Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 05:27 am BST

PDB ID	:	2C1L
Title	:	Structure of the BfiI restriction endonuclease
Authors	:	Grazulis, S.; Manakova, E.; Roessle, M.; Bochtler, M.; Tamulaitiene, G.; Huber, R.; Siksnys, V.
Deposited on	:	2005-09-15
Resolution	:	1.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2
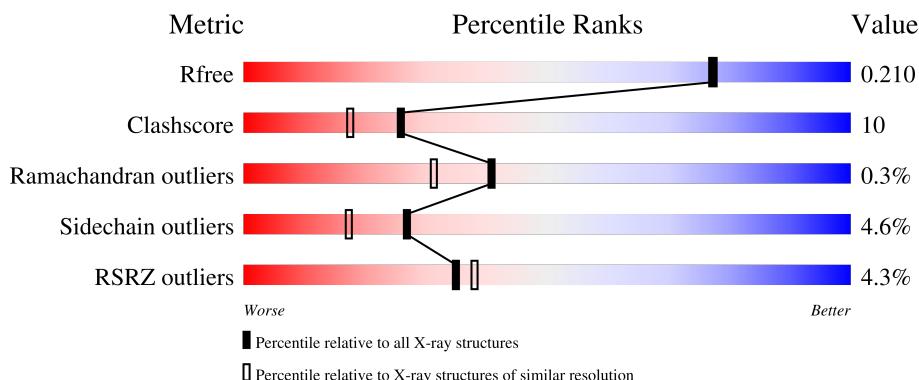
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*
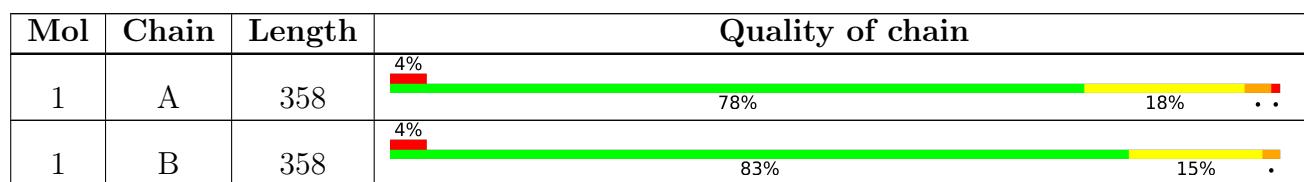
The reported resolution of this entry is 1.90 Å.

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	Percentile Ranks	Value
Rfree		0.210
Clashscore		10
Ramachandran outliers		0.3%
Sidechain outliers		4.6%
RSRZ outliers		4.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	358	4% / 78% / 18% / · ·
1	B	358	4% / 83% / 15% / ·

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
5	SRT	B	1362	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6457 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.
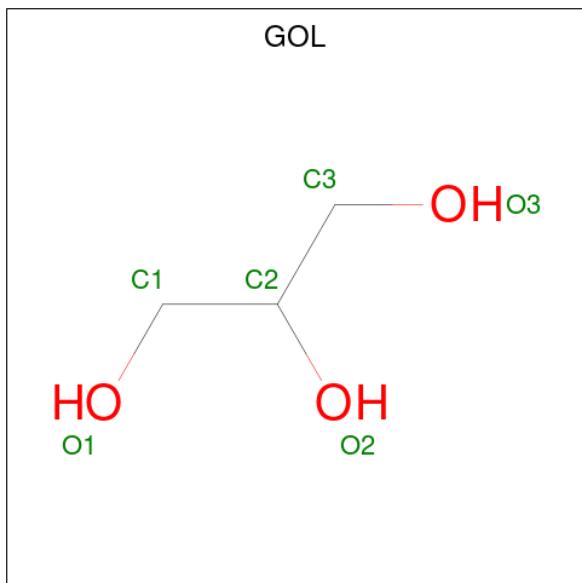
- Molecule 1 is a protein called RESTRICTION ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	17	0
			2966	1850	529	576	11			
1	B	358	Total	C	N	O	S	0	10	0
			2897	1811	512	565	9			
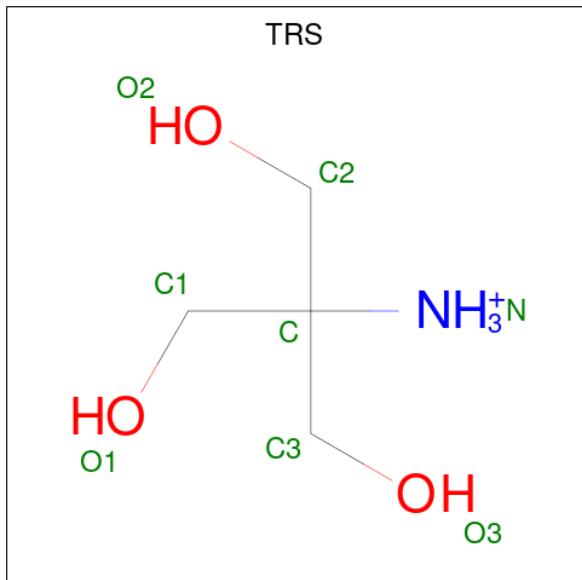
- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
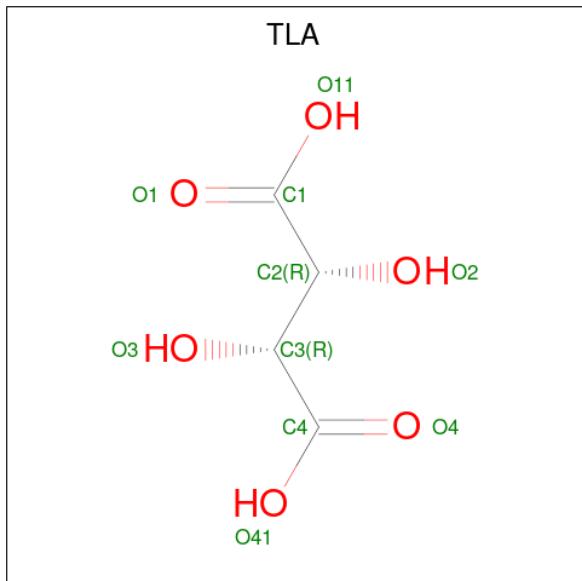
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	4	1	3	0	0

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).
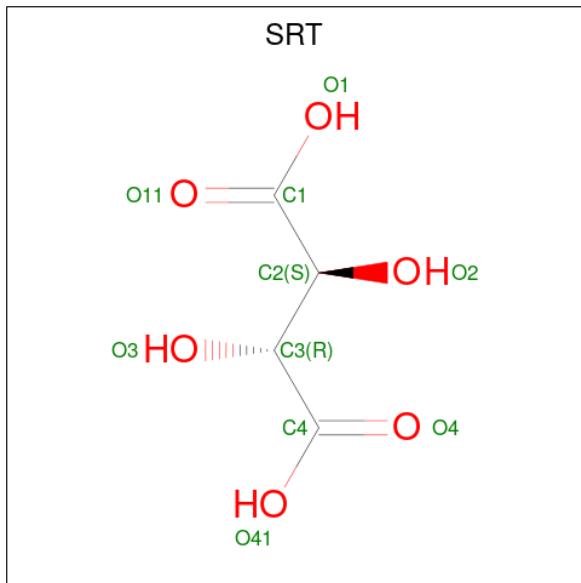
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	4	6	0	0

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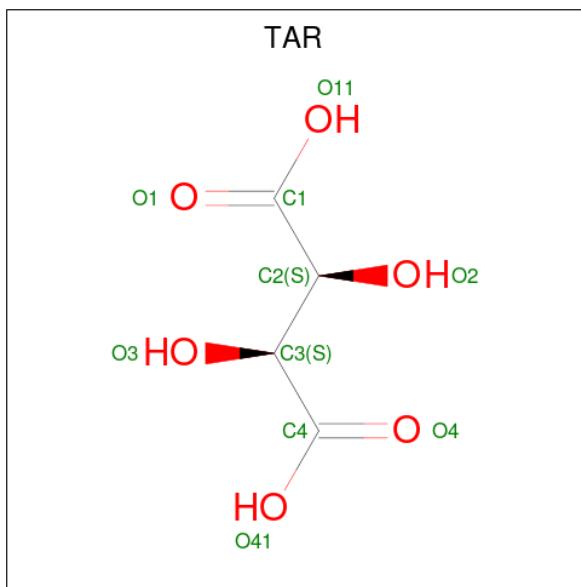
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total C O 10 4 6			0	0

- Molecule 5 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: $C_4H_6O_6$).
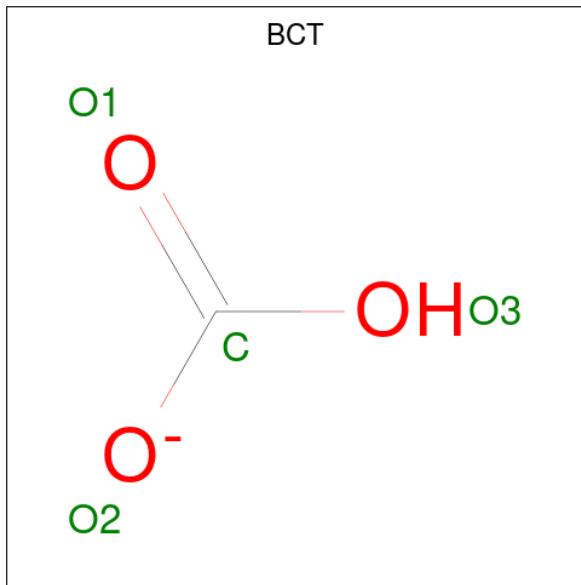
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total C O 10 4 6			0	0
5	B	1	Total C O 10 4 6			0	0

- Molecule 6 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 10	C 4	O 6	0	0
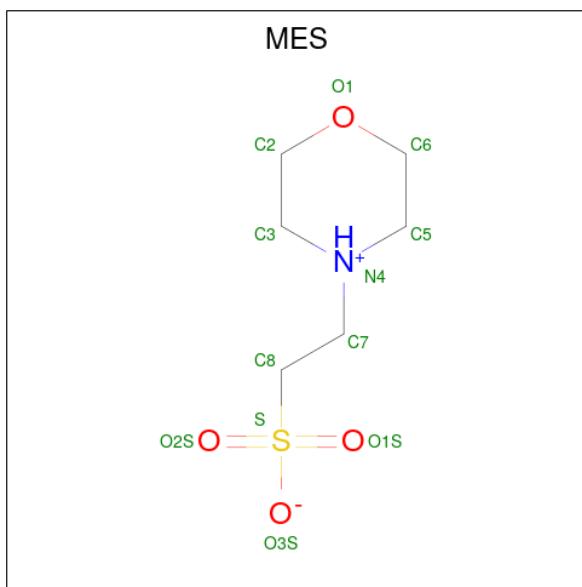
- Molecule 7 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

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

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: $C_6H_{13}NO_4S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
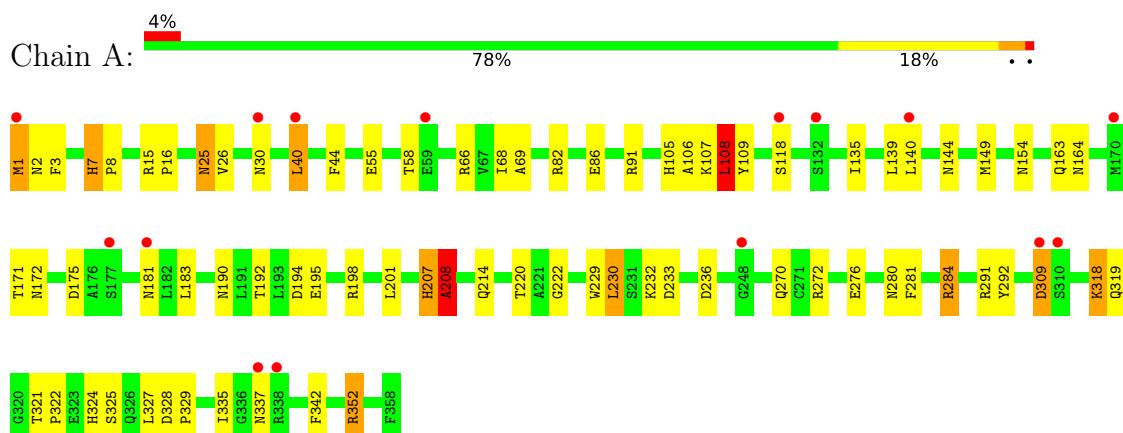
• Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	254	Total	O	0	0
			254	254		
9	B	226	Total	O	0	0
			226	226		
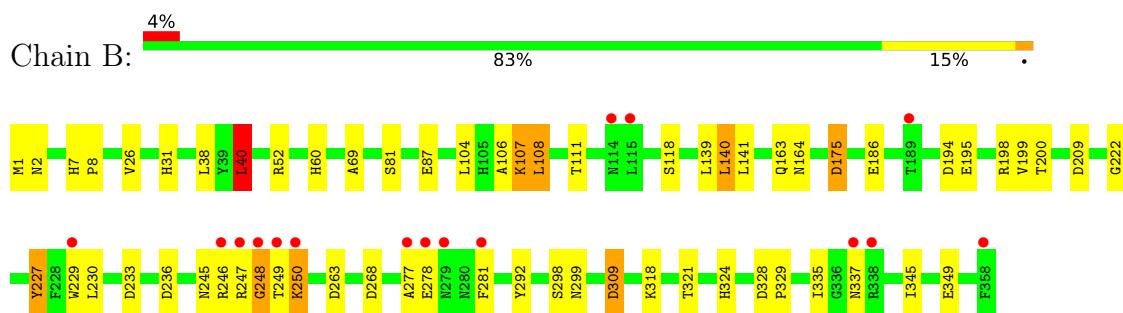
3 Residue-property plots ⓘ

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: RESTRICTION ENDONUCLEASE

Chain A:

• Molecule 1: RESTRICTION ENDONUCLEASE

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	138.93Å　　138.93Å　　94.14Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	28.01　–　1.90 51.85　–　1.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.01-1.90) 99.7 (51.85-1.77)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.72 (at 1.76Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.188　,　0.217 0.180　,　0.210	Depositor DCC
R_{free} test set	7018 reflections (8.04%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6457	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: BCT, MES, GOL, TAR, SRT, TLA, TRS

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	0.80	2/3026 (0.1%)	0.87	9/4099 (0.2%)
1	B	0.70	0/2957	0.83	8/4009 (0.2%)
All	All	0.75	2/5983 (0.0%)	0.85	17/8108 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	ALA	N-CA	10.75	1.67	1.46
1	A	86	GLU	CD-OE1	6.28	1.32	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ALA	N-CA-C	6.40	128.27	111.00
1	A	236	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	207	HIS	C-N-CA	-6.24	106.10	121.70
1	B	236	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	230	LEU	CB-CG-CD1	6.04	121.28	111.00
1	B	175	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	108	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	268	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	209	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309[A]	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	309[B]	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	309	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	40	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	233	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	233	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	263	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	149	MET	CB-CA-C	-5.04	100.32	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	227	TYR	Peptide
1	B	248	GLY	Peptide

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	2966	0	2858	73	0
1	B	2897	0	2787	48	0
2	A	18	0	24	3	0
2	B	6	0	8	2	0
3	A	8	0	12	0	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
5	A	10	0	4	2	0
5	B	10	0	4	2	0
6	A	10	0	4	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	B	24	0	26	1	0
9	A	254	0	0	12	0
9	B	226	0	0	4	0
All	All	6457	0	5735	120	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 10.

All (120) 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:208:ALA:CA	1:A:208:ALA:N	1.67	1.54
1:A:318:LYS:O	1:A:321:THR:HG22	1.56	1.03
1:B:309:ASP:OD2	9:B:2188:HOH:O	1.76	1.01
1:A:214:GLN:HE22	2:A:1361:GOL:H32	1.27	0.99
1:A:144[B]:ASN:ND2	9:A:2113:HOH:O	2.06	0.89
1:A:207:HIS:C	1:A:208:ALA:CA	2.43	0.87
1:B:245:ASN:ND2	1:B:250:LYS:O	2.11	0.83
2:B:1359:GOL:O3	9:B:2213:HOH:O	1.92	0.82
1:B:106:ALA:HB1	1:B:108[B]:LEU:HD11	1.61	0.80
1:A:214:GLN:HE22	2:A:1361:GOL:C3	1.95	0.79
1:B:321:THR:HG23	1:B:324:HIS:H	1.50	0.77
1:A:318:LYS:O	1:A:321:THR:CG2	2.32	0.76
1:A:25:ASN:C	1:A:25:ASN:HD22	1.90	0.74
1:B:175:ASP:O	8:B:1361:MES:H32	1.89	0.73
1:A:208:ALA:N	1:A:208:ALA:CB	2.52	0.71
1:B:318:LYS:O	1:B:321:THR:HG22	1.92	0.70
1:A:154[A]:ASN:ND2	9:A:2115:HOH:O	2.24	0.69
1:B:163:GLN:O	1:B:164[B]:ASN:HB3	1.93	0.68
1:A:139:LEU:HD23	1:B:139:LEU:HD23	1.75	0.68
1:A:309[B]:ASP:OD2	9:A:2219:HOH:O	2.10	0.67
1:A:82[A]:ARG:NH2	9:A:2071:HOH:O	2.29	0.65
1:B:277:ALA:O	1:B:281:PHE:CE2	2.50	0.65
1:A:335:ILE:HD11	1:A:342:PHE:CD2	2.32	0.65
1:B:140[A]:LEU:HD12	1:B:141:LEU:N	2.12	0.64
1:A:190:ASN:OD1	1:A:192:THR:O	2.15	0.64
1:B:106:ALA:HB1	1:B:108[B]:LEU:CD1	2.26	0.64
1:A:328:ASP:N	1:A:329:PRO:CD	2.61	0.64
1:A:321:THR:HG23	1:A:324:HIS:H	1.64	0.63
1:A:44:PHE:CE1	5:B:1362:SRT:H2	2.34	0.62
1:A:1[A]:MET:HG3	1:A:2:ASN:N	2.12	0.62
1:A:175:ASP:OD1	5:A:1364:SRT:O3	2.18	0.62
1:A:229:TRP:CZ3	1:A:284:ARG:HG2	2.35	0.61
1:A:321:THR:OG1	1:A:322:PRO:HD2	2.01	0.61
1:A:181[B]:ASN:ND2	9:A:2135:HOH:O	2.33	0.60
1:A:352:ARG:HG3	1:A:352:ARG:HH11	1.65	0.60
1:B:1:MET:CE	1:B:2:ASN:H	2.14	0.60
1:B:195:GLU:HA	1:B:198:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232[A]:LYS:HG2	1:A:281:PHE:O	2.02	0.60
1:A:40[B]:LEU:HD12	1:A:109:TYR:CD2	2.37	0.60
1:A:195:GLU:HA	1:A:198:ARG:HD2	1.84	0.59
1:A:229:TRP:CE3	1:A:284:ARG:HG2	2.38	0.59
1:A:229:TRP:CH2	1:A:284:ARG:HD2	2.37	0.59
1:A:232[B]:LYS:NZ	1:A:280:ASN:O	2.36	0.58
1:A:106:ALA:HB1	1:A:108:LEU:HD11	1.86	0.58
1:B:52:ARG:NH1	1:B:281:PHE:CZ	2.71	0.58
1:B:7:HIS:HB2	1:B:8:PRO:HA	1.85	0.57
1:A:25:ASN:C	1:A:25:ASN:ND2	2.57	0.57
1:B:247:ARG:NH2	9:B:2162:HOH:O	2.38	0.57
1:B:107:LYS:C	1:B:108[B]:LEU:HD12	2.25	0.57
1:B:108[B]:LEU:HD12	1:B:108[B]:LEU:N	2.19	0.56
1:A:214:GLN:NE2	2:A:1361:GOL:H32	2.09	0.56
1:A:201:LEU:HD22	9:A:2167:HOH:O	2.05	0.56
1:A:175:ASP:N	5:A:1364:SRT:O1	2.39	0.56
1:B:26:VAL:HG12	1:B:118[A]:SER:OG	2.06	0.55
1:A:1[B]:MET:HG2	1:A:3:PHE:CZ	2.42	0.55
1:A:280:ASN:ND2	9:A:2209:HOH:O	2.39	0.54
1:B:247:ARG:NH1	9:B:2163:HOH:O	2.06	0.54
1:B:81:SER:HB2	1:B:186:GLU:HG3	1.88	0.54
1:A:40[B]:LEU:HD12	1:A:109:TYR:CE2	2.43	0.54
1:B:1:MET:HE2	1:B:2:ASN:H	1.73	0.54
1:B:52:ARG:NH1	1:B:281:PHE:CE2	2.76	0.54
1:B:87:GLU:OE2	2:B:1359:GOL:H12	2.07	0.54
1:A:15:ARG:HB3	1:A:16:PRO:HD3	1.89	0.53
1:B:163:GLN:O	1:B:164[B]:ASN:CB	2.53	0.53
1:B:52:ARG:CZ	1:B:281:PHE:CZ	2.92	0.53
1:A:222:GLY:HA3	1:A:292:TYR:CE2	2.46	0.51
1:B:1:MET:HE3	1:B:1:MET:HA	1.92	0.51
1:A:82[B]:ARG:CZ	1:A:82[B]:ARG:HB2	2.40	0.51
1:A:30[B]:ASN:CG	1:A:30[B]:ASN:O	2.49	0.50
1:A:207:HIS:O	1:A:208:ALA:CA	2.58	0.50
1:B:163:GLN:O	1:B:164[A]:ASN:HB2	2.12	0.50
1:A:270:GLN:NE2	9:A:2201:HOH:O	2.45	0.50
1:B:222:GLY:HA3	1:B:292:TYR:CE2	2.47	0.49
1:A:7:HIS:HB2	1:A:8:PRO:HA	1.95	0.49
1:B:321:THR:HG22	1:B:324:HIS:HB2	1.93	0.49
1:A:25:ASN:HD22	1:A:26:VAL:N	2.11	0.49
1:A:276:GLU:OE2	1:A:284:ARG:HD3	2.13	0.49
1:A:154[A]:ASN:ND2	9:A:2116:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82[C]:ARG:HG2	1:A:183:LEU:HB2	1.95	0.48
1:A:163:GLN:O	1:A:164[A]:ASN:CB	2.60	0.48
1:A:201:LEU:CD2	9:A:2167:HOH:O	2.61	0.47
1:A:319:GLN:HA	1:A:324:HIS:CD2	2.48	0.47
1:A:82[A]:ARG:HD3	9:A:2072:HOH:O	2.15	0.47
1:B:199:VAL:HG12	1:B:200:THR:N	2.30	0.47
1:B:328:ASP:N	1:B:329:PRO:CD	2.77	0.47
1:A:321:THR:OG1	1:A:322:PRO:CD	2.64	0.46
1:B:245:ASN:OD1	1:B:245:ASN:O	2.34	0.46
1:B:26:VAL:O	1:B:111:THR:HG21	2.16	0.46
1:A:135:ILE:HB	1:B:104:LEU:HA	1.97	0.45
1:B:38:LEU:HD22	1:B:111:THR:HG22	1.98	0.45
1:B:140[B]:LEU:HD23	1:B:141:LEU:N	2.32	0.44
1:A:291:ARG:O	1:A:292:TYR:HB2	2.17	0.44
1:A:328:ASP:N	1:A:329:PRO:HD3	2.33	0.44
1:A:1[B]:MET:HG2	1:A:3:PHE:CE2	2.52	0.44
1:A:106:ALA:HB1	1:A:108:LEU:CD1	2.48	0.44
1:A:105:HIS:CD2	5:B:1362:SRT:HB	2.28	0.43
1:A:327:LEU:C	1:A:329:PRO:HD2	2.39	0.43
1:B:345:ILE:HD11	1:B:349:GLU:HG3	1.99	0.43
1:A:171:THR:O	1:A:172:ASN:HB2	2.19	0.43
1:A:163:GLN:O	1:A:164[A]:ASN:HB3	2.18	0.43
1:B:40:LEU:O	1:B:69:ALA:HA	2.19	0.43
1:B:81:SER:CB	1:B:186:GLU:HG3	2.48	0.42
1:A:40[A]:LEU:O	1:A:69:ALA:HA	2.20	0.42
1:A:154[A]:ASN:CG	9:A:2115:HOH:O	2.57	0.42
1:B:318:LYS:O	1:B:321:THR:CG2	2.66	0.42
1:B:298:SER:O	1:B:299:ASN:HB2	2.19	0.42
1:A:66:ARG:HD3	1:A:68:ILE:HD11	2.01	0.41
1:B:245:ASN:HD22	1:B:248:GLY:HA3	1.85	0.41
1:B:1:MET:HE3	1:B:2:ASN:H	1.84	0.41
1:B:31:HIS:HE2	1:B:60:HIS:CE1	2.38	0.41
1:B:227:TYR:HB2	1:B:229:TRP:CZ3	2.56	0.41
1:A:26:VAL:CG1	1:A:140[B]:LEU:HD11	2.51	0.41
1:B:321:THR:HG22	1:B:324:HIS:CB	2.50	0.41
1:A:26:VAL:CG1	1:A:140[B]:LEU:CD1	2.99	0.41
1:A:284:ARG:HE	1:A:284:ARG:HB2	1.55	0.41
1:A:40[B]:LEU:CD1	1:A:109:TYR:CE2	3.04	0.41
1:B:199:VAL:CG1	1:B:200:THR:N	2.84	0.40
1:A:58:THR:OG1	1:A:91:ARG:HD2	2.22	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	373/358 (104%)	360 (96%)	12 (3%)	1 (0%)	41	31
1	B	366/358 (102%)	355 (97%)	10 (3%)	1 (0%)	41	31
All	All	739/716 (103%)	715 (97%)	22 (3%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	246	ARG
1	A	208	ALA

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	324/306 (106%)	304 (94%)	20 (6%)	18	9
1	B	316/306 (103%)	303 (96%)	13 (4%)	30	21
All	All	640/612 (105%)	607 (95%)	33 (5%)	27	14

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	7	HIS
1	A	25	ASN

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Mol	Chain	Res	Type
1	A	40[A]	LEU
1	A	40[B]	LEU
1	A	55	GLU
1	A	107	LYS
1	A	108	LEU
1	A	118[A]	SER
1	A	118[B]	SER
1	A	194	ASP
1	A	220	THR
1	A	230	LEU
1	A	272	ARG
1	A	284	ARG
1	A	318	LYS
1	A	325	SER
1	A	337	ASN
1	A	352	ARG
1	B	40	LEU
1	B	107	LYS
1	B	108[A]	LEU
1	B	108[B]	LEU
1	B	140[A]	LEU
1	B	140[B]	LEU
1	B	194	ASP
1	B	230	LEU
1	B	249	THR
1	B	250	LYS
1	B	278	GLU
1	B	335	ILE
1	B	337	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	62	ASN
1	A	77	GLN
1	A	90	ASN
1	A	143	ASN
1	A	214	GLN
1	B	133	GLN
1	B	181	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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
7	BCT	A	1366	-	2,3,3	0.14	0	2,3,3	0.24	0
4	TLA	A	1363	-	9,9,9	2.72	1 (11%)	12,12,12	1.58	3 (25%)
3	TRS	A	1362	-	7,7,7	1.34	2 (28%)	9,9,9	1.50	2 (22%)
7	BCT	B	1364	-	2,3,3	0.18	0	2,3,3	1.08	0
8	MES	B	1360	-	12,12,12	1.98	4 (33%)	14,16,16	1.47	2 (14%)
8	MES	B	1361	-	12,12,12	2.62	4 (33%)	14,16,16	0.86	0
6	TAR	A	1365	-	9,9,9	0.84	0	12,12,12	1.86	4 (33%)
2	GOL	A	1361	-	5,5,5	0.35	0	5,5,5	0.53	0
2	GOL	A	1359	-	5,5,5	0.39	0	5,5,5	0.54	0
5	SRT	A	1364	-	9,9,9	0.89	1 (11%)	12,12,12	1.79	4 (33%)
2	GOL	B	1359	-	5,5,5	0.54	0	5,5,5	0.30	0
4	TLA	B	1363	-	9,9,9	0.90	0	12,12,12	1.46	3 (25%)
2	GOL	A	1360	-	5,5,5	0.37	0	5,5,5	0.41	0
5	SRT	B	1362	-	9,9,9	1.14	1 (11%)	12,12,12	3.20	7 (58%)

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	TLA	A	1363	-	-	0/12/12/12	-
3	TRS	A	1362	-	-	4/9/9/9	-
8	MES	B	1360	-	-	3/6/14/14	0/1/1/1
8	MES	B	1361	-	-	2/6/14/14	0/1/1/1
6	TAR	A	1365	-	-	4/12/12/12	-
2	GOL	A	1361	-	-	0/4/4/4	-
2	GOL	A	1359	-	-	2/4/4/4	-
5	SRT	A	1364	-	-	6/12/12/12	-
2	GOL	B	1359	-	-	2/4/4/4	-
4	TLA	B	1363	-	-	0/12/12/12	-
2	GOL	A	1360	-	-	3/4/4/4	-
5	SRT	B	1362	-	-	7/12/12/12	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1363	TLA	C3-C4	-7.85	1.41	1.52
8	B	1361	MES	C8-S	5.16	1.84	1.77
8	B	1361	MES	C7-N4	4.34	1.57	1.47
8	B	1360	MES	C3-N4	4.02	1.58	1.46
8	B	1361	MES	C3-N4	3.58	1.56	1.46
8	B	1361	MES	C5-N4	3.36	1.56	1.46
8	B	1360	MES	C5-N4	3.33	1.56	1.46
8	B	1360	MES	C7-N4	2.92	1.54	1.47
8	B	1360	MES	C8-S	2.82	1.81	1.77
5	B	1362	SRT	C2-C1	-2.75	1.48	1.52
3	A	1362	TRS	O2-C2	2.38	1.50	1.42
5	A	1364	SRT	C3-C4	-2.12	1.49	1.52
3	A	1362	TRS	O1-C1	2.07	1.49	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1362	SRT	C3-C2-C1	-4.98	98.75	109.87
5	B	1362	SRT	O2-C2-C3	4.79	119.74	110.23
5	B	1362	SRT	O41-C4-O4	-4.46	113.97	124.09
5	B	1362	SRT	O3-C3-C4	4.14	119.33	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1362	SRT	O41-C4-C3	4.12	124.41	113.27
4	A	1363	TLA	C3-C2-C1	-3.86	101.27	109.87
8	B	1360	MES	O1S-S-C8	3.47	111.09	106.92
5	A	1364	SRT	O41-C4-C3	3.46	122.62	113.27
6	A	1365	TAR	O41-C4-C3	3.11	121.67	113.27
3	A	1362	TRS	C3-C-C1	-2.96	101.64	110.81
6	A	1365	TAR	O11-C1-C2	2.94	121.22	113.27
5	A	1364	SRT	O1-C1-O11	-2.85	117.62	124.09
5	B	1362	SRT	O1-C1-C2	2.70	120.56	113.27
5	B	1362	SRT	C2-C3-C4	2.64	115.77	109.87
6	A	1365	TAR	O11-C1-O1	-2.63	118.12	124.09
8	B	1360	MES	O1-C6-C5	-2.61	106.06	111.80
4	B	1363	TLA	O11-C1-C2	2.58	120.24	113.27
5	A	1364	SRT	O41-C4-O4	-2.40	118.64	124.09
6	A	1365	TAR	O2-C2-C3	-2.34	105.58	110.23
4	B	1363	TLA	O11-C1-O1	-2.22	119.05	124.09
5	A	1364	SRT	O1-C1-C2	2.20	119.23	113.27
4	B	1363	TLA	O41-C4-C3	2.14	119.06	113.27
3	A	1362	TRS	C1-C-N	2.11	114.28	107.98
4	A	1363	TLA	O3-C3-C4	-2.05	106.36	110.66
4	A	1363	TLA	C2-C3-C4	-2.00	105.40	109.87

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1359	GOL	O1-C1-C2-C3
2	A	1360	GOL	O1-C1-C2-C3
2	B	1359	GOL	C1-C2-C3-O3
5	A	1364	SRT	C1-C2-C3-C4
5	A	1364	SRT	O2-C2-C3-O3
5	A	1364	SRT	O2-C2-C3-C4
8	B	1360	MES	N4-C7-C8-S
5	B	1362	SRT	C1-C2-C3-O3
5	A	1364	SRT	O3-C3-C4-O4
5	A	1364	SRT	O3-C3-C4-O41
5	B	1362	SRT	O1-C1-C2-C3
5	B	1362	SRT	O11-C1-C2-C3
5	A	1364	SRT	C1-C2-C3-O3
5	B	1362	SRT	O1-C1-C2-O2
5	B	1362	SRT	O11-C1-C2-O2
6	A	1365	TAR	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
6	A	1365	TAR	O3-C3-C4-O41
2	A	1359	GOL	O1-C1-C2-O2
2	A	1360	GOL	O1-C1-C2-O2
2	B	1359	GOL	O2-C2-C3-O3
5	B	1362	SRT	O2-C2-C3-O3
8	B	1360	MES	C8-C7-N4-C5
8	B	1361	MES	C8-C7-N4-C3
8	B	1361	MES	C8-C7-N4-C5
5	B	1362	SRT	C1-C2-C3-C4
3	A	1362	TRS	N-C-C2-O2
8	B	1360	MES	C8-C7-N4-C3
3	A	1362	TRS	C3-C-C2-O2
3	A	1362	TRS	C1-C-C3-O3
3	A	1362	TRS	C1-C-C2-O2
2	A	1360	GOL	C1-C2-C3-O3
6	A	1365	TAR	O1-C1-C2-C3
6	A	1365	TAR	O11-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1361	MES	1	0
2	A	1361	GOL	3	0
5	A	1364	SRT	2	0
2	B	1359	GOL	2	0
5	B	1362	SRT	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	358/358 (100%)	0.01	15 (4%)	36	39	12, 23, 42, 65	29 (8%)
1	B	358/358 (100%)	0.01	16 (4%)	33	36	12, 24, 48, 82	20 (5%)
All	All	716/716 (100%)	0.01	31 (4%)	35	38	12, 24, 44, 82	49 (6%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ARG	10.0
1	B	248	GLY	8.1
1	B	249	THR	6.4
1	A	40[A]	LEU	5.5
1	A	181[A]	ASN	5.2
1	A	177[A]	SER	5.2
1	B	115	LEU	5.1
1	A	337	ASN	4.7
1	A	170[A]	MET	4.2
1	A	132[A]	SER	4.0
1	A	310[A]	SER	3.9
1	A	309[A]	ASP	3.7
1	B	114	ASN	3.3
1	B	358	PHE	3.3
1	B	337	ASN	3.2
1	A	140[A]	LEU	3.2
1	A	1[A]	MET	3.1
1	A	248	GLY	3.0
1	B	229	TRP	2.8
1	A	30[A]	ASN	2.8
1	B	281	PHE	2.8
1	B	277	ALA	2.7
1	B	278	GLU	2.6
1	B	247	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	338	ARG	2.4
1	A	59[A]	GLU	2.2
1	B	250	LYS	2.2
1	A	118[A]	SER	2.2
1	B	189	THR	2.1
1	B	279	ASN	2.1
1	B	338	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	GOL	A	1361	6/6	0.28	0.37	75,76,77,77	0
6	TAR	A	1365	10/10	0.58	0.26	69,72,76,76	0
8	MES	B	1361	12/12	0.67	0.28	95,96,96,96	0
3	TRS	A	1362	8/8	0.73	0.20	41,50,50,53	0
5	SRT	A	1364	10/10	0.78	0.27	66,68,71,71	0
2	GOL	A	1360	6/6	0.79	0.15	51,55,55,56	0
5	SRT	B	1362	10/10	0.80	0.20	29,40,43,43	0
4	TLA	B	1363	10/10	0.81	0.18	56,58,59,59	0
7	BCT	A	1366	4/4	0.82	0.13	58,59,60,60	0
2	GOL	A	1359	6/6	0.83	0.13	40,41,44,48	0
7	BCT	B	1364	4/4	0.86	0.11	35,36,37,37	0
2	GOL	B	1359	6/6	0.87	0.16	57,57,58,59	0
4	TLA	A	1363	10/10	0.90	0.15	19,27,33,36	0
8	MES	B	1360	12/12	0.96	0.13	33,39,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.