



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:59 AM UTC

PDB ID : 7MS2 / pdb_00007ms2
Title : Three-dimensional structure of a GH3 Beta-glucosidase from *Clostridium thermocellum* in complex with glycerol
Authors : Almeida, L.R.; Muniz, J.R.C.
Deposited on : 2021-05-10
Resolution : 2.04 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

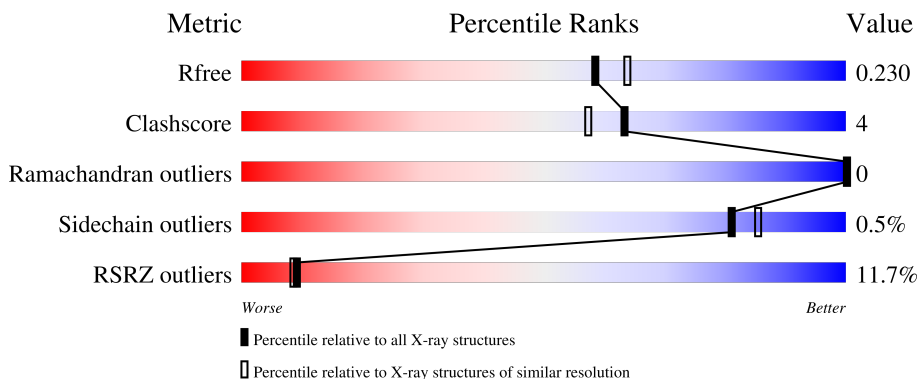
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	755	
1	B	755	

2 Entry composition i

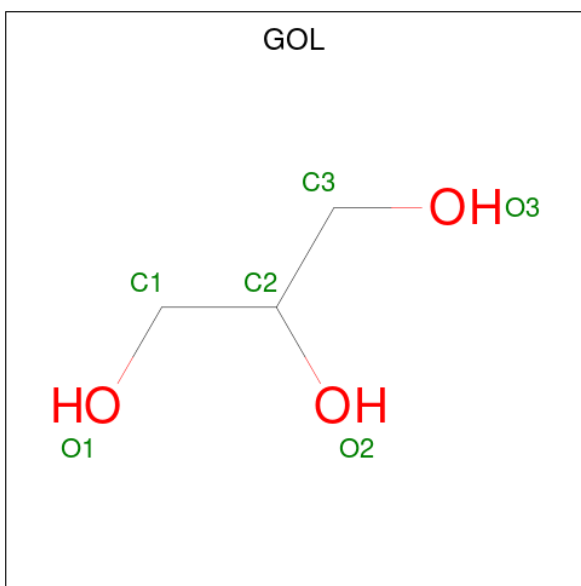
There are 5 unique types of molecules in this entry. The entry contains 11772 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thermostable beta-glucosidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	750	Total 5673	C 3578	N 959	O 1110	P 1	S 25	1	0	0
1	B	745	Total 5654	C 3560	N 964	O 1104	P 1	S 25	0	0	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



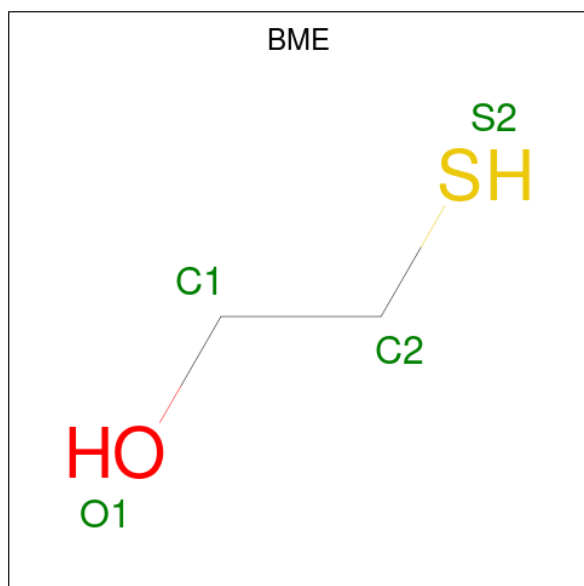
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

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

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

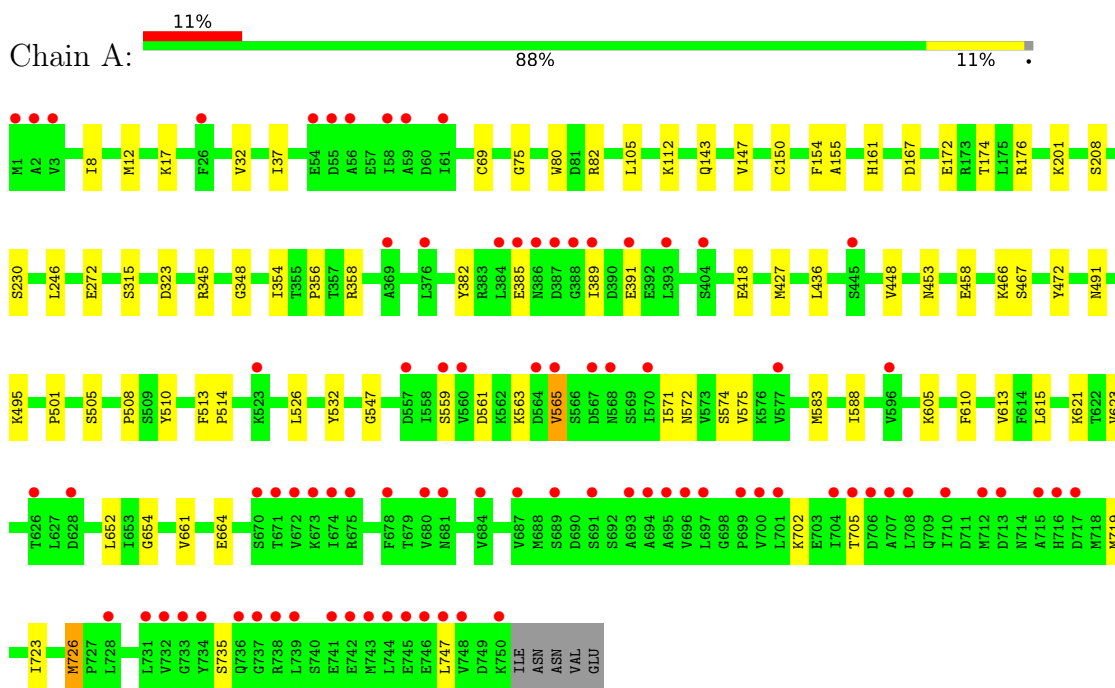
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	1
			204	204		
5	B	200	Total	O	0	1
			201	201		

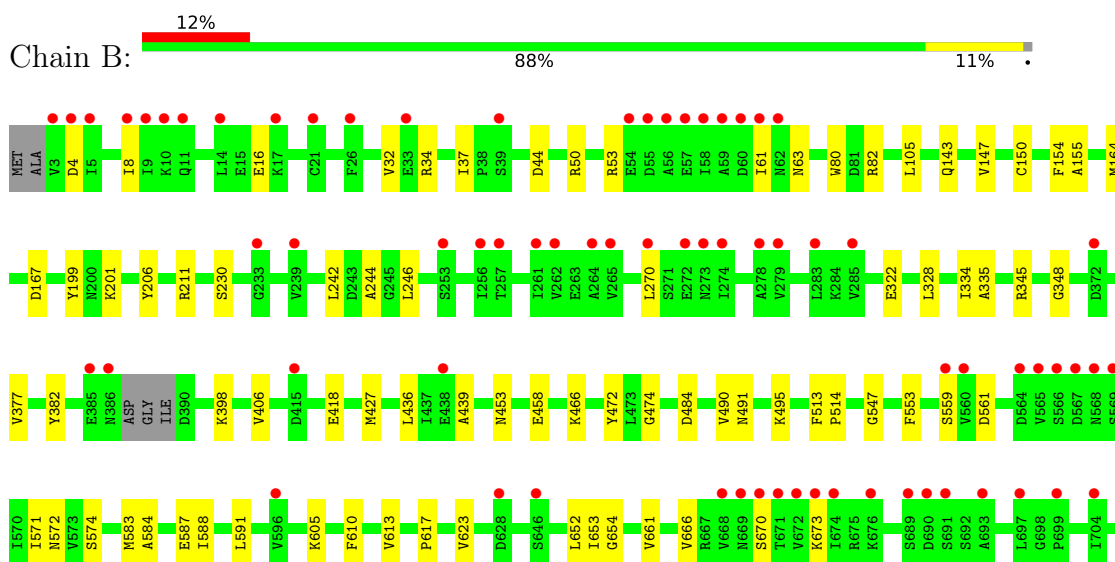
3 Residue-property plots [i](#)

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: Thermostable beta-glucosidase B



- Molecule 1: Thermostable beta-glucosidase B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.84Å 148.06Å 198.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.44 – 2.04 60.44 – 2.04	Depositor EDS
% Data completeness (in resolution range)	57.3 (60.44-2.04) 51.4 (60.44-2.04)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.03Å)	Xtrriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.202 , 0.230 0.202 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtrriage
Anisotropy	0.920	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11772	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, GOL, CL, BME

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	0.10	0/5766	0.29	0/7819
1	B	0.10	0/5746	0.29	0/7788
All	All	0.10	0/11512	0.29	0/15607

There are no bond length outliers.

There are no bond angle outliers.

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	5673	0	5437	45	0
1	B	5654	0	5416	44	0
2	A	18	0	24	1	0
2	B	12	0	16	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	204	0	0	1	0
5	B	201	0	0	1	0
All	All	11772	0	10905	89	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 4.

All (89) 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:559:SER:HB3	1:A:574:SER:HB2	1.70	0.73
1:A:654:GLY:HA2	1:A:661:VAL:HG22	1.76	0.67
1:A:561:ASP:HB2	1:A:572:ASN:HB2	1.78	0.66
1:A:17:LYS:NZ	1:A:272:GLU:OE2	2.30	0.65
1:B:491:ASN:HB2	1:B:583:MET:HE2	1.79	0.65
1:A:723:ILE:HA	1:A:726:MET:HE2	1.79	0.64
1:A:565:VAL:HG21	1:A:571:ILE:HG12	1.79	0.64
1:B:726:MET:HG3	1:B:730:SER:HB2	1.80	0.62
1:A:323:ASP:OD2	1:A:466:LYS:NZ	2.33	0.60
1:B:654:GLY:HA2	1:B:661:VAL:HG22	1.83	0.59
1:A:82:ARG:NH2	1:A:610:PHE:O	2.36	0.59
1:B:82:ARG:NH2	1:B:610:PHE:O	2.36	0.59
1:A:491:ASN:HB2	1:A:583:MET:HE2	1.87	0.57
1:A:161:HIS:HA	2:A:803:GOL:H12	1.88	0.56
1:B:32:VAL:HB	1:B:37:ILE:HB	1.89	0.55
1:B:242:LEU:HD23	1:B:270:LEU:HD21	1.90	0.53
1:B:605:LYS:HD3	1:B:652:LEU:HD12	1.90	0.53
1:A:427:MET:HE1	1:A:501:PRO:HG2	1.89	0.53
1:B:453:ASN:O	1:B:472:TYR:HA	2.08	0.53
1:B:427:MET:HE2	1:B:458:GLU:HG3	1.91	0.53
1:B:398:LYS:HD3	1:B:439:ALA:HB1	1.90	0.53
1:A:32:VAL:HB	1:A:37:ILE:HB	1.91	0.53
1:A:605:LYS:HD3	1:A:652:LEU:HD12	1.92	0.52
1:B:167:ASP:HA	1:B:201:LYS:HB2	1.92	0.52
1:A:702:LYS:HA	1:A:705:THR:HG22	1.91	0.51
1:A:382:TYR:HD2	1:A:436:LEU:HD22	1.76	0.51
1:A:448:VAL:HG22	1:A:467:SER:HB2	1.94	0.50
1:B:495:LYS:HG2	1:B:547:GLY:HA3	1.94	0.50
1:B:591:LEU:HD12	1:B:653:ILE:HD11	1.93	0.50
1:A:427:MET:HE2	1:A:458:GLU:HG3	1.92	0.50
1:A:453:ASN:O	1:A:472:TYR:HA	2.11	0.50
1:B:559:SER:HB3	1:B:574:SER:HB2	1.94	0.50
1:A:613:VAL:HG11	1:A:623:VAL:HG22	1.93	0.49
1:B:44:ASP:OD2	1:B:50:ARG:NH2	2.44	0.49
1:B:328:LEU:HD13	1:B:334:ILE:HD13	1.94	0.49
1:A:563:LYS:NZ	1:A:664:GLU:OE2	2.45	0.49
1:B:571:ILE:HD13	1:B:666:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:VAL:HG11	1:B:623:VAL:HG22	1.94	0.49
1:B:561:ASP:HB2	1:B:572:ASN:HB2	1.93	0.49
1:A:495:LYS:HG2	1:A:547:GLY:HA3	1.95	0.49
1:A:230:SER:HB3	1:A:246:LEU:HD21	1.94	0.48
1:B:143:GLN:HA	1:B:147:VAL:O	2.14	0.48
1:A:167:ASP:HA	1:A:201:LYS:HB2	1.96	0.47
1:B:53:ARG:HD3	1:B:63:ASN:OD1	2.14	0.47
1:A:208:SER:HB2	1:A:246:LEU:HD22	1.96	0.47
1:B:105:LEU:HA	1:B:150:CYS:HB3	1.95	0.47
1:A:345:ARG:HH21	1:A:348:GLY:HA2	1.79	0.47
1:A:719:MET:O	1:A:723:ILE:HG12	2.15	0.47
1:B:382:TYR:HD2	1:B:436:LEU:HD22	1.80	0.46
1:B:335:ALA:HA	1:B:377:VAL:HG13	1.98	0.46
1:A:356:PRO:HB2	1:A:358:ARG:O	2.16	0.45
1:A:105:LEU:HA	1:A:150:CYS:HB3	1.98	0.45
1:B:736:GLN:CD	1:B:737:GLY:H	2.24	0.45
1:A:143:GLN:HA	1:A:147:VAL:O	2.16	0.45
1:A:154:PHE:CD1	1:A:155:ALA:HB2	2.52	0.45
1:B:230:SER:HB3	1:B:246:LEU:HD21	1.98	0.45
1:B:345:ARG:HH21	1:B:348:GLY:HA2	1.82	0.44
1:A:172:GLU:O	1:A:176:ARG:HG2	2.18	0.44
1:B:211:ARG:HG3	1:B:244:ALA:HA	1.99	0.44
1:B:670:SER:O	1:B:673:LYS:NZ	2.50	0.44
1:B:154:PHE:CD1	1:B:155:ALA:HB2	2.53	0.44
1:B:553:PHE:CD2	1:B:587:GLU:HB2	2.53	0.44
1:B:16:GLU:CD	1:B:34:ARG:HH21	2.24	0.43
1:A:69:CYS:HA	1:A:354:ILE:HD13	2.01	0.43
1:B:201:LYS:HE2	1:B:206:TYR:CE2	2.53	0.43
1:A:508:PRO:HB3	1:A:532:TYR:CG	2.53	0.43
1:B:513:PHE:HA	1:B:514:PRO:HA	1.89	0.43
1:A:112:LYS:NZ	5:A:925[A]:HOH:O	2.51	0.42
1:A:615:LEU:HD23	1:A:621:LYS:HE2	2.01	0.42
1:B:4:ASP:O	1:B:8:ILE:HG13	2.19	0.42
1:A:495:LYS:HD2	1:A:588:ILE:HB	2.00	0.42
1:A:174:THR:HA	1:A:526:LEU:HD23	2.01	0.42
1:B:80:TRP:HB2	1:B:588:ILE:HD13	2.01	0.42
1:A:8:ILE:O	1:A:12:MET:HG3	2.20	0.42
1:A:80:TRP:HB2	1:A:588:ILE:HD13	2.02	0.42
1:A:385:GLU:H	1:A:385:GLU:CD	2.28	0.41
1:B:484:ASP:HB3	1:B:490:VAL:HG23	2.02	0.41
1:A:505:SER:HA	1:A:510:TYR:CG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LEU:HD22	1:B:406:VAL:HG11	2.02	0.41
1:A:513:PHE:HA	1:A:514:PRO:HA	1.91	0.41
1:B:495:LYS:HD2	1:B:588:ILE:HB	2.01	0.41
1:A:345:ARG:HH22	1:A:418:GLU:HB2	1.86	0.41
1:B:322:GLU:HB3	1:B:466:LYS:HG3	2.02	0.41
1:A:389:ILE:HD11	1:A:391:GLU:OE2	2.20	0.41
1:A:75:GLY:O	1:A:315:SER:HB2	2.21	0.40
1:B:474:GLY:O	5:B:901:HOH:O	2.22	0.40
1:B:164:MET:HA	1:B:199:TYR:HB3	2.04	0.40
1:B:345:ARG:HH22	1:B:418:GLU:HB2	1.87	0.40
1:B:584:ALA:HB2	1:B:617:PRO:HD3	2.03	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	747/755 (99%)	735 (98%)	12 (2%)	0	100	100
1	B	740/755 (98%)	726 (98%)	14 (2%)	0	100	100
All	All	1487/1510 (98%)	1461 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	586/643 (91%)	582 (99%)	4 (1%)	76	80
1	B	584/643 (91%)	582 (100%)	2 (0%)	86	90
All	All	1170/1286 (91%)	1164 (100%)	6 (0%)	81	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	VAL
1	A	575	VAL
1	A	726	MET
1	A	747	LEU
1	B	61	ILE
1	B	736	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	62	ASN
1	A	446	ASN
1	B	145	GLN
1	B	157	ASN
1	B	375	ASN
1	B	616	ASN
1	B	669	ASN
1	B	716	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](#)

2 non-standard protein/DNA/RNA residues 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
1	SEP	A	735	1	8,9,10	1.62	1 (12%)	7,12,14	1.51	1 (14%)
1	SEP	B	735	1	8,9,10	1.62	1 (12%)	7,12,14	1.68	2 (28%)

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
1	SEP	A	735	1	-	2/6/8/10	-
1	SEP	B	735	1	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	735	SEP	P-O1P	3.54	1.61	1.50
1	B	735	SEP	P-O1P	3.54	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	SEP	OG-CB-CA	3.67	111.72	108.14
1	A	735	SEP	OG-CB-CA	3.32	111.38	108.14
1	B	735	SEP	O3P-P-OG	2.05	112.01	106.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	735	SEP	CA-CB-OG-P
1	B	735	SEP	CA-CB-OG-P
1	A	735	SEP	N-CA-CB-OG
1	B	735	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
3	BME	B	803	-	3,3,3	0.29	0	2,2,2	0.40	0
2	GOL	A	801	-	5,5,5	0.97	0	5,5,5	1.05	0
2	GOL	A	803	-	5,5,5	0.97	0	5,5,5	0.96	0
2	GOL	B	801	-	5,5,5	0.93	0	5,5,5	1.10	0
2	GOL	B	802	-	5,5,5	0.94	0	5,5,5	1.04	0
3	BME	A	804	-	3,3,3	0.31	0	2,2,2	0.35	0
2	GOL	A	802	-	5,5,5	0.82	0	5,5,5	1.09	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	BME	B	803	-	-	1/1/1/1	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	A	803	-	-	4/4/4/4	-
2	GOL	B	801	-	-	1/4/4/4	-
2	GOL	B	802	-	-	2/4/4/4	-
3	BME	A	804	-	-	0/1/1/1	-
2	GOL	A	802	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	803	GOL	C1-C2-C3-O3
2	A	803	GOL	O2-C2-C3-O3
2	A	801	GOL	C1-C2-C3-O3
2	A	803	GOL	O1-C1-C2-C3
2	B	802	GOL	O1-C1-C2-C3
2	A	803	GOL	O1-C1-C2-O2
3	B	803	BME	O1-C1-C2-S2
2	B	802	GOL	O1-C1-C2-O2
2	A	801	GOL	O2-C2-C3-O3
2	B	801	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	749/755 (99%)	0.75	85 (11%) 10 9	17, 37, 89, 121	1 (0%)
1	B	744/755 (98%)	0.82	90 (12%) 8 8	17, 41, 79, 127	1 (0%)
All	All	1493/1510 (98%)	0.79	175 (11%) 9 8	17, 39, 84, 127	2 (0%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	THR	7.2
1	B	734	TYR	6.7
1	A	732	VAL	6.5
1	B	3	VAL	5.9
1	B	61	ILE	5.9
1	A	1	MET	5.8
1	B	733	GLY	5.3
1	A	58	ILE	5.2
1	A	670	SER	5.1
1	A	696	VAL	5.0
1	A	387	ASP	5.0
1	B	750	LYS	5.0
1	B	59	ALA	4.8
1	B	737	GLY	4.8
1	A	738	ARG	4.7
1	B	732	VAL	4.7
1	A	389	ILE	4.6
1	A	734	TYR	4.6
1	A	55	ASP	4.3
1	A	697	LEU	4.2
1	A	3	VAL	4.2
1	B	54	GLU	4.1
1	B	739	LEU	4.1
1	B	62	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	739	LEU	4.1
1	A	747	LEU	4.0
1	B	741	GLU	4.0
1	B	58	ILE	3.9
1	A	695	ALA	3.9
1	B	386	ASN	3.9
1	B	57	GLU	3.9
1	B	415	ASP	3.8
1	A	748	VAL	3.8
1	B	14	LEU	3.7
1	A	715	ALA	3.7
1	B	568	ASN	3.7
1	B	262	VAL	3.6
1	A	728	LEU	3.6
1	B	673	LYS	3.6
1	A	704	ILE	3.6
1	A	386	ASN	3.5
1	A	680	VAL	3.5
1	B	747	LEU	3.5
1	B	55	ASP	3.5
1	B	740	SER	3.5
1	B	674	ILE	3.4
1	B	744	LEU	3.4
1	B	372	ASP	3.4
1	A	672	VAL	3.4
1	B	670	SER	3.4
1	A	56	ALA	3.4
1	A	694	ALA	3.4
1	A	388	GLY	3.3
1	A	689	SER	3.3
1	A	705	THR	3.2
1	A	2	ALA	3.2
1	B	672	VAL	3.2
1	A	746	GLU	3.2
1	A	737	GLY	3.2
1	A	54	GLU	3.1
1	B	748	VAL	3.1
1	B	704	ILE	3.1
1	A	673	LYS	3.1
1	A	708	LEU	3.1
1	A	744	LEU	3.1
1	B	671	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	691	SER	3.0
1	B	689	SER	3.0
1	B	285	VAL	3.0
1	A	742	GLU	3.0
1	B	278	ALA	2.9
1	B	646	SER	2.9
1	A	628	ASP	2.9
1	A	699	PRO	2.9
1	A	691	SER	2.9
1	A	568	ASN	2.9
1	A	713	ASP	2.9
1	B	261	ILE	2.9
1	B	26	PHE	2.9
1	A	716	HIS	2.9
1	B	239	VAL	2.8
1	B	669	ASN	2.8
1	B	693	ALA	2.8
1	A	678	PHE	2.8
1	B	560	VAL	2.8
1	A	61	ILE	2.8
1	B	5	ILE	2.8
1	A	733	GLY	2.8
1	B	56	ALA	2.8
1	A	701	LEU	2.8
1	A	404	SER	2.7
1	B	564	ASP	2.7
1	A	731	LEU	2.7
1	B	728	LEU	2.7
1	A	684	VAL	2.7
1	B	743	MET	2.7
1	B	742	GLU	2.7
1	B	4	ASP	2.6
1	B	438	GLU	2.6
1	A	707	ALA	2.6
1	A	736	GLN	2.6
1	A	710	ILE	2.5
1	A	557	ASP	2.5
1	B	668	VAL	2.5
1	A	741	GLU	2.5
1	A	750	LYS	2.5
1	A	626	THR	2.5
1	B	233	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	736	GLN	2.4
1	B	746	GLU	2.4
1	A	674	ILE	2.4
1	B	9	ILE	2.4
1	B	60	ASP	2.4
1	B	256	ILE	2.4
1	B	265	VAL	2.4
1	B	596	VAL	2.4
1	A	675	ARG	2.4
1	A	393	LEU	2.3
1	B	270	LEU	2.3
1	B	628	ASP	2.3
1	A	570	ILE	2.3
1	A	59	ALA	2.3
1	A	26	PHE	2.3
1	A	687	VAL	2.3
1	A	745	GLU	2.3
1	A	596	VAL	2.3
1	B	10	LYS	2.3
1	B	283	LEU	2.3
1	B	253	SER	2.2
1	B	559	SER	2.2
1	B	566	SER	2.2
1	B	569	SER	2.2
1	A	564	ASP	2.2
1	A	567	ASP	2.2
1	B	690	ASP	2.2
1	A	369	ALA	2.2
1	A	712	MET	2.2
1	A	376	LEU	2.2
1	B	697	LEU	2.2
1	B	274	ILE	2.2
1	A	565	VAL	2.2
1	A	559	SER	2.2
1	B	738	ARG	2.2
1	B	8	ILE	2.2
1	B	257	THR	2.2
1	B	273	ASN	2.2
1	B	567	ASP	2.2
1	A	560	VAL	2.1
1	A	693	ALA	2.1
1	B	264	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	523	LYS	2.1
1	A	743	MET	2.1
1	A	385	GLU	2.1
1	A	391	GLU	2.1
1	B	21	CYS	2.1
1	B	39	SER	2.1
1	B	699	PRO	2.1
1	B	731	LEU	2.1
1	B	33	GLU	2.1
1	B	385	GLU	2.1
1	A	681	ASN	2.1
1	A	717	ASP	2.1
1	A	577	VAL	2.1
1	B	279	VAL	2.1
1	B	565	VAL	2.1
1	A	384	LEU	2.0
1	A	706	ASP	2.0
1	B	11	GLN	2.0
1	B	676	LYS	2.0
1	A	700	VAL	2.0
1	B	272	GLU	2.0
1	B	745	GLU	2.0
1	A	445	SER	2.0
1	B	707	ALA	2.0
1	B	17	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	735	10/11	0.60	0.16	106,122,128,137	0
1	SEP	B	735	10/11	0.63	0.19	91,95,112,115	0

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	GOL	B	802	6/6	0.66	0.16	77,79,80,80	0
2	GOL	A	802	6/6	0.81	0.16	27,33,34,36	0
2	GOL	B	801	6/6	0.85	0.18	34,42,47,50	0
2	GOL	A	801	6/6	0.85	0.13	27,32,36,41	0
3	BME	A	804	4/4	0.90	0.12	25,34,36,46	0
3	BME	B	803	4/4	0.91	0.11	26,35,37,50	0
2	GOL	A	803	6/6	0.93	0.10	20,38,39,42	0
4	CL	A	805	1/1	0.97	0.12	24,24,24,24	0
4	CL	B	804	1/1	0.98	0.06	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.