Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 03:16 PM EST

PDB ID	:	3NAI
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 (i) 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 (i)) were used in the production of this report:

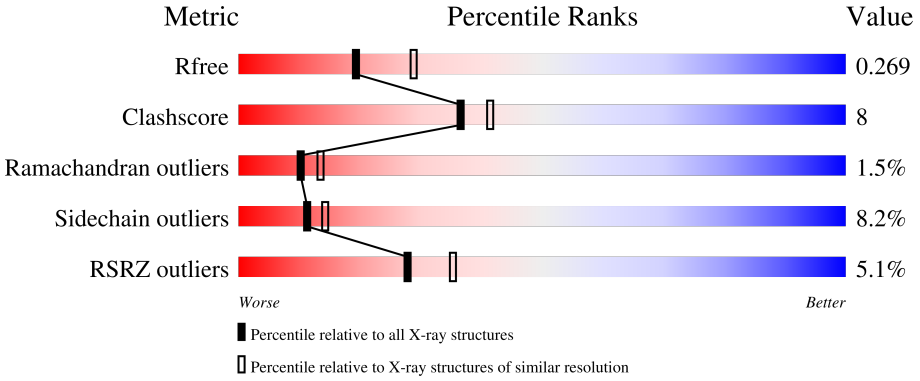
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 <=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% 73% 17% • 6%
1	B	517	4% 74% 18% • 6%
1	C	517	5% 74% 16% • 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 (i)

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
			Total	C	N	O	S			
1	A	486	3857	2437	679	716	25	0	0	0
1	B	486	3857	2437	679	716	25	0	0	0
1	C	486	3857	2437	679	716	25	0	0	0

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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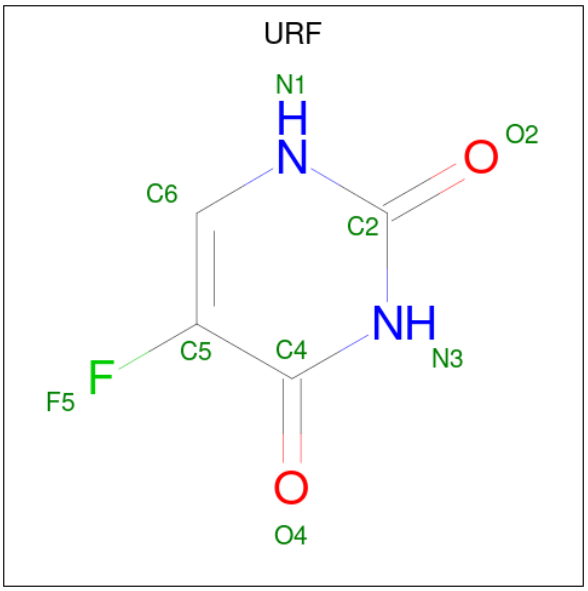
Chain	Residue	Modelled	Actual	Comment	Reference
C	511	ALA	-	expression tag	UNP Q80J95
C	512	ALA	-	expression tag	UNP Q80J95
C	513	LEU	-	expression tag	UNP Q80J95
C	514	GLU	-	expression tag	UNP Q80J95
C	515	HIS	-	expression tag	UNP Q80J95
C	516	HIS	-	expression tag	UNP Q80J95
C	517	HIS	-	expression tag	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 MAGNESIUM ION (three-letter code: 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 (three-letter code: URF) (formula: $C_4H_3FN_2O_2$).



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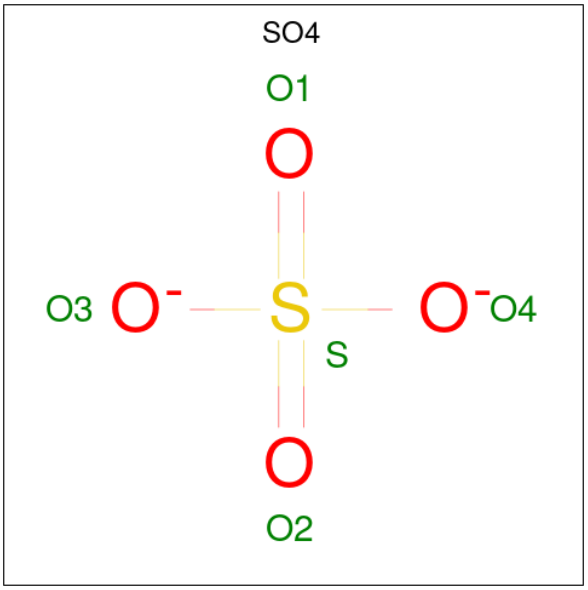
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	B	1	9	4	1	2	2	0	0
3	C	1	9	4	1	2	2	0	0

- Molecule 4 is MANGANESE (III) ION (three-letter code: MN3) (formula: Mn).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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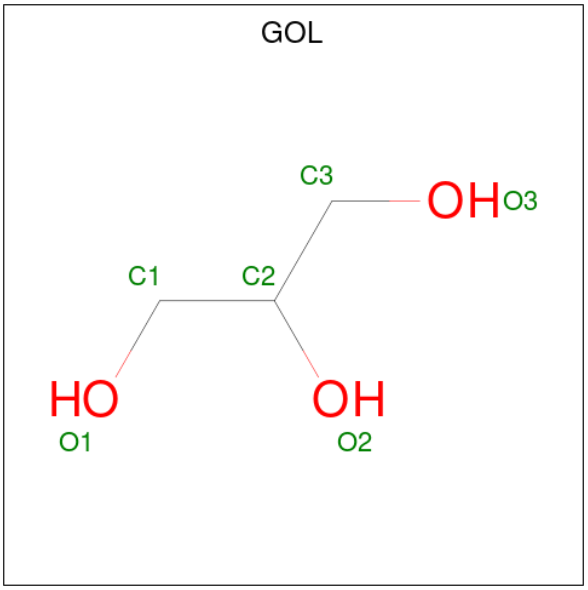
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	C	1	5	4	1	0	0
			Total	O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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is water.

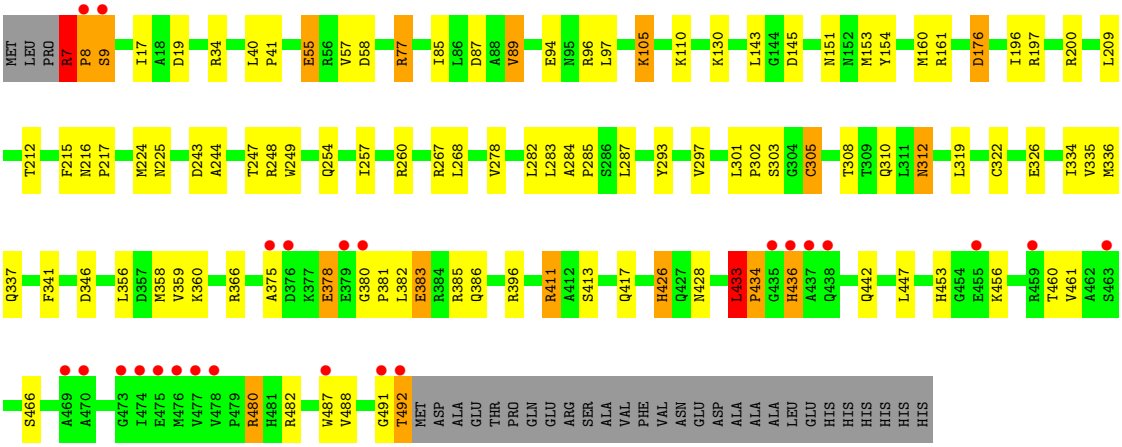
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	130	130	130	0	0
			Total	O		
7	B	106	106	106	0	0
			Total	O		
7	C	112	112	112	0	0

3 Residue-property plots (i)

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

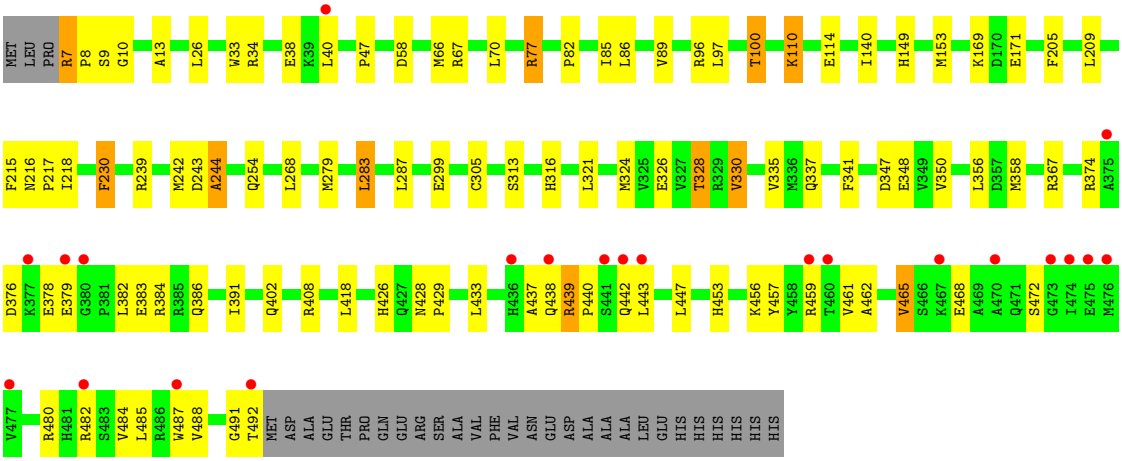
• Molecule 1: RNA dependent RNA polymerase

Chain A:



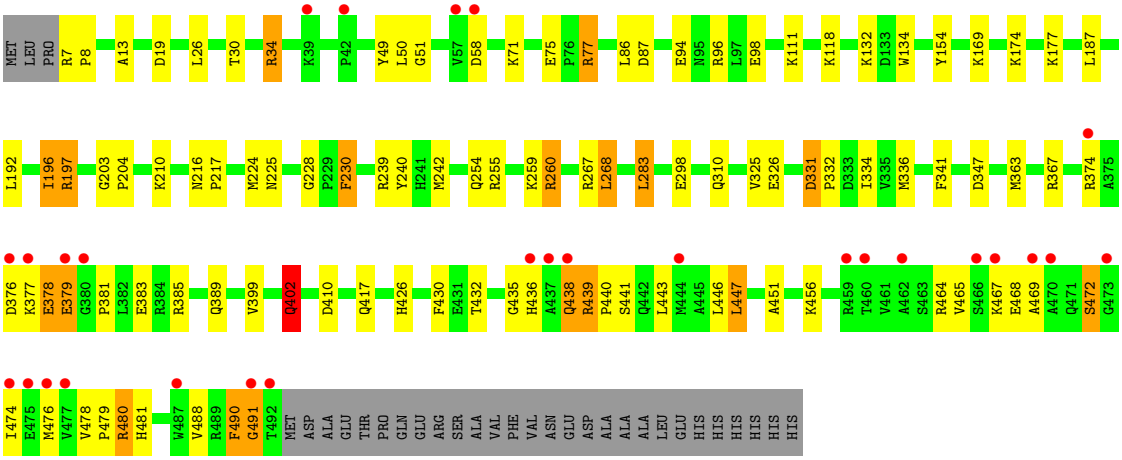
• Molecule 1: RNA dependent RNA polymerase

Chain B:



• Molecule 1: RNA dependent RNA polymerase

Chain C:


MET LEU PRO R7 P8 A13 D19 L26 T30 R34 K39 P42 Y49 L50 G51 V57 D58 K71 E75 P76 R77 L86 D87 E94 N95 R96 L97 E98 K111 K118 K132 D133 W134 Y154 K169 K174 K177 L187
L192 I196 R197 G203 P204 K210 N216 P217 M224 N225 G228 P229 F230 R239 Y240 H241 M242 Q254 R255 K259 R260 R267 L268 L283 E298 Q310 V325 E326 D331 P332 D333 I334 V335 M336 F341 D347 M363 R367 R374 A375
D376 K377 E378 E379 G380 P381 L382 E383 R384 R385 Q389 V399 Q402 D410 Q417 H426 F430 E431 T432 G435 H436 A437 Q438 R439 P440 S441 Q442 L443 M444 A445 L446 L447 A451 K456 R459 T460 V461 A462 S463 R464 V465 S466 K467 E468 A469 A470 Q471 S472 G473
I474 E475 M476 V477 V478 P479 R480 H481 W487 V488 R489 F490 G491 T492 MET ASP ALA GLU THR PRO GLN GLU ARG SER ALA VAL PHE VAL ASN GLU ASP ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.53-2.56) 98.7 (39.53-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SO4, MN3, GOL, URF

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	0.49	0/3952	0.64	1/5355 (0.0%)
1	B	0.48	0/3952	0.61	0/5355
1	C	0.48	0/3952	0.60	0/5355
All	All	0.48	0/11856	0.62	1/16065 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	ARG	C-N-CD	-5.01	109.58	120.60

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	66	0
1	B	3857	0	3812	59	0
1	C	3857	0	3812	58	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	183	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 (183) 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: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: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
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:B:358:MET:HE3	1:B:384:ARG:HB3	1.70	0.72
1:C:87:ASP:OD1	1:C:260:ARG:NH2	2.23	0.72
1:A:257:ILE:HD13	1:A:319:LEU:HD21	1.73	0.70
1:A:356:LEU:HD23	1:A:358:MET:HE1	1.75	0.69
1:C:439:ARG:H	1:C:440:PRO:HD3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ALA:HB2	1:B:67:ARG:HG2	1.76	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: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:A:40:LEU:HD12	1:A:41:PRO:HD2	1.84	0.59
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:346:ASP:CG	3:A:521:URF:HN3	2.07	0.56
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: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
1:B:456:LYS:HG3	1:B:457:TYR:H	1.73	0.54
1:A:105:LYS:H	1:A:105:LYS:NZ	2.05	0.54
1:C:326:GLU:CD	1:C:367:ARG:HH22	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:169:LYS:HD3	1:B:171:GLU:CD	2.32	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:C:436:HIS:CE1	1:C:439:ARG:HD3	2.47	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
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:437:ALA:C	1:B:439:ARG:H	2.14	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: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:A:491:GLY:HA3	1:A:492:THR:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:149:HIS:NE2	1:B:153:MET:HE2	2.30	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:B:356:LEU:HD23	1:B:358:MET:CE	2.45	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: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:B:243:ASP:O	1:B:244:ALA:C	2.54	0.45
1:A:426:HIS:CE1	1:A:428:ASN:O	2.69	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
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:C:383:GLU:HG2	1:C:385:ARG:NH1	2.32	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:A:284:ALA:O	1:A:285:PRO:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:C:374:ARG:HE	1:C:377:LYS:H	1.70	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	484/517 (94%)	460 (95%)	18 (4%)	6 (1%)	13 17
1	B	484/517 (94%)	465 (96%)	13 (3%)	6 (1%)	13 17
1	C	484/517 (94%)	454 (94%)	20 (4%)	10 (2%)	7 8
All	All	1452/1551 (94%)	1379 (95%)	51 (4%)	22 (2%)	10 13

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%)	377 (91%)	37 (9%)	9 12
1	B	414/440 (94%)	384 (93%)	30 (7%)	14 18
1	C	414/440 (94%)	379 (92%)	35 (8%)	10 13
All	All	1242/1320 (94%)	1140 (92%)	102 (8%)	11 14

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	34	ARG
1	A	55	GLU
1	A	57	VAL
1	A	77	ARG
1	A	89	VAL
1	A	97	LEU
1	A	105	LYS
1	A	143	LEU
1	A	145	ASP
1	A	161	ARG
1	A	176	ASP
1	A	196	ILE
1	A	268	LEU
1	A	283	LEU
1	A	287	LEU
1	A	297	VAL
1	A	305	CYS
1	A	312	ASN
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

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Mol	Chain	Res	Type
1	A	386	GLN
1	A	411	ARG
1	A	413	SER
1	A	426	HIS
1	A	433	LEU
1	A	436	HIS
1	A	447	LEU
1	A	461	VAL
1	A	466	SER
1	A	480	ARG
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	230	PHE
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	347	ASP
1	B	378	GLU
1	B	382	LEU
1	B	402	GLN
1	B	418	LEU
1	B	439	ARG
1	B	442	GLN
1	B	447	LEU
1	B	459	ARG
1	B	465	VAL
1	B	468	GLU
1	B	484	VAL
1	C	26	LEU

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Mol	Chain	Res	Type
1	C	34	ARG
1	C	58	ASP
1	C	71	LYS
1	C	75	GLU
1	C	77	ARG
1	C	86	LEU
1	C	111	LYS
1	C	196	ILE
1	C	197	ARG
1	C	210	LYS
1	C	230	PHE
1	C	242	MET
1	C	260	ARG
1	C	268	LEU
1	C	283	LEU
1	C	331	ASP
1	C	336	MET
1	C	347	ASP
1	C	378	GLU
1	C	379	GLU
1	C	402	GLN
1	C	410	ASP
1	C	426	HIS
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	472	SER
1	C	474	ILE
1	C	476	MET
1	C	480	ARG
1	C	490	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	83	GLN
1	A	146	GLN
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	152	ASN
1	A	216	ASN
1	A	225	ASN
1	A	253	GLN
1	A	254	GLN
1	A	312	ASN
1	A	427	GLN
1	A	442	GLN
1	A	481	HIS
1	B	63	GLN
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	417	GLN
1	B	442	GLN
1	C	63	GLN
1	C	104	GLN
1	C	216	ASN
1	C	225	ASN
1	C	254	GLN
1	C	436	HIS
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 monosaccharides 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	A	526	-	4,4,4	0.14	0	6,6,6	0.30	0
6	GOL	C	2	-	5,5,5	0.35	0	5,5,5	0.22	0
5	SO4	A	3	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	B	526	-	4,4,4	0.12	0	6,6,6	0.12	0
6	GOL	A	528	-	5,5,5	0.42	0	5,5,5	0.37	0
3	URF	A	521	2	9,9,9	2.92	4 (44%)	12,12,12	3.65	8 (66%)
5	SO4	C	525	-	4,4,4	0.14	0	6,6,6	0.17	0
5	SO4	C	524	-	4,4,4	0.10	0	6,6,6	0.26	0
3	URF	C	521	-	9,9,9	2.75	4 (44%)	12,12,12	4.08	8 (66%)
5	SO4	A	527	-	4,4,4	0.16	0	6,6,6	0.14	0
5	SO4	B	527	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	C	526	-	4,4,4	0.12	0	6,6,6	0.23	0
5	SO4	A	524	-	4,4,4	0.16	0	6,6,6	0.31	0
5	SO4	B	528	-	4,4,4	0.12	0	6,6,6	0.23	0
5	SO4	B	525	-	4,4,4	0.11	0	6,6,6	0.27	0
5	SO4	B	524	-	4,4,4	0.15	0	6,6,6	0.17	0
5	SO4	A	2	-	4,4,4	0.15	0	6,6,6	0.17	0
3	URF	B	521	2	9,9,9	2.93	3 (33%)	12,12,12	3.85	8 (66%)
5	SO4	A	525	-	4,4,4	0.18	0	6,6,6	0.12	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
3	URF	C	521	-	-	-	0/1/1/1
6	GOL	C	2	-	-	2/4/4/4	-
3	URF	A	521	2	-	-	0/1/1/1
3	URF	B	521	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	528	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	521	URF	C6-C5	6.75	1.39	1.33
3	A	521	URF	C6-C5	6.70	1.39	1.33
3	C	521	URF	C6-C5	5.91	1.39	1.33
3	B	521	URF	C4-C5	4.33	1.49	1.44
3	C	521	URF	C4-C5	4.27	1.49	1.44
3	A	521	URF	C4-C5	3.79	1.49	1.44
3	A	521	URF	C4-N3	-2.95	1.33	1.38
3	C	521	URF	C4-N3	-2.70	1.33	1.38
3	B	521	URF	C4-N3	-2.66	1.33	1.38
3	A	521	URF	C2-N3	-2.23	1.33	1.37
3	C	521	URF	C2-N3	-2.02	1.34	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	521	URF	N1-C2-N3	6.70	122.72	115.13
3	C	521	URF	C5-C4-N3	6.62	119.07	112.56
3	C	521	URF	F5-C5-C4	6.46	122.39	116.40
3	A	521	URF	N1-C2-N3	6.19	122.14	115.13
3	C	521	URF	N1-C2-N3	6.08	122.02	115.13
3	A	521	URF	C5-C4-N3	5.94	118.41	112.56
3	B	521	URF	F5-C5-C4	5.84	121.81	116.40
3	B	521	URF	C5-C4-N3	5.82	118.29	112.56
3	A	521	URF	F5-C5-C4	4.91	120.95	116.40
3	A	521	URF	C6-C5-C4	-4.47	117.41	122.12
3	C	521	URF	C6-C5-C4	-4.40	117.48	122.12
3	C	521	URF	O4-C4-C5	-4.38	121.77	125.72
3	C	521	URF	C4-N3-C2	-4.31	120.13	126.34
3	A	521	URF	O4-C4-C5	-4.27	121.86	125.72
3	B	521	URF	C6-C5-C4	-4.19	117.70	122.12
3	B	521	URF	C4-N3-C2	-4.01	120.56	126.34
3	B	521	URF	O4-C4-C5	-3.78	122.30	125.72
3	A	521	URF	C4-N3-C2	-3.58	121.18	126.34
3	C	521	URF	O2-C2-N1	-3.33	119.12	122.79
3	B	521	URF	O2-C2-N1	-2.68	119.84	122.79
3	B	521	URF	O2-C2-N3	-2.32	117.43	121.82
3	A	521	URF	O2-C2-N3	-2.29	117.51	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	521	URF	F5-C5-C6	-2.25	120.13	121.73
3	A	521	URF	O2-C2-N1	-2.23	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
6	C	2	GOL	1	0
5	A	3	SO4	1	0
6	A	528	GOL	3	0
3	A	521	URF	1	0
3	C	521	URF	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	486/517 (94%)	0.06	24 (4%)	29	37	12, 24, 57, 76	2 (0%)
1	B	486/517 (94%)	0.09	22 (4%)	33	42	15, 28, 62, 78	1 (0%)
1	C	486/517 (94%)	0.17	28 (5%)	23	29	17, 29, 63, 81	1 (0%)
All	All	1458/1551 (94%)	0.11	74 (5%)	28	35	12, 28, 61, 81	4 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	PRO	7.0
1	B	476	MET	6.5
1	A	474	ILE	6.3
1	C	492	THR	6.2
1	C	438	GLN	5.2
1	C	476	MET	5.2
1	C	477	VAL	5.1
1	B	477	VAL	5.0
1	A	477	VAL	5.0
1	B	492	THR	4.8
1	C	469	ALA	4.7
1	B	474	ILE	4.7
1	C	473	GLY	4.5
1	C	437	ALA	4.3
1	C	377	LYS	4.2
1	A	473	GLY	4.2
1	A	476	MET	4.2
1	B	473	GLY	4.0
1	A	438	GLN	3.9
1	C	474	ILE	3.8
1	A	376	ASP	3.8
1	A	492	THR	3.8
1	A	459	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	436	HIS	3.6
1	B	475	GLU	3.6
1	C	470	ALA	3.5
1	B	470	ALA	3.4
1	C	491	GLY	3.4
1	A	478	VAL	3.4
1	C	475	GLU	3.4
1	B	443	LEU	3.3
1	C	42	PRO	3.3
1	A	380	GLY	3.2
1	A	437	ALA	3.2
1	C	57	VAL	3.1
1	B	482	ARG	3.0
1	C	39	LYS	3.0
1	B	377	LYS	2.9
1	A	470	ALA	2.9
1	C	462	ALA	2.9
1	B	438	GLN	2.8
1	A	435	GLY	2.8
1	C	379	GLU	2.8
1	C	487	TRP	2.7
1	B	459	ARG	2.7
1	C	467	LYS	2.6
1	C	466	SER	2.6
1	C	380	GLY	2.6
1	B	442	GLN	2.6
1	B	487	TRP	2.6
1	C	58	ASP	2.5
1	C	376	ASP	2.5
1	A	455	GLU	2.5
1	B	467	LYS	2.4
1	C	374	ARG	2.4
1	A	469	ALA	2.3
1	B	441	SER	2.3
1	A	491	GLY	2.3
1	A	379	GLU	2.3
1	C	444	MET	2.2
1	B	375	ALA	2.2
1	A	475	GLU	2.2
1	A	9	SER	2.2
1	A	463	SER	2.2
1	C	459	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	40	LEU	2.2
1	A	436	HIS	2.1
1	C	436	HIS	2.1
1	C	460	THR	2.1
1	A	375	ALA	2.1
1	A	487	TRP	2.1
1	B	460	THR	2.0
1	B	380	GLY	2.0
1	B	379	GLU	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 monosaccharides 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	0.77	0.26	56,56,57,58	9
3	URF	A	521	9/9	0.79	0.27	70,71,71,72	0
5	SO4	A	527	5/5	0.79	0.24	104,104,104,104	0
3	URF	C	521	9/9	0.83	0.26	71,71,72,72	0
5	SO4	C	525	5/5	0.88	0.22	70,70,71,71	0
2	MG	B	2	1/1	0.89	0.13	33,33,33,33	0
6	GOL	C	2	6/6	0.90	0.15	53,54,55,55	0
6	GOL	A	528	6/6	0.91	0.19	37,39,39,40	0
5	SO4	A	2	5/5	0.91	0.20	80,80,80,80	0
5	SO4	A	526	5/5	0.92	0.21	69,70,70,70	0
5	SO4	C	526	5/5	0.92	0.17	77,77,78,78	0
5	SO4	A	3	5/5	0.92	0.19	75,76,76,76	0
5	SO4	B	528	5/5	0.92	0.23	87,87,87,88	0
2	MG	C	3	1/1	0.93	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	527	5/5	0.94	0.32	86,86,86,86	0
5	SO4	B	525	5/5	0.95	0.14	52,52,53,53	0
5	SO4	B	526	5/5	0.95	0.18	70,71,71,71	0
4	MN3	C	523	1/1	0.96	0.11	55,55,55,55	0
5	SO4	A	525	5/5	0.96	0.21	52,53,53,53	0
5	SO4	B	524	5/5	0.97	0.14	46,46,47,47	0
5	SO4	C	524	5/5	0.97	0.12	46,46,47,47	0
2	MG	A	1	1/1	0.97	0.15	26,26,26,26	0
5	SO4	A	524	5/5	0.98	0.10	40,40,40,41	0
4	MN3	B	523	1/1	0.98	0.09	40,40,40,40	0
4	MN3	C	522	1/1	0.98	0.08	46,46,46,46	0
4	MN3	A	522	1/1	0.98	0.08	47,47,47,47	0
4	MN3	A	523	1/1	0.99	0.12	40,40,40,40	0
4	MN3	B	522	1/1	1.00	0.07	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.