



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:32 AM UTC

PDB ID : 6MAG / pdb_00006mag
Title : native BbvCI B2 dimer in space group C222
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2018-08-27
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

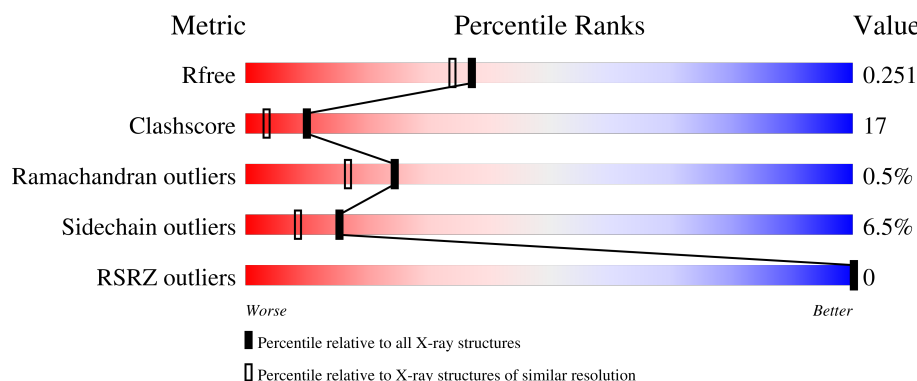
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	
1	B	285	
1	C	285	

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	GOL	B	307	-	-	X	-

2 Entry composition [i](#)

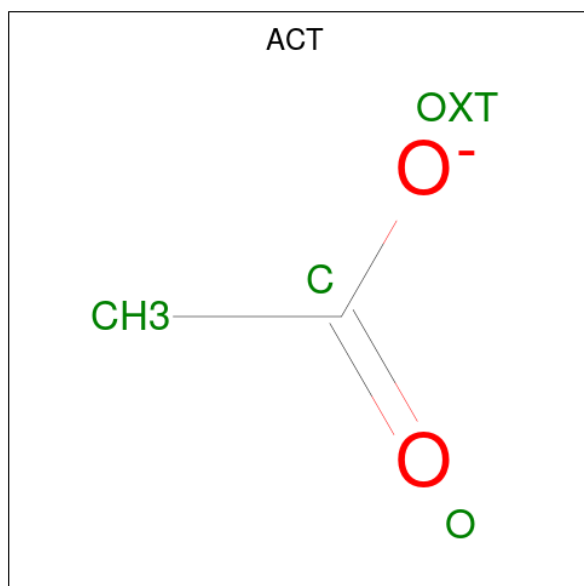
There are 5 unique types of molecules in this entry. The entry contains 7609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BbvCI endonuclease subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	12	0
			2377	1509	410	449	9			
1	B	282	Total	C	N	O	S	0	8	0
			2339	1485	403	442	9			
1	C	282	Total	C	N	O	S	0	11	0
			2364	1498	407	450	9			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



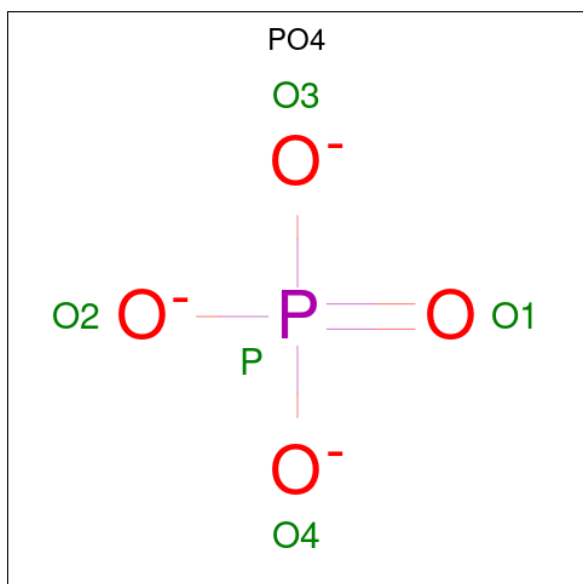
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

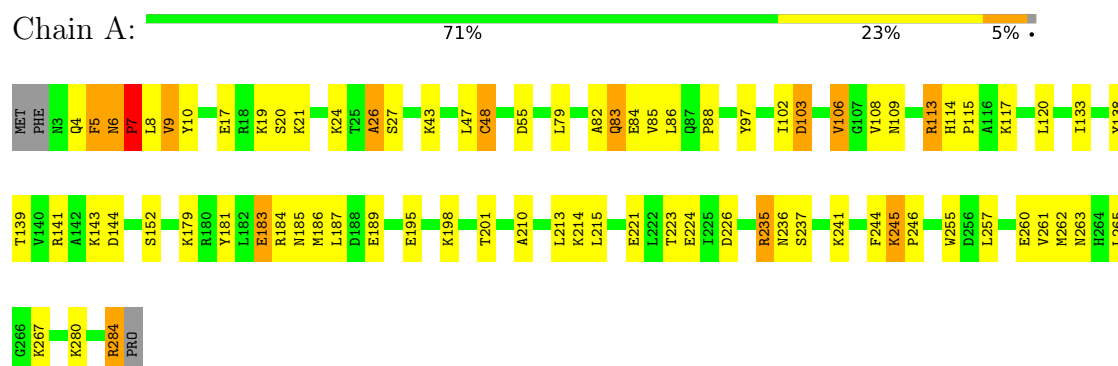
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total 141	O 141	0	0
5	B	128	Total 128	O 128	0	0
5	C	109	Total 109	O 109	0	0

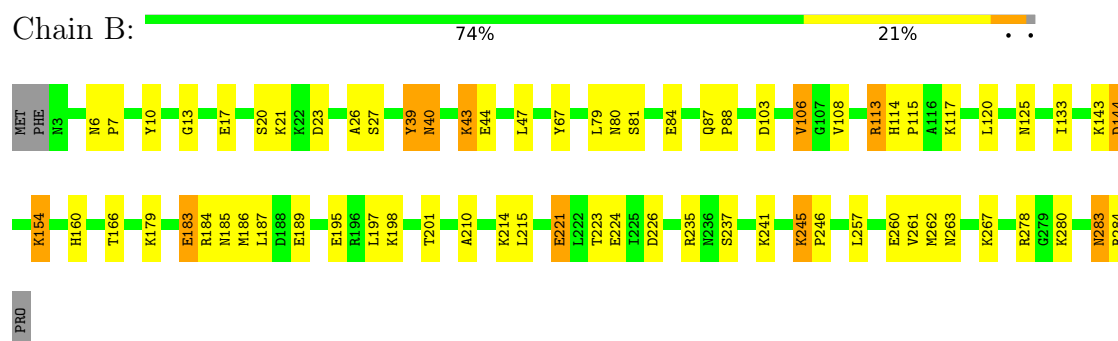
3 Residue-property plots

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.

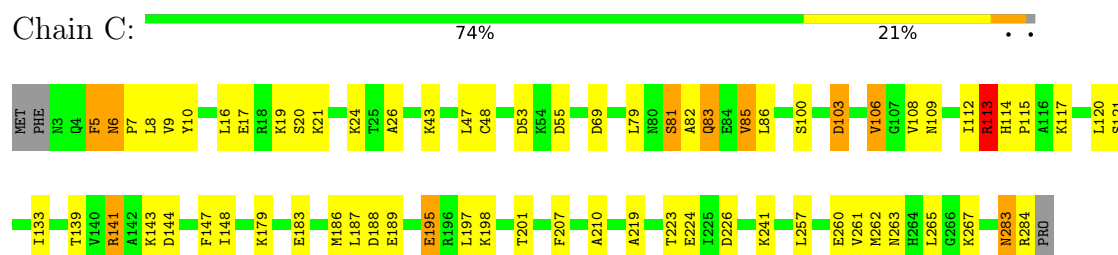
• Molecule 1: BbvCI endonuclease subunit 2



• Molecule 1: BbvCI endonuclease subunit 2



• Molecule 1: BbvCI endonuclease subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.71Å 165.71Å 141.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.65 – 2.07 28.65 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.0 (28.65-2.07) 96.1 (28.65-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.196 , 0.243 0.210 , 0.251	Depositor DCC
R_{free} test set	3219 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.470 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.458 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7609	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, PO4

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	5/2433 (0.2%)	1.21	12/3291 (0.4%)
1	B	0.76	2/2392 (0.1%)	1.18	8/3238 (0.2%)
1	C	0.72	1/2417 (0.0%)	1.15	7/3271 (0.2%)
All	All	0.76	8/7242 (0.1%)	1.18	27/9800 (0.3%)

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	A	0	2
1	B	0	5
All	All	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	ASP	C-N	-11.68	1.18	1.33
1	B	40	ASN	C-N	-10.67	1.19	1.33
1	A	245	LYS	C-N	-10.10	1.22	1.33
1	A	235[A]	ARG	CA-C	9.70	1.65	1.52
1	A	235[B]	ARG	CA-C	9.70	1.65	1.52
1	B	39	TYR	C-N	8.50	1.45	1.34
1	A	26	ALA	C-N	6.10	1.42	1.33
1	A	244	PHE	C-N	-5.09	1.26	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	ASP	O-C-N	12.18	135.24	122.09
1	B	40	ASN	O-C-N	-11.31	108.99	122.22
1	A	235[A]	ARG	N-CA-C	9.98	124.94	109.96
1	A	235[B]	ARG	N-CA-C	9.98	124.94	109.96
1	C	55	ASP	CA-CB-CG	-6.87	105.73	112.60
1	B	40	ASN	CA-C-N	6.86	130.04	120.29
1	B	40	ASN	C-N-CA	6.86	130.04	120.29
1	A	245	LYS	O-C-N	-6.62	115.03	121.38
1	A	55	ASP	CA-CB-CG	-6.20	106.41	112.60
1	B	23	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	188	ASP	CA-C-N	-5.61	112.77	120.28
1	C	188	ASP	C-N-CA	-5.61	112.77	120.28
1	A	245	LYS	CA-C-N	5.56	125.74	119.90
1	A	245	LYS	C-N-CA	5.56	125.74	119.90
1	A	9	VAL	CA-C-N	-5.46	114.75	122.34
1	A	9	VAL	C-N-CA	-5.46	114.75	122.34
1	B	221	GLU	CB-CA-C	5.45	118.64	109.48
1	C	103	ASP	CB-CA-C	5.45	119.43	110.88
1	B	201	THR	CA-CB-OG1	5.35	117.63	109.60
1	A	201	THR	CA-CB-OG1	5.29	117.54	109.60
1	A	26	ALA	O-C-N	5.26	127.49	122.07
1	B	154	LYS	CB-CA-C	5.24	118.79	109.72
1	B	144	ASP	CB-CA-C	-5.13	102.92	110.06
1	A	103	ASP	CB-CA-C	5.11	118.90	110.88
1	A	7	PRO	N-CA-CB	-5.09	97.91	103.25
1	C	195	GLU	CB-CG-CD	5.08	121.24	112.60
1	C	201	THR	CA-CB-OG1	5.06	117.19	109.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Mainchain
1	B	113	ARG	Mainchain
1	B	43	LYS	Mainchain
1	B	44[B]	GLU	Mainchain

5.2 Too-close contacts

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	2377	0	2332	96	0
1	B	2339	0	2290	60	0
1	C	2364	0	2306	102	0
2	A	4	0	3	0	0
3	A	36	0	48	3	0
3	B	54	0	72	8	0
3	C	42	0	56	4	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	141	0	0	10	0
5	B	128	0	0	2	0
5	C	109	0	0	3	0
All	All	7609	0	7107	249	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 17.

All (249) 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:10:TYR:CZ	1:A:43:LYS:HE3	1.73	1.21
1:B:237:SER:HB3	3:B:307:GOL:H2	1.24	1.19
1:C:6:ASN:H	1:C:7:PRO:HD3	1.02	1.11
1:A:235[B]:ARG:HD3	1:A:236:ASN:N	1.64	1.10
1:C:82:ALA:HA	1:C:85:VAL:CG1	1.81	1.09
1:C:6:ASN:H	1:C:7:PRO:CD	1.65	1.09
1:A:245:LYS:HD2	1:A:246:PRO:HD2	1.35	1.08
1:C:7:PRO:HG3	1:C:113:ARG:CZ	1.84	1.07
1:C:7:PRO:HG3	1:C:113:ARG:NH1	1.71	1.06
1:C:5:PHE:HE1	1:C:8:LEU:HG	1.17	1.04
1:B:154:LYS:HG3	1:B:166:THR:CG2	1.86	1.03
1:C:82:ALA:HA	1:C:85:VAL:HG13	1.39	1.02
1:C:17:GLU:OE2	1:C:21:LYS:NZ	1.92	1.01
1:A:83:GLN:NE2	5:A:401:HOH:O	1.93	1.01
1:A:235[B]:ARG:HD2	1:A:237:SER:H	1.24	1.01
1:A:235[B]:ARG:HH11	1:A:237:SER:N	1.61	0.99
1:C:5:PHE:CE1	1:C:8:LEU:HG	1.98	0.98
1:B:278:ARG:HD2	1:B:283:ASN:OD1	1.63	0.98
1:B:214:LYS:HG3	3:B:307:GOL:H12	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ASN:H	1:C:283:ASN:HD22	1.03	0.95
1:A:235[B]:ARG:HD3	1:A:236:ASN:H	1.32	0.93
1:A:183:GLU:O	1:A:215:LEU:HD21	1.68	0.93
1:C:114:HIS:HB2	1:C:115:PRO:HD2	1.51	0.90
1:C:6:ASN:N	1:C:7:PRO:HD3	1.86	0.89
1:C:53:ASP:HB2	3:C:304:GOL:H2	1.55	0.88
1:A:5:PHE:HB2	1:A:7:PRO:HD3	1.53	0.88
1:A:235[B]:ARG:NH1	1:A:237:SER:N	2.22	0.87
1:C:6:ASN:N	1:C:7:PRO:CD	2.33	0.87
1:C:82:ALA:CA	1:C:85:VAL:HG13	2.06	0.86
1:C:8:LEU:HD13	1:C:10:TYR:CZ	2.11	0.85
1:C:5:PHE:CZ	1:C:8:LEU:HD12	2.10	0.85
1:B:215:LEU:O	1:B:235:ARG:NH2	2.09	0.85
1:B:195:GLU:HG2	1:B:224:GLU:OE2	1.77	0.85
1:A:10:TYR:OH	1:A:43:LYS:HE3	1.78	0.84
1:C:5:PHE:HZ	1:C:8:LEU:HD12	1.43	0.84
1:A:235[B]:ARG:CD	1:A:237:SER:H	1.91	0.84
1:A:263[B]:ASN:HD21	1:A:267:LYS:NZ	1.76	0.84
1:C:82:ALA:HA	1:C:85:VAL:HG11	1.57	0.83
1:C:207:PHE:CE2	1:C:257:LEU:CD1	2.61	0.83
1:C:263[B]:ASN:HD21	1:C:267:LYS:HZ3	1.23	0.82
1:A:235[B]:ARG:CD	1:A:236:ASN:N	2.42	0.81
1:C:5:PHE:HE1	1:C:8:LEU:CG	1.90	0.81
1:A:255:TRP:HE1	3:A:307:GOL:H2	1.46	0.80
1:C:263[B]:ASN:HD21	1:C:267:LYS:NZ	1.77	0.80
1:A:48:CYS:SG	5:A:453:HOH:O	2.40	0.78
1:B:154:LYS:HG3	1:B:166:THR:HG21	1.65	0.78
1:B:154:LYS:CG	1:B:166:THR:CG2	2.61	0.77
1:C:69:ASP:OD2	3:C:306:GOL:H31	1.84	0.77
1:A:263[B]:ASN:HD21	1:A:267:LYS:HZ3	1.28	0.77
1:C:195:GLU:HG2	1:C:224[A]:GLU:OE1	1.86	0.76
1:A:213:LEU:HD11	1:A:215:LEU:HD12	1.68	0.75
1:A:181:TYR:HE1	5:A:503:HOH:O	1.69	0.75
1:B:154:LYS:HG3	1:B:166:THR:HG23	1.67	0.75
1:B:40:ASN:OD1	3:B:309:GOL:O2	2.04	0.75
1:C:114:HIS:HB2	1:C:115:PRO:CD	2.17	0.75
1:A:10:TYR:CZ	1:A:43:LYS:CE	2.65	0.74
1:C:5:PHE:HB2	1:C:100:SER:O	1.87	0.74
1:A:10:TYR:CE2	1:A:43:LYS:HE3	2.23	0.74
1:A:17:GLU:HG3	1:C:21:LYS:CE	2.18	0.74
1:A:7:PRO:HG3	1:A:113:ARG:NH2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:PHE:CD2	1:C:257:LEU:HD11	2.23	0.73
1:A:195:GLU:HG2	1:A:224[A]:GLU:OE1	1.88	0.73
1:B:6:ASN:HB3	1:B:7:PRO:HD2	1.70	0.73
1:C:283:ASN:H	1:C:283:ASN:ND2	1.82	0.73
1:A:235[B]:ARG:HH11	1:A:236:ASN:C	1.97	0.72
1:B:237:SER:CB	3:B:307:GOL:H2	2.13	0.72
1:C:207:PHE:CD2	1:C:257:LEU:CD1	2.72	0.72
1:B:245:LYS:HD2	1:B:246:PRO:HD2	1.71	0.71
1:C:8:LEU:HD13	1:C:10:TYR:CE1	2.24	0.71
1:A:7:PRO:HG3	1:A:113:ARG:CZ	2.20	0.71
1:A:84:GLU:HG3	1:A:88:PRO:HG2	1.73	0.71
1:A:235[B]:ARG:HD2	1:A:237:SER:N	2.04	0.69
1:C:8:LEU:HD13	1:C:10:TYR:OH	1.92	0.69
1:A:221:GLU:HG2	1:A:223:THR:HG23	1.74	0.69
1:B:160:HIS:CD2	3:B:305:GOL:H2	2.28	0.69
1:C:5:PHE:CE1	1:C:8:LEU:CG	2.71	0.68
1:A:262[A]:MET:HA	1:A:262[A]:MET:HE2	1.75	0.68
1:A:284:ARG:HD3	1:A:284:ARG:N	2.07	0.68
1:A:6:ASN:N	1:A:7:PRO:HD3	2.08	0.68
1:C:82:ALA:C	1:C:85:VAL:HG13	2.20	0.67
1:B:154:LYS:CG	1:B:166:THR:HG21	2.24	0.67
1:A:17:GLU:HG3	1:C:21:LYS:HE2	1.76	0.67
1:C:121:SER:OG	1:C:141:ARG:HB2	1.95	0.67
1:A:235[B]:ARG:HH11	1:A:237:SER:H	1.44	0.66
1:B:262[A]:MET:HE2	1:B:262[A]:MET:HA	1.77	0.66
1:B:7:PRO:HB3	1:B:113:ARG:NH2	2.11	0.66
1:C:262[A]:MET:HE2	1:C:262[A]:MET:HA	1.77	0.65
1:A:235[B]:ARG:NH1	1:A:236:ASN:HB3	2.12	0.65
1:B:154:LYS:CG	1:B:166:THR:HG23	2.27	0.65
1:A:106:VAL:HG12	1:A:108:VAL:HG12	1.79	0.64
1:C:16:LEU:O	1:C:20:SER:CB	2.45	0.64
1:C:19:LYS:HD3	1:C:85:VAL:HG21	1.80	0.64
1:C:17:GLU:OE2	1:C:21:LYS:CE	2.45	0.63
1:B:214:LYS:HA	3:B:307:GOL:H32	1.80	0.63
1:B:6:ASN:HB3	1:B:7:PRO:CD	2.30	0.62
1:C:283:ASN:HD22	1:C:283:ASN:N	1.86	0.61
1:A:214:LYS:O	1:A:214:LYS:HG2	1.99	0.61
1:B:154:LYS:CD	1:B:166:THR:HG21	2.31	0.61
1:A:139:THR:HA	3:A:305:GOL:H12	1.83	0.60
1:A:85:VAL:HG12	1:A:86:LEU:HG	1.83	0.60
1:B:183:GLU:O	1:B:215:LEU:HD21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LYS:NZ	1:C:82:ALA:HB2	2.18	0.59
1:C:7:PRO:CG	1:C:113:ARG:NH1	2.59	0.58
1:C:106:VAL:HG23	1:C:108:VAL:HG12	1.85	0.58
1:B:214:LYS:HA	3:B:307:GOL:C3	2.35	0.57
1:C:85:VAL:HG22	1:C:86:LEU:HG	1.87	0.57
1:C:81:SER:O	1:C:81:SER:OG	2.22	0.56
1:C:113:ARG:O	1:C:147:PHE:CE1	2.58	0.56
1:C:5:PHE:CZ	1:C:8:LEU:CD1	2.85	0.56
1:A:214:LYS:HB2	1:A:236:ASN:HB3	1.88	0.56
1:C:261:VAL:HG12	1:C:262[A]:MET:CE	2.36	0.55
1:A:6:ASN:ND2	1:C:24:LYS:NZ	2.55	0.55
1:C:8:LEU:CD1	1:C:10:TYR:OH	2.55	0.55
1:C:207:PHE:CE2	1:C:257:LEU:HD12	2.41	0.55
1:C:19:LYS:HZ2	1:C:82:ALA:CB	2.19	0.55
1:A:24:LYS:HA	1:A:27:SER:HB3	1.90	0.54
1:A:261:VAL:HG12	1:A:262[A]:MET:CE	2.38	0.54
1:C:113:ARG:NH2	5:C:401:HOH:O	2.07	0.54
1:B:87:GLN:HB3	1:B:88:PRO:HD3	1.90	0.54
1:A:83:GLN:OE1	1:A:83:GLN:HA	2.05	0.54
1:B:261:VAL:HG12	1:B:262[A]:MET:CE	2.38	0.54
1:C:19:LYS:NZ	1:C:82:ALA:CB	2.71	0.53
1:C:207:PHE:HD2	1:C:257:LEU:HD11	1.72	0.53
1:B:283:ASN:O	1:B:284:ARG:O	2.27	0.53
1:A:5:PHE:CD2	5:A:439:HOH:O	2.54	0.53
1:C:183:GLU:HG2	1:C:186:MET:SD	2.49	0.53
1:B:106:VAL:HG12	1:B:108:VAL:HG12	1.89	0.52
1:A:114[A]:HIS:HD2	5:A:411:HOH:O	1.91	0.52
1:C:8:LEU:HD11	1:C:47:LEU:HD21	1.92	0.52
1:C:112:ILE:HG21	1:C:148:ILE:HG22	1.92	0.52
1:B:10:TYR:CE1	1:B:43:LYS:HE3	2.44	0.52
1:C:198:LYS:NZ	1:C:226:ASP:OD2	2.40	0.52
1:A:117:LYS:HG2	1:A:144:ASP:OD1	2.10	0.52
1:C:113:ARG:O	1:C:147:PHE:HE1	1.93	0.52
1:B:197:LEU:C	1:B:197:LEU:HD23	2.35	0.51
1:C:16:LEU:O	1:C:20:SER:HB2	2.10	0.51
1:A:183:GLU:O	1:A:215:LEU:CD2	2.52	0.51
1:B:117:LYS:HG2	1:B:144:ASP:OD1	2.11	0.51
1:A:5:PHE:HB3	5:A:439:HOH:O	2.10	0.51
1:B:262[A]:MET:HE2	1:B:262[A]:MET:CA	2.41	0.50
1:C:139:THR:HA	3:C:301:GOL:H31	1.93	0.50
1:C:262[A]:MET:HE2	1:C:262[A]:MET:CA	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PRO:CG	1:A:113:ARG:NH2	2.74	0.50
1:A:181:TYR:CE1	5:A:503:HOH:O	2.54	0.50
1:C:83:GLN:C	1:C:85:VAL:H	2.20	0.50
1:A:10:TYR:CE2	1:A:43:LYS:CE	2.91	0.50
1:C:5:PHE:CE1	1:C:8:LEU:CD1	2.95	0.50
1:C:197:LEU:HD23	1:C:197:LEU:C	2.37	0.50
1:A:24:LYS:O	1:A:27:SER:HB3	2.12	0.50
1:B:7:PRO:O	5:B:401:HOH:O	2.20	0.50
1:A:114[B]:HIS:HB2	1:A:115:PRO:HD2	1.93	0.49
1:B:13:GLY:HA3	1:B:39:TYR:OH	2.12	0.49
1:C:17:GLU:OE2	1:C:21:LYS:HE2	2.11	0.49
1:B:114[A]:HIS:HB2	1:B:115:PRO:HD2	1.93	0.49
1:A:6:ASN:N	1:A:7:PRO:CD	2.73	0.49
1:A:114[A]:HIS:HB2	1:A:115:PRO:HD2	1.93	0.49
1:B:114[B]:HIS:HB2	1:B:115:PRO:HD2	1.94	0.49
1:A:235[B]:ARG:HH11	1:A:236:ASN:CA	2.26	0.48
1:C:7:PRO:CG	1:C:113:ARG:CZ	2.75	0.48
1:A:235[B]:ARG:NH1	1:A:237:SER:H	2.02	0.48
1:A:262[A]:MET:HE2	1:A:262[A]:MET:CA	2.41	0.48
1:A:6:ASN:ND2	1:C:24:LYS:HE3	2.28	0.47
1:C:5:PHE:CD1	1:C:7:PRO:HD2	2.49	0.47
1:A:214:LYS:HB2	1:A:236:ASN:CB	2.44	0.47
1:B:43:LYS:O	1:B:47:LEU:HG	2.14	0.47
1:B:103:ASP:HB2	5:B:438:HOH:O	2.14	0.47
1:A:5:PHE:CG	5:A:439:HOH:O	2.67	0.47
1:B:183:GLU:C	1:B:215:LEU:HD21	2.38	0.47
1:A:10:TYR:OH	1:A:47:LEU:HD11	2.15	0.47
1:A:198:LYS:NZ	1:A:226:ASP:OD2	2.41	0.47
1:B:198:LYS:NZ	1:B:226:ASP:OD2	2.40	0.47
1:C:83:GLN:C	1:C:85:VAL:N	2.70	0.47
1:C:5:PHE:HD1	1:C:7:PRO:HD2	1.80	0.47
1:A:263[B]:ASN:HD21	1:A:267:LYS:HZ2	1.61	0.46
1:B:20:SER:O	1:B:27:SER:HB2	2.15	0.46
1:C:19:LYS:HZ1	1:C:82:ALA:HB2	1.80	0.46
1:C:207:PHE:HE2	1:C:257:LEU:HD12	1.81	0.46
1:C:261:VAL:HG12	1:C:262[A]:MET:HE2	1.96	0.46
1:C:103:ASP:OD2	1:C:109:ASN:ND2	2.47	0.46
1:A:179:LYS:HE3	1:A:186:MET:SD	2.56	0.46
1:A:138:TYR:O	3:A:305:GOL:H32	2.15	0.46
1:C:16:LEU:O	1:C:20:SER:HB3	2.14	0.45
1:C:198:LYS:HG3	1:C:224[A]:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:HB2	5:A:471:HOH:O	2.15	0.45
1:A:10:TYR:CE2	1:A:43:LYS:NZ	2.83	0.45
1:A:6:ASN:HD21	1:C:24:LYS:NZ	2.14	0.45
1:B:26:ALA:HA	1:B:79:LEU:HD21	1.97	0.45
1:A:235[B]:ARG:CZ	1:A:237:SER:HB3	2.47	0.45
1:B:13:GLY:HA3	1:B:39:TYR:CZ	2.52	0.45
1:B:261:VAL:HG12	1:B:262[A]:MET:HE2	1.98	0.45
1:B:278:ARG:HD2	1:B:283:ASN:CG	2.38	0.45
1:B:120:LEU:HD11	1:B:143:LYS:HB2	1.98	0.45
1:A:7:PRO:CB	1:A:113:ARG:NH2	2.80	0.44
1:A:223:THR:O	1:A:224[A]:GLU:HB2	2.16	0.44
1:A:6:ASN:ND2	1:C:24:LYS:HZ2	2.15	0.44
1:B:179:LYS:O	1:B:210:ALA:HA	2.18	0.44
1:C:179:LYS:O	1:C:210:ALA:HA	2.18	0.44
1:A:179:LYS:O	1:A:210:ALA:HA	2.19	0.43
1:B:198:LYS:HG3	1:B:224:GLU:HG2	1.98	0.43
1:C:8:LEU:HD23	1:C:8:LEU:HA	1.86	0.43
1:C:10:TYR:CE1	1:C:43:LYS:HE3	2.53	0.43
1:A:114[B]:HIS:HE1	5:A:440:HOH:O	2.01	0.43
1:A:198:LYS:HG3	1:A:224[A]:GLU:HG2	2.00	0.43
1:A:245:LYS:CD	1:A:246:PRO:HD2	2.26	0.43
1:B:257:LEU:HD23	1:B:257:LEU:C	2.42	0.43
1:A:257:LEU:C	1:A:257:LEU:HD23	2.43	0.43
1:A:4:GLN:HA	1:A:4:GLN:OE1	2.19	0.43
1:A:20:SER:O	1:A:27:SER:HB2	2.18	0.43
1:B:223[B]:THR:O	1:B:224:GLU:HB2	2.19	0.43
1:C:5:PHE:CD1	1:C:100:SER:HB2	2.53	0.43
1:B:125:ASN:ND2	1:C:219:ALA:HB3	2.34	0.43
1:C:69:ASP:CG	3:C:306:GOL:H31	2.42	0.43
1:C:117:LYS:HG2	1:C:144:ASP:OD1	2.19	0.43
1:C:263[B]:ASN:ND2	1:C:267:LYS:NZ	2.57	0.43
1:C:223:THR:O	1:C:224[A]:GLU:HB2	2.18	0.42
1:A:26:ALA:HA	1:A:79:LEU:HD21	2.01	0.42
1:B:263[B]:ASN:HD21	1:B:267:LYS:NZ	2.17	0.42
1:A:19:LYS:NZ	1:A:82:ALA:HB2	2.33	0.42
1:A:103:ASP:OD2	1:A:109:ASN:ND2	2.49	0.42
1:A:261:VAL:HG12	1:A:262[A]:MET:HE2	2.00	0.42
1:B:223[A]:THR:O	1:B:224:GLU:HB2	2.20	0.42
1:C:120:LEU:HD11	1:C:143:LYS:HB2	2.00	0.42
1:A:6:ASN:ND2	1:C:24:LYS:CE	2.83	0.42
1:A:17:GLU:HG3	1:C:21:LYS:HE3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:HD2	5:C:427:HOH:O	2.19	0.42
1:B:7:PRO:HB3	1:B:113:ARG:HH21	1.81	0.42
1:C:16:LEU:O	1:C:20:SER:N	2.53	0.42
1:C:112:ILE:CG2	1:C:148:ILE:HG22	2.50	0.42
1:C:262[A]:MET:HE1	1:C:265:LEU:HD12	2.02	0.41
1:B:84:GLU:HG3	1:B:88:PRO:HG2	2.03	0.41
1:A:10:TYR:HE1	1:A:97:TYR:CE1	2.39	0.41
1:A:262[A]:MET:HE1	1:A:265:LEU:HD12	2.02	0.41
1:B:179:LYS:HE3	1:B:186:MET:HE3	2.02	0.41
1:A:120:LEU:HD11	1:A:143:LYS:HB2	2.03	0.41
1:B:39:TYR:HA	1:B:67:TYR:CE1	2.55	0.41
1:B:235:ARG:HB3	3:B:307:GOL:O3	2.19	0.41
1:C:103:ASP:HB2	5:C:401:HOH:O	2.20	0.41
1:A:183:GLU:HB2	1:A:184:ARG:H	1.77	0.41
1:A:185:ASN:O	1:A:189:GLU:HG3	2.21	0.41
1:B:13:GLY:O	1:B:17:GLU:HG2	2.21	0.41
1:C:19:LYS:HZ2	1:C:82:ALA:HB1	1.83	0.41
1:A:102:ILE:HD11	1:A:113:ARG:HD3	2.03	0.40
1:C:112:ILE:HG22	1:C:148:ILE:O	2.21	0.40
1:B:13:GLY:CA	1:B:39:TYR:CZ	3.05	0.40
1:C:26:ALA:HA	1:C:79:LEU:HD21	2.04	0.40
1:B:183:GLU:C	1:B:215:LEU:CD2	2.95	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	292/285 (102%)	280 (96%)	11 (4%)	1 (0%)	36	30
1	B	288/285 (101%)	272 (94%)	15 (5%)	1 (0%)	36	30
1	C	291/285 (102%)	275 (94%)	14 (5%)	2 (1%)	18	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	871/855 (102%)	827 (95%)	40 (5%)	4 (0%)	24 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	ASN
1	B	81	SER
1	A	7	PRO
1	C	113	ARG

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	259/250 (104%)	242 (93%)	17 (7%)	15 8
1	B	255/250 (102%)	240 (94%)	15 (6%)	18 10
1	C	258/250 (103%)	242 (94%)	16 (6%)	16 9
All	All	772/750 (103%)	724 (94%)	48 (6%)	15 9

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	6	ASN
1	A	7	PRO
1	A	8	LEU
1	A	9	VAL
1	A	21	LYS
1	A	48	CYS
1	A	83	GLN
1	A	106	VAL
1	A	133	ILE
1	A	141	ARG
1	A	183	GLU

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Mol	Chain	Res	Type
1	A	187	LEU
1	A	241	LYS
1	A	260	GLU
1	A	280	LYS
1	A	284	ARG
1	B	21	LYS
1	B	80	ASN
1	B	106	VAL
1	B	133	ILE
1	B	183	GLU
1	B	184	ARG
1	B	185	ASN
1	B	187	LEU
1	B	189	GLU
1	B	221	GLU
1	B	241	LYS
1	B	245	LYS
1	B	260	GLU
1	B	280	LYS
1	B	283	ASN
1	C	5	PHE
1	C	9	VAL
1	C	48	CYS
1	C	81	SER
1	C	83	GLN
1	C	85	VAL
1	C	106	VAL
1	C	113	ARG
1	C	133	ILE
1	C	141	ARG
1	C	187	LEU
1	C	189	GLU
1	C	241	LYS
1	C	260	GLU
1	C	283	ASN
1	C	284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	134	GLN

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Mol	Chain	Res	Type
1	B	4	GLN
1	B	125	ASN
1	C	125	ASN
1	C	134	GLN
1	C	283	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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	$\# Z > 2$
3	GOL	C	301	-	5,5,5	0.29	0	5,5,5	0.36	0
3	GOL	B	308	-	5,5,5	0.35	0	5,5,5	0.56	0
3	GOL	B	306	-	5,5,5	0.42	0	5,5,5	0.47	0
3	GOL	A	305	-	5,5,5	0.27	0	5,5,5	0.45	0
3	GOL	A	304	-	5,5,5	0.50	0	5,5,5	0.21	0
3	GOL	C	303	-	5,5,5	0.23	0	5,5,5	0.88	0
4	PO4	C	308	-	4,4,4	0.84	0	6,6,6	0.63	0
4	PO4	A	308	-	4,4,4	1.03	0	6,6,6	0.54	0
3	GOL	B	302	-	5,5,5	0.29	0	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	304	-	5,5,5	0.32	0	5,5,5	0.29	0
3	GOL	C	304	-	5,5,5	0.44	0	5,5,5	0.22	0
3	GOL	B	303	-	5,5,5	0.29	0	5,5,5	0.56	0
3	GOL	A	302	-	5,5,5	0.32	0	5,5,5	0.32	0
4	PO4	B	310	-	4,4,4	0.97	0	6,6,6	0.41	0
3	GOL	A	306	-	5,5,5	0.37	0	5,5,5	0.19	0
3	GOL	C	306	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	A	303	-	5,5,5	0.31	0	5,5,5	0.81	0
3	GOL	A	307	-	5,5,5	0.25	0	5,5,5	0.31	0
3	GOL	C	307	-	5,5,5	0.26	0	5,5,5	0.41	0
3	GOL	B	307	-	5,5,5	0.34	0	5,5,5	0.57	0
3	GOL	B	309	-	5,5,5	0.15	0	5,5,5	0.55	0
3	GOL	B	305	-	5,5,5	0.59	0	5,5,5	0.68	0
3	GOL	B	301	-	5,5,5	0.23	0	5,5,5	0.45	0
3	GOL	C	305	-	5,5,5	0.32	0	5,5,5	0.18	0
3	GOL	C	302	-	5,5,5	0.31	0	5,5,5	0.37	0
2	ACT	A	301	-	3,3,3	0.92	0	3,3,3	0.57	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	GOL	C	301	-	-	1/4/4/4	-
3	GOL	B	308	-	-	2/4/4/4	-
3	GOL	B	306	-	-	2/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	A	304	-	-	2/4/4/4	-
3	GOL	C	303	-	-	0/4/4/4	-
3	GOL	B	302	-	-	2/4/4/4	-
3	GOL	B	304	-	-	2/4/4/4	-
3	GOL	C	304	-	-	4/4/4/4	-
3	GOL	B	303	-	-	4/4/4/4	-
3	GOL	A	302	-	-	4/4/4/4	-
3	GOL	A	306	-	-	0/4/4/4	-
3	GOL	C	306	-	-	0/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-
3	GOL	A	307	-	-	0/4/4/4	-
3	GOL	C	307	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	307	-	-	3/4/4/4	-
3	GOL	B	309	-	-	4/4/4/4	-
3	GOL	B	305	-	-	0/4/4/4	-
3	GOL	B	301	-	-	0/4/4/4	-
3	GOL	C	305	-	-	2/4/4/4	-
3	GOL	C	302	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
3	A	303	GOL	O1-C1-C2-C3
3	A	304	GOL	O1-C1-C2-C3
3	B	302	GOL	O1-C1-C2-C3
3	B	303	GOL	O1-C1-C2-C3
3	B	304	GOL	O1-C1-C2-C3
3	B	307	GOL	C1-C2-C3-O3
3	B	309	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-C3
3	C	304	GOL	C1-C2-C3-O3
3	C	305	GOL	C1-C2-C3-O3
3	C	307	GOL	C1-C2-C3-O3
3	B	309	GOL	O1-C1-C2-O2
3	C	304	GOL	O1-C1-C2-O2
3	C	304	GOL	O2-C2-C3-O3
3	A	302	GOL	O1-C1-C2-C3
3	B	306	GOL	C1-C2-C3-O3
3	B	308	GOL	C1-C2-C3-O3
3	B	309	GOL	O1-C1-C2-C3
3	C	302	GOL	C1-C2-C3-O3
3	C	304	GOL	O1-C1-C2-C3
3	C	307	GOL	O1-C1-C2-C3
3	A	304	GOL	O1-C1-C2-O2
3	B	302	GOL	O1-C1-C2-O2
3	B	309	GOL	O2-C2-C3-O3
3	C	305	GOL	O2-C2-C3-O3
3	C	307	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	303	GOL	O1-C1-C2-O2
3	B	304	GOL	O1-C1-C2-O2
3	C	302	GOL	O2-C2-C3-O3
3	A	302	GOL	O1-C1-C2-O2
3	A	302	GOL	O2-C2-C3-O3
3	A	303	GOL	O1-C1-C2-O2
3	B	307	GOL	O1-C1-C2-O2
3	C	302	GOL	O1-C1-C2-O2
3	C	307	GOL	O2-C2-C3-O3
3	A	305	GOL	O2-C2-C3-O3
3	B	306	GOL	O2-C2-C3-O3
3	B	307	GOL	O2-C2-C3-O3
3	B	308	GOL	O2-C2-C3-O3
3	B	303	GOL	C1-C2-C3-O3
3	B	303	GOL	O2-C2-C3-O3
3	A	305	GOL	C1-C2-C3-O3
3	C	301	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	GOL	1	0
3	A	305	GOL	2	0
3	C	304	GOL	1	0
3	C	306	GOL	2	0
3	A	307	GOL	1	0
3	B	307	GOL	6	0
3	B	309	GOL	1	0
3	B	305	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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Mol	Chain	Number of breaks
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Mol	Chain	Number of breaks
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	40:ASN	C	41:CYS	N	1.19
1	C	188:ASP	C	189:GLU	N	1.18

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	282/285 (98%)	-1.17	0 100 100	12, 36, 81, 132	12 (4%)
1	B	282/285 (98%)	-1.20	0 100 100	14, 36, 80, 133	8 (2%)
1	C	282/285 (98%)	-1.17	0 100 100	14, 37, 79, 139	11 (3%)
All	All	846/855 (98%)	-1.18	0 100 100	12, 36, 81, 139	31 (3%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	A	301	4/4	0.97	0.09	73,73,74,75	0
3	GOL	B	303	6/6	0.97	0.06	65,71,75,77	0
3	GOL	B	304	6/6	0.97	0.07	73,80,84,85	0
3	GOL	B	305	6/6	0.97	0.06	49,53,58,58	0
3	GOL	C	307	6/6	0.97	0.07	74,84,86,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	301	6/6	0.98	0.05	45,55,56,64	0
3	GOL	B	302	6/6	0.98	0.07	35,48,51,54	0
3	GOL	A	303	6/6	0.98	0.06	38,46,47,50	0
3	GOL	A	304	6/6	0.98	0.05	63,69,73,73	0
3	GOL	A	306	6/6	0.98	0.04	65,65,66,67	0
3	GOL	B	307	6/6	0.98	0.06	62,63,66,74	0
3	GOL	C	302	6/6	0.98	0.06	71,71,75,76	0
3	GOL	C	304	6/6	0.98	0.05	46,59,63,65	0
3	GOL	C	306	6/6	0.98	0.07	67,71,74,75	0
3	GOL	A	307	6/6	0.98	0.05	72,76,77,85	0
4	PO4	C	308	5/5	0.98	0.04	71,75,80,85	0
3	GOL	C	301	6/6	0.99	0.03	47,56,58,62	0
3	GOL	A	302	6/6	0.99	0.05	56,69,71,71	0
3	GOL	C	303	6/6	0.99	0.08	40,46,47,52	0
3	GOL	B	306	6/6	0.99	0.07	35,46,52,62	0
3	GOL	C	305	6/6	0.99	0.04	73,75,79,79	0
3	GOL	A	305	6/6	0.99	0.09	41,49,51,52	0
3	GOL	B	308	6/6	0.99	0.05	54,69,71,73	0
4	PO4	A	308	5/5	0.99	0.04	68,70,77,79	0
4	PO4	B	310	5/5	0.99	0.03	73,78,80,86	0
3	GOL	B	309	6/6	0.99	0.10	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.