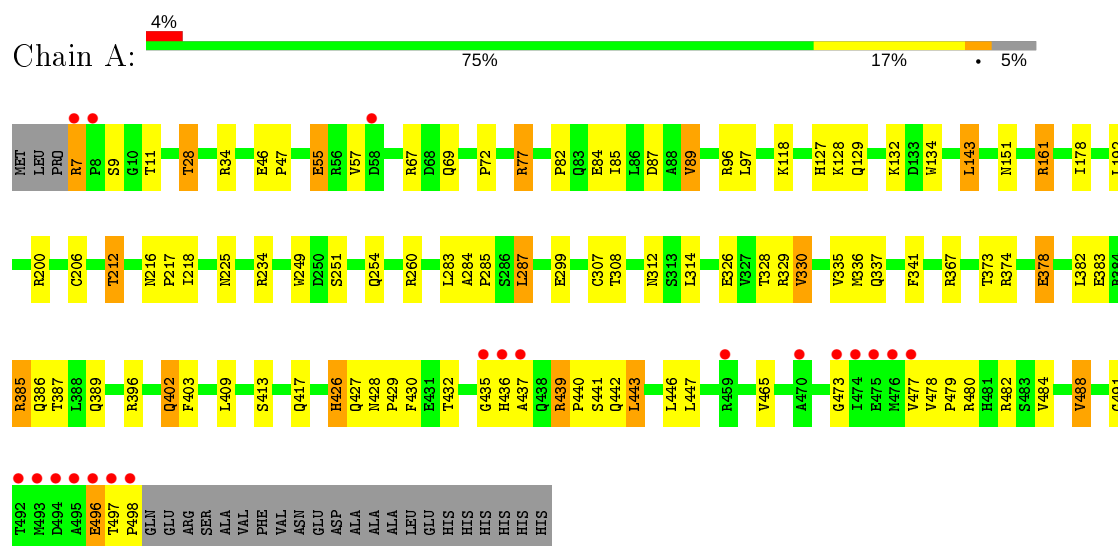
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	132	Total	O	0	0
			132	132		
5	C	149	Total	O	0	0
			149	149		

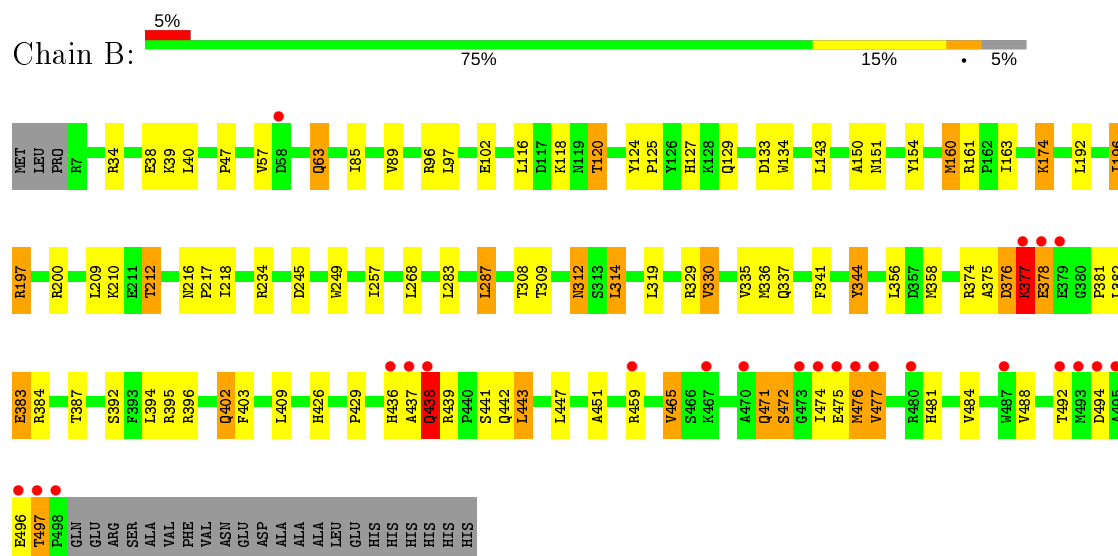
### 3 Residue-property plots

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

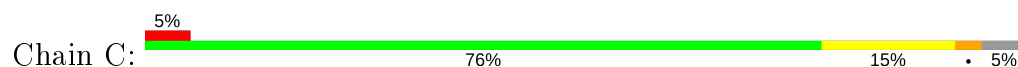
#### • Molecule 1: RNA dependent RNA polymerase



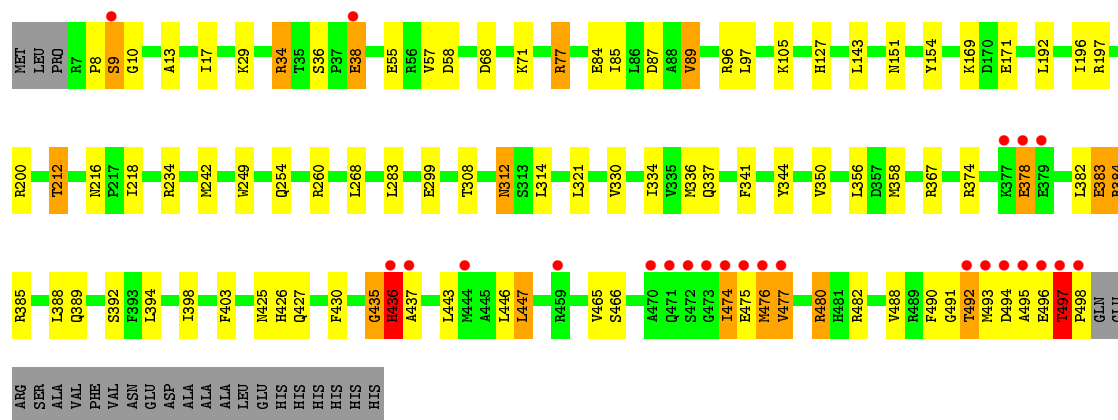
#### • Molecule 1: RNA dependent RNA polymerase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	120.56Å 196.26Å 109.34Å 90.00° 114.23° 90.00°	Depositor
Resolution (Å)	49.07 – 2.50 49.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.07-2.50) 98.8 (49.07-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.46 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.199 , 0.245 0.200 , 0.246	Depositor DCC
$R_{free}$ test set	3946 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12360	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 3.30% 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, 0.333 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: GOL, MN3, 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	0.47	0/3997	0.63	0/5417
1	B	0.47	0/3997	0.62	0/5417
1	C	0.46	0/3997	0.65	2/5417 (0.0%)
All	All	0.47	0/11991	0.63	2/16251 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	367	ARG	NE-CZ-NH1	5.25	122.92	120.30

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	3901	0	3851	69	1
1	B	3901	0	3851	70	0
1	C	3901	0	3851	75	0
2	A	60	0	0	1	0
2	B	45	0	0	2	0
2	C	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	18	0	24	2	0
4	B	24	0	32	1	0
4	C	18	0	24	4	0
5	A	173	0	0	6	0
5	B	132	0	0	5	0
5	C	149	0	0	2	0
All	All	12360	0	11633	208	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 9.

All (208) 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:C:480:ARG:HH11	1:C:480:ARG:HG2	1.12	1.15
1:A:385:ARG:HD3	1:A:386:GLN:H	1.01	1.08
1:C:151:ASN:HD21	1:C:200:ARG:HH11	1.01	0.99
1:B:436:HIS:HB2	1:B:437:ALA:HA	1.44	0.98
1:A:385:ARG:HD3	1:A:386:GLN:N	1.80	0.96
1:C:493:MET:HB3	1:C:494:ASP:HB3	1.45	0.95
1:B:151:ASN:HD21	1:B:200:ARG:HH11	1.12	0.92
1:B:436:HIS:CB	1:B:437:ALA:HA	2.00	0.91
1:C:495:ALA:HB3	1:C:496:GLU:HA	1.53	0.91
1:C:497:THR:HB	1:C:498:PRO:HD3	1.52	0.88
1:B:438:GLN:HG3	1:B:439:ARG:H	1.38	0.87
1:C:356:LEU:HB3	1:C:358:MET:HE1	1.54	0.86
1:C:474:ILE:HA	1:C:475:GLU:HB2	1.57	0.86
1:A:151:ASN:HD21	1:A:200:ARG:HH11	1.25	0.84
1:C:436:HIS:HB2	1:C:437:ALA:CA	2.07	0.83
1:B:374:ARG:O	1:B:376:ASP:N	2.10	0.83
1:C:480:ARG:HH11	1:C:480:ARG:CG	1.93	0.82
1:C:480:ARG:NH1	1:C:480:ARG:HG2	1.91	0.82
1:C:474:ILE:HG23	1:C:476:MET:HB2	1.62	0.82
1:C:436:HIS:HB2	1:C:437:ALA:HB3	1.64	0.80
1:C:493:MET:HB3	1:C:494:ASP:CB	2.12	0.79
1:C:436:HIS:HB2	1:C:437:ALA:CB	2.12	0.78
1:C:497:THR:CB	1:C:498:PRO:HD3	2.14	0.78
1:A:337:GLN:HE21	1:B:329:ARG:HH12	1.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:HIS:CB	1:C:437:ALA:HB3	2.15	0.76
1:B:151:ASN:ND2	1:B:200:ARG:HH11	1.85	0.75
1:C:383:GLU:HG3	5:C:642:HOH:O	1.87	0.74
1:B:234:ARG:NH2	1:C:403:PHE:O	2.15	0.73
1:B:475:GLU:H	1:B:476:MET:HA	1.55	0.72
1:B:438:GLN:HG3	1:B:439:ARG:N	2.05	0.72
1:C:242:MET:HE1	1:C:358:MET:SD	2.31	0.71
1:C:10:GLY:HA2	1:C:17:ILE:HD12	1.73	0.69
1:B:403:PHE:O	1:C:234:ARG:NH2	2.19	0.69
1:C:151:ASN:ND2	1:C:200:ARG:HH11	1.85	0.68
1:A:87:ASP:OD1	1:A:260:ARG:NH2	2.26	0.68
1:A:28:THR:CG2	1:A:427:GLN:HE22	2.06	0.68
1:B:151:ASN:HD21	1:B:200:ARG:NH1	1.91	0.67
1:C:374:ARG:HD3	1:C:378:GLU:HA	1.76	0.67
1:A:84:GLU:H	1:A:84:GLU:CD	2.00	0.66
1:A:28:THR:HG23	1:A:427:GLN:HE22	1.59	0.66
1:C:374:ARG:CD	1:C:378:GLU:HA	2.26	0.65
1:C:474:ILE:CA	1:C:475:GLU:HB2	2.24	0.65
1:B:443:LEU:HG	1:B:465:VAL:HG22	1.79	0.65
1:A:96:ARG:HE	1:A:216:ASN:ND2	1.95	0.64
1:C:436:HIS:HB2	1:C:437:ALA:C	2.17	0.64
1:C:68:ASP:HA	1:C:71:LYS:HE2	1.81	0.62
1:C:427:GLN:H	4:C:529:GOL:H2	1.63	0.62
1:A:385:ARG:HD2	1:A:387:THR:HG22	1.81	0.62
1:C:493:MET:HB3	1:C:494:ASP:CA	2.30	0.61
1:C:495:ALA:CB	1:C:496:GLU:HA	2.23	0.61
1:C:10:GLY:HA3	1:C:17:ILE:HB	1.82	0.60
1:A:443:LEU:HG	1:A:465:VAL:HG13	1.83	0.59
1:C:435:GLY:HA2	1:C:436:HIS:O	2.02	0.59
1:A:337:GLN:NE2	1:B:329:ARG:HH12	2.01	0.58
1:C:491:GLY:O	1:C:492:THR:HB	2.02	0.58
1:B:257:ILE:HD13	1:B:319:LEU:HD21	1.86	0.58
1:A:127:HIS:HE1	5:A:544:HOH:O	1.86	0.58
1:C:356:LEU:HB3	1:C:358:MET:CE	2.30	0.58
1:B:133:ASP:HB2	1:B:143:LEU:HD22	1.86	0.58
1:C:497:THR:HB	1:C:498:PRO:CD	2.30	0.57
1:C:29:LYS:HD2	4:C:1:GOL:H31	1.86	0.57
1:B:396:ARG:HE	1:B:409:LEU:HD13	1.67	0.57
1:B:436:HIS:CB	1:B:437:ALA:CA	2.79	0.57
1:B:218:ILE:HD11	1:B:314:LEU:HD13	1.86	0.57
1:A:329:ARG:HH22	1:B:337:GLN:NE2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HE	1:A:216:ASN:HD22	1.52	0.56
1:C:425:ASN:HD22	4:C:1:GOL:H32	1.70	0.56
1:C:77:ARG:HG2	1:C:254:GLN:HG2	1.87	0.56
1:A:151:ASN:HD21	1:A:200:ARG:NH1	2.00	0.55
1:B:209:LEU:O	1:B:212:THR:HG22	2.06	0.55
1:B:374:ARG:HE	1:B:377:LYS:HB2	1.71	0.55
1:B:358:MET:HE3	1:B:384:ARG:HB3	1.89	0.55
1:B:330:VAL:HG22	1:B:335:VAL:HG23	1.87	0.55
1:B:474:ILE:HG23	1:B:475:GLU:H	1.72	0.55
1:A:249:TRP:HE1	1:A:312:ASN:HD21	1.54	0.55
1:A:128:LYS:HD3	1:A:132:LYS:HD2	1.89	0.55
1:B:496:GLU:HG3	1:B:497:THR:HG22	1.87	0.55
1:B:436:HIS:HB2	1:B:437:ALA:CA	2.26	0.54
1:A:326:GLU:OE1	1:A:367:ARG:NH2	2.34	0.54
1:A:85:ILE:O	1:A:89:VAL:HG13	2.06	0.54
1:A:225:ASN:HB2	4:A:534:GOL:H2	1.90	0.53
1:B:212:THR:HG23	1:B:216:ASN:HB2	1.90	0.53
1:B:476:MET:O	1:B:477:VAL:HG22	2.08	0.53
1:A:374:ARG:HD3	1:A:378:GLU:O	2.08	0.53
1:A:402:GLN:HE21	1:A:402:GLN:H	1.56	0.53
1:A:143:LEU:HG	1:A:192:LEU:HD22	1.91	0.53
1:B:330:VAL:HG22	1:B:335:VAL:CG2	2.38	0.53
1:A:7:ARG:HD2	1:A:7:ARG:N	2.24	0.53
1:B:102:GLU:OE1	1:C:496:GLU:HG3	2.09	0.53
1:B:436:HIS:CG	1:B:472:SER:HB3	2.45	0.52
1:A:330:VAL:HG22	1:A:335:VAL:HG23	1.92	0.52
1:B:160:MET:HE3	1:B:197:ARG:CD	2.39	0.52
1:C:10:GLY:CA	1:C:17:ILE:HD12	2.40	0.52
1:A:151:ASN:ND2	1:A:200:ARG:HH11	2.00	0.52
1:B:356:LEU:HD23	1:B:358:MET:HE1	1.92	0.52
1:C:356:LEU:HD23	1:C:358:MET:HE1	1.92	0.52
1:C:8:PRO:O	1:C:9:SER:HB2	2.10	0.52
1:B:374:ARG:HB3	1:B:377:LYS:HD3	1.91	0.52
1:C:85:ILE:O	1:C:89:VAL:HG13	2.10	0.52
1:C:358:MET:CE	1:C:384:ARG:HD3	2.40	0.51
1:A:77:ARG:HG2	1:A:254:GLN:HG2	1.93	0.51
1:A:249:TRP:HE1	1:A:312:ASN:ND2	2.08	0.51
1:A:396:ARG:HE	1:A:409:LEU:HD13	1.76	0.50
1:A:67:ARG:NH2	2:A:529:SO4:O3	2.39	0.50
1:B:143:LEU:HG	1:B:192:LEU:HD22	1.93	0.50
1:A:206:CYS:HG	1:A:307:CYS:HG	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:HG22	1:A:335:VAL:CG2	2.42	0.50
1:C:87:ASP:OD1	1:C:260:ARG:NH2	2.36	0.50
1:C:497:THR:CB	1:C:498:PRO:CD	2.87	0.50
1:C:249:TRP:HE1	1:C:312:ASN:HD21	1.59	0.49
1:C:34:ARG:HG3	1:C:430:PHE:HA	1.93	0.49
1:A:77:ARG:HD2	1:A:299:GLU:CG	2.43	0.49
1:B:344:TYR:CD2	1:B:394:LEU:HD21	2.48	0.49
2:B:527:SO4:O3	5:B:571:HOH:O	2.20	0.49
1:C:374:ARG:H	1:C:378:GLU:HB3	1.78	0.48
1:C:9:SER:HA	1:C:10:GLY:HA3	1.65	0.48
1:C:96:ARG:HE	1:C:216:ASN:HD22	1.61	0.48
1:B:377:LYS:O	1:B:378:GLU:HB2	2.14	0.47
1:A:409:LEU:HG	1:A:413:SER:HB2	1.96	0.47
1:A:47:PRO:HG2	1:A:429:PRO:HB3	1.96	0.47
1:B:96:ARG:HE	1:B:216:ASN:HD22	1.61	0.47
1:C:474:ILE:CG2	1:C:476:MET:HB2	2.39	0.47
1:C:249:TRP:HE1	1:C:312:ASN:ND2	2.13	0.47
1:C:443:LEU:HG	1:C:465:VAL:HG13	1.97	0.47
1:C:96:ARG:HE	1:C:216:ASN:ND2	2.12	0.47
1:A:161:ARG:HD2	1:A:287:LEU:HD22	1.96	0.47
1:C:436:HIS:HB3	1:C:437:ALA:HB3	1.94	0.47
1:A:435:GLY:C	1:A:437:ALA:H	2.19	0.47
1:B:475:GLU:N	1:B:476:MET:HA	2.25	0.47
1:B:160:MET:HE3	1:B:197:ARG:NE	2.31	0.46
1:C:341:PHE:CE1	1:C:350:VAL:HG13	2.51	0.46
1:A:132:LYS:HD3	1:A:132:LYS:O	2.15	0.46
1:B:154:TYR:HB2	1:B:197:ARG:HG3	1.97	0.46
1:B:451:ALA:O	1:B:481:HIS:HE1	1.98	0.46
1:A:402:GLN:NE2	1:A:402:GLN:H	2.13	0.46
1:B:127:HIS:HD2	5:B:600:HOH:O	1.98	0.46
1:C:36:SER:OG	1:C:38:GLU:HB2	2.16	0.46
1:B:374:ARG:NH1	1:B:381:PRO:O	2.40	0.46
1:B:150:ALA:HA	1:B:160:MET:HE1	1.98	0.46
1:C:344:TYR:CD2	1:C:394:LEU:HD21	2.51	0.46
1:A:217:PRO:HB3	1:A:341:PHE:HB2	1.98	0.46
1:C:77:ARG:CG	1:C:254:GLN:HG2	2.45	0.46
1:A:212:THR:HG23	1:A:216:ASN:HB2	1.98	0.45
1:C:154:TYR:HB2	1:C:197:ARG:HG3	1.97	0.45
1:C:143:LEU:HG	1:C:192:LEU:HD22	1.97	0.45
1:A:77:ARG:HD2	1:A:299:GLU:HG3	1.98	0.45
1:B:120:THR:HG21	2:B:522:SO4:S	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HH12	1:B:337:GLN:HE21	1.63	0.45
1:B:47:PRO:HG2	1:B:429:PRO:HB3	1.97	0.45
1:A:11:THR:HG22	5:A:568:HOH:O	2.16	0.45
1:A:34:ARG:HG3	1:A:430:PHE:HA	1.98	0.45
1:A:497:THR:HB	1:A:498:PRO:HD2	1.99	0.44
1:B:402:GLN:H	1:B:402:GLN:HG3	1.44	0.44
1:B:217:PRO:HB3	1:B:341:PHE:HB2	2.00	0.44
1:B:438:GLN:CG	1:B:439:ARG:N	2.77	0.44
1:A:69:GLN:HG2	5:A:607:HOH:O	2.17	0.44
1:B:471:GLN:N	1:B:471:GLN:HE21	2.15	0.44
1:A:367:ARG:NH2	5:A:581:HOH:O	2.31	0.44
1:B:63:GLN:NE2	5:B:544:HOH:O	2.50	0.44
1:C:358:MET:HE2	1:C:384:ARG:HD3	1.99	0.44
1:A:478:VAL:HA	1:A:479:PRO:HD3	1.84	0.44
1:A:72:PRO:HB2	1:A:251:SER:HB2	2.00	0.43
1:B:439:ARG:HG2	1:B:442:GLN:H	1.83	0.43
1:B:85:ILE:O	1:B:89:VAL:HG13	2.18	0.43
1:A:439:ARG:HD3	1:A:443:LEU:HD13	1.99	0.43
1:C:218:ILE:HD11	1:C:314:LEU:HD13	1.99	0.43
1:B:116:LEU:HD11	1:B:196:ILE:HG22	2.00	0.43
1:B:163:ILE:HD13	1:B:287:LEU:HD23	2.00	0.43
1:B:484:VAL:O	1:B:488:VAL:HG23	2.18	0.43
1:A:161:ARG:HG3	5:A:592:HOH:O	2.18	0.43
1:A:218:ILE:HD11	1:A:314:LEU:HD13	2.00	0.43
1:A:132:LYS:HD3	1:A:132:LYS:C	2.39	0.43
1:A:55:GLU:HG2	1:A:55:GLU:H	1.41	0.43
1:C:169:LYS:HD3	1:C:171:GLU:CD	2.39	0.43
1:A:426:HIS:CE1	1:A:428:ASN:O	2.71	0.43
1:B:127:HIS:HE1	5:B:540:HOH:O	2.00	0.43
1:C:77:ARG:HD2	1:C:299:GLU:CD	2.39	0.43
1:B:163:ILE:CD1	1:B:287:LEU:HD23	2.49	0.42
1:C:13:ALA:H	4:C:528:GOL:H2	1.84	0.42
1:C:212:THR:O	1:C:212:THR:CG2	2.67	0.42
1:C:447:LEU:HD13	1:C:465:VAL:HG21	2.01	0.42
1:C:127:HIS:HE1	5:C:533:HOH:O	2.03	0.42
1:C:374:ARG:CG	1:C:378:GLU:HA	2.49	0.42
1:A:129:GLN:HG3	5:A:656:HOH:O	2.19	0.42
1:B:374:ARG:C	1:B:376:ASP:N	2.72	0.42
1:A:82:PRO:HA	4:A:533:GOL:H2	2.02	0.42
1:A:212:THR:O	1:A:212:THR:HG23	2.21	0.41
1:B:377:LYS:HE2	1:B:383:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:THR:HA	4:B:530:GOL:H32	2.01	0.41
1:A:118:LYS:HE2	1:A:134:TRP:CE2	2.55	0.41
1:A:284:ALA:O	1:A:285:PRO:C	2.59	0.41
1:A:484:VAL:O	1:A:488:VAL:HG22	2.21	0.41
1:C:480:ARG:NH1	1:C:480:ARG:CG	2.63	0.41
1:A:77:ARG:CG	1:A:254:GLN:HG2	2.51	0.41
1:B:174:LYS:HD2	5:B:558:HOH:O	2.20	0.41
1:B:34:ARG:NH1	1:B:38:GLU:O	2.54	0.41
1:B:394:LEU:O	1:B:395:ARG:HB2	2.21	0.41
1:A:128:LYS:CD	1:A:132:LYS:HD2	2.51	0.41
1:B:249:TRP:HE1	1:B:312:ASN:ND2	2.18	0.41
1:C:388:LEU:HG	1:C:398:ILE:HG21	2.02	0.41
1:C:358:MET:HE3	1:C:384:ARG:HD3	2.03	0.41
1:B:436:HIS:CD2	1:B:472:SER:HB3	2.56	0.40
1:C:334:ILE:HA	1:C:337:GLN:HG2	2.03	0.40
1:B:124:TYR:HA	1:B:125:PRO:HA	1.87	0.40
1:A:206:CYS:SG	1:A:307:CYS:SG	3.15	0.40
1:A:46:GLU:HB2	1:A:178:ILE:CD1	2.51	0.40
1:A:417:GLN:HE21	1:A:442:GLN:NE2	2.19	0.40
1:B:118:LYS:HE2	1:B:134:TRP:CD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:NH2	1:A:403:PHE:O 2_656	2.09	0.11

## 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	490/517 (95%)	465 (95%)	21 (4%)	4 (1%)	19 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	490/517 (95%)	460 (94%)	20 (4%)	10 (2%)	7	12
1	C	490/517 (95%)	459 (94%)	24 (5%)	7 (1%)	11	20
All	All	1470/1551 (95%)	1384 (94%)	65 (4%)	21 (1%)	11	20

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	ALA
1	B	438	GLN
1	B	472	SER
1	B	494	ASP
1	B	497	THR
1	C	492	THR
1	C	497	THR
1	A	491	GLY
1	A	496	GLU
1	B	377	LYS
1	B	378	GLU
1	C	435	GLY
1	C	9	SER
1	C	436	HIS
1	B	245	ASP
1	B	376	ASP
1	B	477	VAL
1	A	440	PRO
1	C	474	ILE
1	A	473	GLY
1	C	477	VAL

### 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	419/440 (95%)	383 (91%)	36 (9%)	10	20
1	B	419/440 (95%)	379 (90%)	40 (10%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	419/440 (95%)	381 (91%)	38 (9%)	9	18
All	All	1257/1320 (95%)	1143 (91%)	114 (9%)	9	18

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	9	SER
1	A	28	THR
1	A	55	GLU
1	A	57	VAL
1	A	77	ARG
1	A	89	VAL
1	A	97	LEU
1	A	143	LEU
1	A	161	ARG
1	A	212	THR
1	A	283	LEU
1	A	287	LEU
1	A	308	THR
1	A	330	VAL
1	A	336	MET
1	A	373	THR
1	A	378	GLU
1	A	382	LEU
1	A	383	GLU
1	A	385	ARG
1	A	389	GLN
1	A	402	GLN
1	A	426	HIS
1	A	432	THR
1	A	436	HIS
1	A	439	ARG
1	A	441	SER
1	A	443	LEU
1	A	446	LEU
1	A	447	LEU
1	A	477	VAL
1	A	480	ARG
1	A	482	ARG
1	A	488	VAL
1	A	496	GLU

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Mol	Chain	Res	Type
1	B	39	LYS
1	B	40	LEU
1	B	57	VAL
1	B	63	GLN
1	B	97	LEU
1	B	120	THR
1	B	129	GLN
1	B	160	MET
1	B	161	ARG
1	B	174	LYS
1	B	196	ILE
1	B	197	ARG
1	B	210	LYS
1	B	212	THR
1	B	268	LEU
1	B	283	LEU
1	B	287	LEU
1	B	308	THR
1	B	309	THR
1	B	312	ASN
1	B	314	LEU
1	B	330	VAL
1	B	336	MET
1	B	344	TYR
1	B	377	LYS
1	B	382	LEU
1	B	383	GLU
1	B	387	THR
1	B	392	SER
1	B	402	GLN
1	B	426	HIS
1	B	438	GLN
1	B	441	SER
1	B	443	LEU
1	B	447	LEU
1	B	459	ARG
1	B	465	VAL
1	B	471	GLN
1	B	476	MET
1	B	492	THR
1	C	34	ARG
1	C	38	GLU

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Mol	Chain	Res	Type
1	C	55	GLU
1	C	57	VAL
1	C	58	ASP
1	C	77	ARG
1	C	84	GLU
1	C	89	VAL
1	C	97	LEU
1	C	105	LYS
1	C	196	ILE
1	C	212	THR
1	C	268	LEU
1	C	283	LEU
1	C	308	THR
1	C	312	ASN
1	C	321	LEU
1	C	330	VAL
1	C	336	MET
1	C	378	GLU
1	C	382	LEU
1	C	383	GLU
1	C	384	ARG
1	C	385	ARG
1	C	389	GLN
1	C	392	SER
1	C	426	HIS
1	C	436	HIS
1	C	446	LEU
1	C	447	LEU
1	C	466	SER
1	C	476	MET
1	C	477	VAL
1	C	480	ARG
1	C	482	ARG
1	C	488	VAL
1	C	490	PHE
1	C	497	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	127	HIS

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Mol	Chain	Res	Type
1	A	151	ASN
1	A	152	ASN
1	A	216	ASN
1	A	312	ASN
1	A	337	GLN
1	A	402	GLN
1	A	417	GLN
1	A	427	GLN
1	A	436	HIS
1	A	481	HIS
1	B	63	GLN
1	B	69	GLN
1	B	127	HIS
1	B	151	ASN
1	B	152	ASN
1	B	216	ASN
1	B	312	ASN
1	B	337	GLN
1	B	417	GLN
1	B	438	GLN
1	B	471	GLN
1	B	481	HIS
1	C	63	GLN
1	C	104	GLN
1	C	127	HIS
1	C	151	ASN
1	C	152	ASN
1	C	216	ASN
1	C	254	GLN
1	C	312	ASN
1	C	425	ASN
1	C	427	GLN
1	C	481	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 41 ligands modelled in this entry, 3 are monoatomic - leaving 38 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	527	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	A	528	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	B	524	-	4,4,4	0.14	0	6,6,6	0.21	0
4	GOL	A	535	-	5,5,5	0.42	0	5,5,5	0.43	0
4	GOL	B	531	-	5,5,5	0.38	0	5,5,5	0.22	0
4	GOL	B	532	-	5,5,5	0.40	0	5,5,5	0.43	0
2	SO4	B	527	-	4,4,4	0.17	0	6,6,6	0.30	0
2	SO4	B	523	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	A	526	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	A	522	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	A	525	-	4,4,4	0.15	0	6,6,6	0.16	0
4	GOL	B	530	-	5,5,5	0.37	0	5,5,5	0.30	0
2	SO4	B	521	-	4,4,4	0.15	0	6,6,6	0.10	0
4	GOL	B	2	-	5,5,5	0.42	0	5,5,5	0.36	0
2	SO4	A	523	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	C	524	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	A	529	-	4,4,4	0.13	0	6,6,6	0.20	0
2	SO4	A	1	-	4,4,4	0.17	0	6,6,6	0.24	0
4	GOL	A	534	-	5,5,5	0.35	0	5,5,5	0.42	0
2	SO4	C	526	-	4,4,4	0.15	0	6,6,6	0.17	0
4	GOL	C	529	-	5,5,5	0.40	0	5,5,5	0.22	0
4	GOL	C	1	-	5,5,5	0.34	0	5,5,5	0.30	0
2	SO4	C	521	-	4,4,4	0.14	0	6,6,6	0.13	0
4	GOL	C	528	-	5,5,5	0.31	0	5,5,5	0.41	0
2	SO4	A	521	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	C	525	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	526	-	4,4,4	0.15	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	533	-	5,5,5	0.40	0	5,5,5	0.34	0
2	SO4	A	531	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	C	523	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	B	3	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	A	530	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	C	2	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	A	524	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	B	528	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	B	522	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	C	522	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	525	-	4,4,4	0.17	0	6,6,6	0.18	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
4	GOL	B	530	-	-	2/4/4/4	-
4	GOL	B	2	-	-	4/4/4/4	-
4	GOL	A	535	-	-	2/4/4/4	-
4	GOL	B	531	-	-	2/4/4/4	-
4	GOL	B	532	-	-	2/4/4/4	-
4	GOL	C	528	-	-	3/4/4/4	-
4	GOL	A	533	-	-	4/4/4/4	-
4	GOL	C	529	-	-	2/4/4/4	-
4	GOL	C	1	-	-	0/4/4/4	-
4	GOL	A	534	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	531	GOL	O1-C1-C2-C3
4	B	2	GOL	O1-C1-C2-O2
4	B	2	GOL	C1-C2-C3-O3
4	A	534	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	530	GOL	C1-C2-C3-O3
4	C	528	GOL	O1-C1-C2-O2
4	C	528	GOL	O1-C1-C2-C3
4	B	2	GOL	O2-C2-C3-O3
4	C	529	GOL	O1-C1-C2-O2
4	A	535	GOL	O1-C1-C2-C3
4	B	532	GOL	O1-C1-C2-C3
4	B	2	GOL	O1-C1-C2-C3
4	C	529	GOL	O1-C1-C2-C3
4	B	531	GOL	O1-C1-C2-O2
4	A	534	GOL	O2-C2-C3-O3
4	B	530	GOL	O2-C2-C3-O3
4	A	533	GOL	O2-C2-C3-O3
4	B	532	GOL	O1-C1-C2-O2
4	A	533	GOL	O1-C1-C2-C3
4	A	533	GOL	C1-C2-C3-O3
4	A	535	GOL	O1-C1-C2-O2
4	C	528	GOL	O2-C2-C3-O3
4	A	533	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	527	SO4	1	0
4	B	530	GOL	1	0
2	A	529	SO4	1	0
4	A	534	GOL	1	0
4	C	529	GOL	1	0
4	C	1	GOL	2	0
4	C	528	GOL	1	0
4	A	533	GOL	1	0
2	B	522	SO4	1	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, 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	492/517 (95%)	-0.00	20 (4%)	37 40	12, 24, 58, 76	4 (0%)
1	B	492/517 (95%)	0.07	24 (4%)	29 31	15, 27, 57, 79	4 (0%)
1	C	492/517 (95%)	0.11	24 (4%)	29 31	14, 27, 63, 81	3 (0%)
All	All	1476/1551 (95%)	0.06	68 (4%)	32 34	12, 26, 60, 81	11 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	ILE	9.0
1	B	497	THR	8.3
1	C	437	ALA	7.9
1	B	477	VAL	7.3
1	C	476	MET	7.3
1	C	497	THR	7.1
1	A	477	VAL	7.0
1	B	495	ALA	6.9
1	C	474	ILE	6.9
1	A	476	MET	6.5
1	A	495	ALA	6.3
1	C	493	MET	6.2
1	A	474	ILE	5.9
1	C	495	ALA	5.8
1	A	497	THR	5.8
1	B	496	GLU	5.8
1	B	475	GLU	5.7
1	A	8	PRO	5.4
1	B	498	PRO	5.3
1	A	493	MET	5.3
1	C	475	GLU	5.0
1	B	493	MET	4.9
1	B	476	MET	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	498	PRO	4.7
1	C	492	THR	4.5
1	C	496	GLU	4.5
1	A	492	THR	4.0
1	A	498	PRO	3.9
1	A	436	HIS	3.9
1	A	475	GLU	3.6
1	A	473	GLY	3.6
1	A	470	ALA	3.6
1	C	473	GLY	3.6
1	C	494	ASP	3.5
1	B	473	GLY	3.3
1	C	436	HIS	3.2
1	A	437	ALA	3.2
1	A	494	ASP	3.2
1	C	472	SER	3.2
1	C	378	GLU	3.1
1	A	496	GLU	3.1
1	A	459	ARG	2.9
1	B	459	ARG	2.9
1	A	58	ASP	2.8
1	C	38	GLU	2.8
1	B	378	GLU	2.8
1	C	477	VAL	2.6
1	A	7	ARG	2.6
1	B	379	GLU	2.6
1	B	492	THR	2.5
1	B	494	ASP	2.5
1	B	436	HIS	2.5
1	B	470	ALA	2.5
1	C	9	SER	2.5
1	C	379	GLU	2.4
1	B	437	ALA	2.3
1	C	377	LYS	2.3
1	C	470	ALA	2.3
1	C	459	ARG	2.2
1	C	444	MET	2.2
1	B	58	ASP	2.2
1	A	435	GLY	2.2
1	B	487	TRP	2.1
1	C	471	GLN	2.1
1	B	480	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	467	LYS	2.1
1	B	438	GLN	2.0
1	B	377	LYS	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	530	5/5	0.70	0.38	118,119,119,119	0
4	GOL	C	528	6/6	0.72	0.28	60,61,61,62	0
4	GOL	C	529	6/6	0.72	0.26	50,50,52,52	0
2	SO4	A	529	5/5	0.76	0.32	98,98,98,98	0
2	SO4	A	528	5/5	0.77	0.27	90,90,90,91	0
2	SO4	B	528	5/5	0.77	0.27	92,92,92,92	0
2	SO4	B	526	5/5	0.81	0.28	100,100,100,100	0
2	SO4	A	527	5/5	0.82	0.27	96,96,97,97	0
4	GOL	B	2	6/6	0.83	0.20	58,59,59,59	0
2	SO4	B	525	5/5	0.83	0.22	74,74,75,75	0
4	GOL	C	1	6/6	0.85	0.18	40,42,43,43	0
4	GOL	A	534	6/6	0.85	0.22	59,60,60,60	0
4	GOL	A	533	6/6	0.86	0.25	52,53,53,53	0
4	GOL	B	531	6/6	0.87	0.20	50,50,51,52	0
2	SO4	C	521	5/5	0.87	0.20	79,79,80,80	0
4	GOL	B	532	6/6	0.87	0.22	50,51,52,52	0
4	GOL	A	535	6/6	0.87	0.25	49,51,51,52	0
2	SO4	A	531	5/5	0.88	0.22	78,79,79,79	0
2	SO4	A	526	5/5	0.89	0.28	80,80,80,80	0
4	GOL	B	530	6/6	0.90	0.24	53,54,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	523	5/5	0.90	0.20	69,70,70,71	0
2	SO4	B	522	5/5	0.91	0.17	89,89,89,90	0
2	SO4	A	521	5/5	0.91	0.21	67,68,68,68	0
2	SO4	A	523	5/5	0.92	0.34	54,55,56,57	0
2	SO4	C	525	5/5	0.92	0.34	94,94,94,95	0
2	SO4	A	522	5/5	0.92	0.15	75,75,76,76	0
2	SO4	C	524	5/5	0.93	0.38	62,63,63,64	0
2	SO4	B	521	5/5	0.93	0.22	72,72,73,73	0
3	MN3	C	527	1/1	0.93	0.13	72,72,72,72	0
2	SO4	B	524	5/5	0.94	0.15	53,53,55,55	0
2	SO4	C	522	5/5	0.94	0.15	72,72,72,72	0
2	SO4	B	527	5/5	0.94	0.30	58,58,59,59	0
3	MN3	A	532	1/1	0.95	0.05	55,55,55,55	0
2	SO4	C	523	5/5	0.95	0.19	80,80,80,81	0
2	SO4	A	525	5/5	0.95	0.14	63,63,64,64	0
2	SO4	A	524	5/5	0.95	0.12	64,64,65,65	0
2	SO4	C	2	5/5	0.96	0.14	54,54,55,55	0
2	SO4	C	526	5/5	0.96	0.14	64,64,65,65	0
3	MN3	B	529	1/1	0.96	0.06	74,74,74,74	0
2	SO4	A	1	5/5	0.97	0.12	46,46,47,47	0
2	SO4	B	3	5/5	0.98	0.11	62,62,63,63	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.