



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:05 AM UTC

PDB ID : 5Z9S / pdb_00005z9s
Title : Functional and Structural Characterization of a beta-Glucosidase Involved in Saponin Metabolism from Intestinal Bacteria
Authors : Yan, S.; Wei, P.C.; Li, J.R.
Deposited on : 2018-02-05
Resolution : 2.30 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

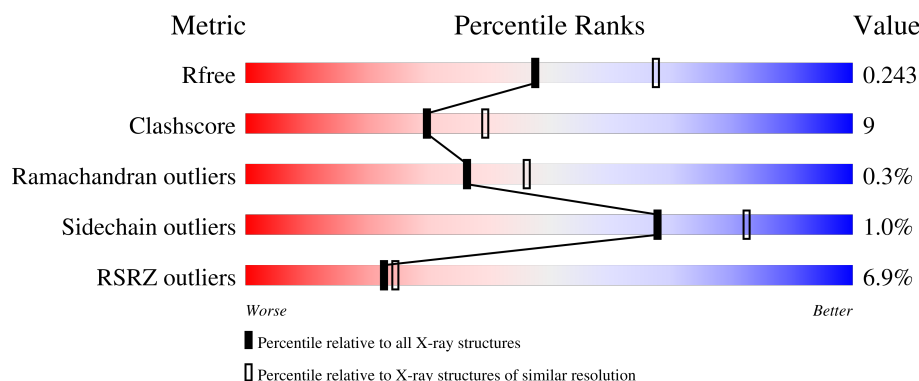
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	796	6% 81% 14% ..
1	B	796	8% 81% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12098 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 Glycosyl hydrolase family 3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			5804	3656	999	1129	20			
1	B	763	Total	C	N	O	S	0	0	0
			5794	3652	997	1125	20			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A0A133LV16
A	2	GLY	-	expression tag	UNP A0A133LV16
A	789	LEU	-	expression tag	UNP A0A133LV16
A	790	GLU	-	expression tag	UNP A0A133LV16
A	791	HIS	-	expression tag	UNP A0A133LV16
A	792	HIS	-	expression tag	UNP A0A133LV16
A	793	HIS	-	expression tag	UNP A0A133LV16
A	794	HIS	-	expression tag	UNP A0A133LV16
A	795	HIS	-	expression tag	UNP A0A133LV16
A	796	HIS	-	expression tag	UNP A0A133LV16
B	1	MET	-	expression tag	UNP A0A133LV16
B	2	GLY	-	expression tag	UNP A0A133LV16
B	789	LEU	-	expression tag	UNP A0A133LV16
B	790	GLU	-	expression tag	UNP A0A133LV16
B	791	HIS	-	expression tag	UNP A0A133LV16
B	792	HIS	-	expression tag	UNP A0A133LV16
B	793	HIS	-	expression tag	UNP A0A133LV16
B	794	HIS	-	expression tag	UNP A0A133LV16
B	795	HIS	-	expression tag	UNP A0A133LV16
B	796	HIS	-	expression tag	UNP A0A133LV16

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

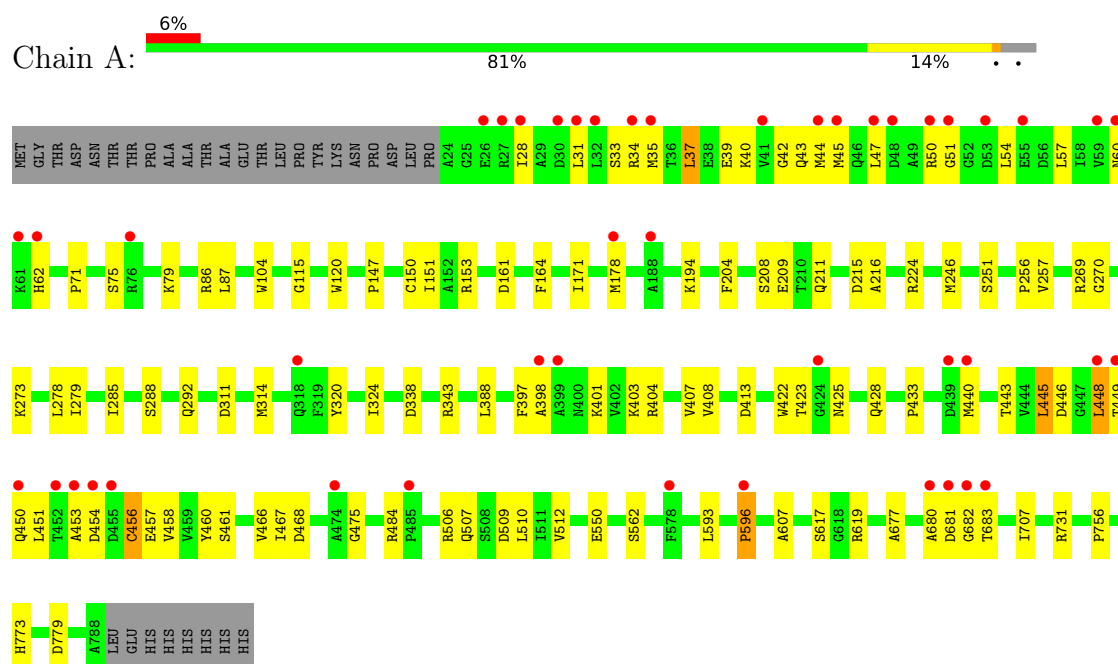
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total	O	0	0
			236	236		
3	B	240	Total	O	0	0
			240	240		

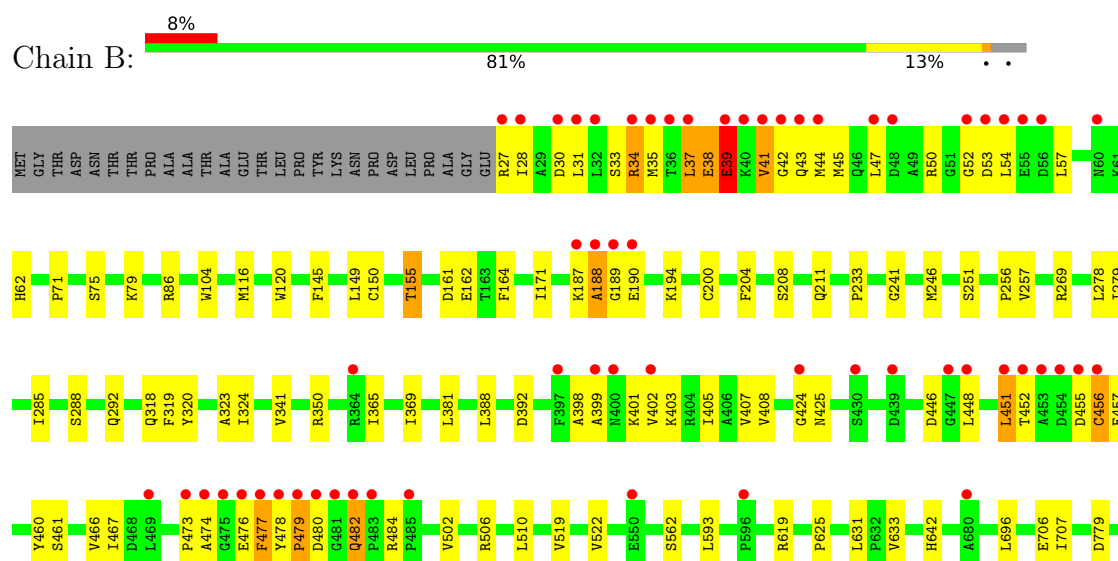
3 Residue-property plots [i](#)

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: Glycosyl hydrolase family 3 protein



- Molecule 1: Glycosyl hydrolase family 3 protein



1789

GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.95Å 134.42Å 90.28Å 90.00° 98.82° 90.00°	Depositor
Resolution (Å)	47.85 – 2.30 47.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.85-2.30) 93.3 (47.85-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.224 , 0.242 0.224 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12098	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: BGC

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	0.15	0/5923	0.40	1/8062 (0.0%)
1	B	0.23	0/5913	0.45	4/8049 (0.0%)
All	All	0.20	0/11836	0.43	5/16111 (0.0%)

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	1
1	B	0	4
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	PHE	N-CA-C	-7.95	97.12	108.96
1	B	39	GLU	N-CA-C	5.60	119.37	107.67
1	B	482	GLN	CA-C-N	-5.53	114.28	120.14
1	B	482	GLN	C-N-CA	-5.53	114.28	120.14
1	A	680	ALA	N-CA-C	5.41	116.94	110.44

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	440	MET	Peptide

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Mol	Chain	Res	Type	Group
1	B	34	ARG	Peptide
1	B	38	GLU	Peptide
1	B	41	VAL	Peptide
1	B	455	ASP	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	5804	0	5718	86	0
1	B	5794	0	5715	112	0
2	A	12	0	11	3	0
2	B	12	0	11	0	0
3	A	236	0	0	11	0
3	B	240	0	0	17	0
All	All	12098	0	11455	197	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 9.

All (197) 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:B:479:PRO:HG3	1:B:484:ARG:HG2	1.20	1.12
1:B:477:PHE:HA	1:B:479:PRO:HD3	1.02	1.02
1:B:479:PRO:HG3	1:B:484:ARG:CG	1.88	1.02
1:B:477:PHE:HA	1:B:479:PRO:CD	1.90	1.01
1:B:478:TYR:CZ	1:B:480:ASP:HB3	1.96	1.00
1:B:477:PHE:CA	1:B:479:PRO:HD3	1.94	0.98
1:B:519:VAL:O	3:B:901:HOH:O	1.81	0.96
1:B:188:ALA:HA	1:B:190:GLU:HB3	1.48	0.96
1:B:478:TYR:C	1:B:480:ASP:HA	1.94	0.93
1:B:478:TYR:CE2	1:B:480:ASP:HB3	2.10	0.87
1:B:30:ASP:O	3:B:902:HOH:O	1.94	0.85
1:B:27:ARG:NH1	3:B:905:HOH:O	2.09	0.83
1:B:50:ARG:NH1	3:B:906:HOH:O	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:TYR:CE1	1:B:480:ASP:HB3	2.17	0.79
1:A:449:THR:H	1:A:458:VAL:HG21	1.48	0.79
1:B:479:PRO:CG	1:B:484:ARG:HG2	2.09	0.78
1:B:211:GLN:OE1	3:B:903:HOH:O	2.01	0.77
1:A:40:LYS:HZ3	1:A:324:ILE:HG23	1.52	0.75
1:B:779:ASP:OD2	3:B:904:HOH:O	2.08	0.72
1:A:468:ASP:OD1	3:A:901:HOH:O	2.09	0.70
1:B:405:ILE:HG12	1:B:510:LEU:HB3	1.74	0.70
1:B:408:VAL:HG12	1:B:461:SER:HB2	1.73	0.70
1:A:408:VAL:HG12	1:A:461:SER:HB2	1.73	0.69
1:B:478:TYR:HA	1:B:480:ASP:O	1.93	0.69
1:A:150:CYS:HB3	1:A:208:SER:HB3	1.76	0.68
1:B:27:ARG:HG2	1:B:28:ILE:H	1.58	0.68
1:A:211:GLN:NE2	3:A:910:HOH:O	2.27	0.68
1:B:34:ARG:O	3:B:907:HOH:O	2.12	0.67
1:A:215:ASP:O	3:A:902:HOH:O	2.13	0.67
1:A:194:LYS:NZ	3:A:913:HOH:O	2.28	0.66
1:B:479:PRO:HD2	1:B:482:GLN:O	1.95	0.66
1:B:41:VAL:HG12	1:B:44:MET:HG2	1.76	0.66
1:A:50:ARG:NE	1:A:51:GLY:O	2.24	0.65
1:A:120:TRP:HB2	1:A:707:ILE:HD13	1.79	0.64
1:B:120:TRP:HB2	1:B:707:ILE:HD13	1.78	0.64
1:B:162:GLU:OE1	3:B:908:HOH:O	2.15	0.64
1:B:39:GLU:HG2	1:B:86:ARG:HH21	1.60	0.64
1:A:507:GLN:NE2	3:A:903:HOH:O	2.19	0.63
1:B:150:CYS:HB3	1:B:208:SER:HB3	1.80	0.62
1:A:44:MET:HB3	1:A:47:LEU:HD13	1.82	0.62
1:B:34:ARG:O	3:B:909:HOH:O	2.15	0.62
1:B:41:VAL:HG11	1:B:44:MET:HE2	1.81	0.62
1:B:155:THR:HG21	1:B:625:PRO:HG3	1.82	0.62
1:B:43:GLN:HB3	1:B:341:VAL:HG21	1.83	0.61
1:A:153:ARG:NH2	3:A:909:HOH:O	2.26	0.60
1:A:147:PRO:HB3	1:A:178:MET:SD	2.41	0.60
1:A:39:GLU:HG3	1:A:42:GLY:H	1.67	0.58
1:A:161:ASP:HB3	1:A:562:SER:HB2	1.85	0.58
1:B:479:PRO:N	1:B:480:ASP:HA	2.14	0.58
1:B:62:HIS:O	3:B:910:HOH:O	2.17	0.58
1:B:190:GLU:HG2	1:B:350:ARG:HE	1.69	0.58
1:B:38:GLU:HA	1:B:39:GLU:HG3	1.85	0.57
1:B:44:MET:HB3	1:B:47:LEU:HD13	1.86	0.57
1:B:452:THR:OG1	1:B:456:CYS:SG	2.60	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ASN:N	3:B:915:HOH:O	2.37	0.56
1:A:34:ARG:NH1	1:A:37:LEU:HD11	2.21	0.56
1:A:398:ALA:H	1:A:401:LYS:NZ	2.04	0.56
1:A:388:LEU:HA	1:A:593:LEU:HD23	1.87	0.56
1:B:31:LEU:HA	1:B:34:ARG:HH12	1.71	0.55
1:B:476:GLU:N	1:B:476:GLU:OE2	2.39	0.55
1:B:388:LEU:HA	1:B:593:LEU:HD23	1.89	0.55
1:A:57:LEU:O	1:A:60:ASN:OD1	2.25	0.54
1:B:39:GLU:HG2	1:B:86:ARG:NH2	2.23	0.54
1:B:478:TYR:CD2	1:B:480:ASP:HB3	2.42	0.54
1:A:40:LYS:HA	1:A:43:GLN:HG3	1.90	0.54
1:A:153:ARG:HD3	1:A:209:GLU:OE2	2.08	0.53
1:B:403:LYS:HA	1:B:456:CYS:HB2	1.91	0.53
1:B:44:MET:HE1	1:B:323:ALA:HB3	1.91	0.53
1:B:466:VAL:HG12	1:B:467:ILE:HG23	1.91	0.53
1:B:251:SER:HA	1:B:256:PRO:HA	1.91	0.53
1:B:405:ILE:HD12	1:B:451:LEU:HD23	1.92	0.52
1:B:479:PRO:N	1:B:480:ASP:CA	2.73	0.52
1:A:681:ASP:HB2	1:A:683:THR:HA	1.91	0.52
1:B:448:LEU:HA	1:B:451:LEU:HD13	1.91	0.52
1:B:54:LEU:HG	1:B:57:LEU:HB3	1.91	0.52
1:A:270:GLY:O	1:A:273:LYS:HE2	2.11	0.51
1:B:424:GLY:C	3:B:915:HOH:O	2.53	0.51
1:B:479:PRO:HG3	1:B:484:ARG:HG3	1.86	0.51
1:A:398:ALA:HB3	1:A:401:LYS:HD3	1.93	0.51
1:A:457:GLU:OE1	3:A:904:HOH:O	2.20	0.50
1:B:164:PHE:HB2	1:B:171:ILE:HG12	1.92	0.50
1:A:448:LEU:HD11	1:A:512:VAL:HG21	1.93	0.50
1:B:31:LEU:C	1:B:34:ARG:HH22	2.20	0.50
1:B:446:ASP:C	1:B:448:LEU:H	2.20	0.50
1:B:39:GLU:H	1:B:42:GLY:H	1.60	0.50
1:A:62:HIS:O	3:A:905:HOH:O	2.20	0.49
1:A:311:ASP:OD1	1:A:343:ARG:NH1	2.43	0.49
1:A:413:ASP:OD1	1:A:443:THR:HG21	2.13	0.49
1:B:31:LEU:CA	1:B:34:ARG:HH22	2.25	0.49
1:B:35:MET:HA	3:B:907:HOH:O	2.11	0.49
1:B:288:SER:HA	1:B:292:GLN:HE21	1.78	0.49
1:A:506:ARG:NH2	1:A:550:GLU:OE2	2.36	0.49
1:B:44:MET:HE3	1:B:324:ILE:HG13	1.95	0.49
1:A:251:SER:HA	1:A:256:PRO:HA	1.94	0.48
1:A:86:ARG:HH21	1:A:87:LEU:HD11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:O	1:A:79:LYS:HG2	2.13	0.48
1:A:204:PHE:O	1:A:257:VAL:HG11	2.13	0.48
1:B:285:ILE:O	1:B:288:SER:OG	2.29	0.48
1:A:115:GLY:HA2	1:A:596:PRO:HG2	1.95	0.48
1:A:314:MET:HE1	2:A:801:BGC:H5	1.94	0.48
1:B:33:SER:O	1:B:35:MET:HB2	2.13	0.48
1:A:28:ILE:HG12	1:A:31:LEU:HD13	1.94	0.47
1:B:318:GLN:H	1:B:318:GLN:CD	2.21	0.47
1:A:443:THR:CG2	1:A:446:ASP:H	2.27	0.47
1:A:194:LYS:HA	1:A:194:LYS:HD3	1.69	0.47
1:A:285:ILE:O	1:A:288:SER:OG	2.29	0.47
1:B:399:ALA:O	1:B:452:THR:HG21	2.14	0.47
1:B:45:MET:HG2	3:B:910:HOH:O	2.14	0.47
1:B:204:PHE:O	1:B:257:VAL:HG11	2.15	0.47
1:B:392:ASP:OD2	3:B:911:HOH:O	2.20	0.47
1:B:452:THR:HB	1:B:456:CYS:HB3	1.96	0.47
1:A:45:MET:HE2	3:A:905:HOH:O	2.13	0.46
1:A:34:ARG:CZ	1:A:37:LEU:HD11	2.46	0.46
1:B:39:GLU:HG2	1:B:86:ARG:HE	1.81	0.46
1:B:631:LEU:HD23	1:B:633:VAL:HG13	1.98	0.46
1:B:478:TYR:CD1	1:B:480:ASP:HB3	2.50	0.46
1:A:398:ALA:H	1:A:401:LYS:HZ2	1.62	0.46
1:B:478:TYR:CD1	1:B:478:TYR:O	2.69	0.46
1:B:246:MET:HA	1:B:279:ILE:O	2.15	0.46
1:B:161:ASP:HB3	1:B:562:SER:HB2	1.99	0.45
1:A:449:THR:HG22	1:A:458:VAL:CG2	2.46	0.45
1:A:224:ARG:HD2	1:A:756:PRO:HA	1.98	0.45
1:A:314:MET:HE1	2:A:801:BGC:C5	2.46	0.45
1:A:449:THR:HG21	1:A:453:ALA:HB3	1.99	0.45
1:B:451:LEU:HA	1:B:452:THR:HA	1.47	0.45
1:A:314:MET:HE1	2:A:801:BGC:H6C2	1.99	0.45
1:B:30:ASP:OD1	1:B:30:ASP:N	2.43	0.45
1:B:145:PHE:HA	1:B:200:CYS:HB3	1.99	0.45
1:A:246:MET:HA	1:A:279:ILE:O	2.17	0.45
1:B:52:GLY:HA2	1:B:53:ASP:HA	1.68	0.45
1:A:292:GLN:HG3	3:A:1095:HOH:O	2.17	0.44
1:B:451:LEU:HB2	1:B:452:THR:OG1	2.18	0.44
1:B:34:ARG:NH1	3:B:902:HOH:O	2.49	0.44
1:B:45:MET:HE3	1:B:45:MET:HB3	1.78	0.44
1:B:75:SER:O	1:B:79:LYS:HG3	2.17	0.44
1:B:502:VAL:O	1:B:506:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PRO:HB3	1:A:104:TRP:CZ3	2.52	0.44
1:B:398:ALA:HB3	1:B:401:LYS:HD3	1.99	0.44
1:B:292:GLN:HE21	1:B:292:GLN:HB2	1.64	0.44
1:A:216:ALA:HB3	1:B:642:HIS:CD2	2.53	0.44
1:A:273:LYS:HA	1:A:273:LYS:HD3	1.87	0.44
1:B:619:ARG:HG2	1:B:707:ILE:HD12	1.98	0.44
1:B:187:LYS:O	1:B:241:GLY:HA3	2.18	0.44
1:A:403:LYS:HG3	1:A:509:ASP:OD2	2.18	0.43
1:B:41:VAL:HA	1:B:43:GLN:HG3	2.00	0.43
1:A:448:LEU:HB2	1:A:607:ALA:HB2	2.00	0.43
1:A:454:ASP:O	1:A:456:CYS:N	2.45	0.43
1:A:677:ALA:HB1	1:A:683:THR:O	2.18	0.43
1:A:425:ASN:ND2	1:A:433:PRO:O	2.38	0.43
1:B:43:GLN:C	1:B:45:MET:H	2.26	0.43
1:A:54:LEU:HG	1:A:57:LEU:HB3	2.00	0.43
1:A:443:THR:HG23	1:A:446:ASP:H	1.83	0.43
1:A:475:GLY:O	1:A:484:ARG:HD2	2.19	0.43
1:A:773:HIS:HB3	1:A:779:ASP:HB3	2.00	0.43
1:B:116:MET:HG2	1:B:381:LEU:HD21	2.01	0.43
1:B:27:ARG:HG2	1:B:28:ILE:N	2.31	0.42
1:A:677:ALA:CB	1:A:683:THR:HG22	2.49	0.42
1:B:35:MET:HG3	1:B:37:LEU:HD13	2.00	0.42
1:A:34:ARG:HH12	1:A:37:LEU:HD21	1.84	0.42
1:A:707:ILE:HG12	1:A:731:ARG:HG2	2.02	0.42
1:B:269:ARG:NH2	1:B:278:LEU:HG	2.34	0.42
1:A:448:LEU:HA	1:A:449:THR:HA	1.59	0.42
1:A:682:GLY:HA3	1:A:683:THR:HA	1.54	0.42
1:A:33:SER:C	1:A:35:MET:H	2.26	0.42
1:A:43:GLN:C	1:A:45:MET:H	2.27	0.42
1:B:696:LEU:HD21	1:B:706:GLU:HB3	2.02	0.42
1:A:164:PHE:HB2	1:A:171:ILE:HG12	2.01	0.42
1:A:449:THR:C	1:A:451:LEU:N	2.78	0.42
1:A:619:ARG:HG2	1:A:707:ILE:HD12	2.02	0.42
1:A:151:ILE:HG23	1:A:153:ARG:HG3	2.02	0.41
1:B:478:TYR:CE1	1:B:480:ASP:CB	2.96	0.41
1:B:71:PRO:HB3	1:B:104:TRP:CZ3	2.56	0.41
1:B:484:ARG:HH21	1:B:484:ARG:HD2	1.74	0.41
1:A:35:MET:HE1	1:A:338:ASP:HB3	2.00	0.41
1:A:407:VAL:O	1:A:460:TYR:HA	2.20	0.41
1:A:422:TRP:CZ3	1:A:428:GLN:HG2	2.56	0.41
1:B:448:LEU:HA	1:B:451:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:PRO:HA	1:B:474:ALA:HA	1.44	0.41
1:B:478:TYR:CZ	1:B:480:ASP:CB	2.85	0.41
1:A:397:PHE:CD2	1:A:510:LEU:HD13	2.56	0.41
1:B:365:ILE:HG23	1:B:369:ILE:HD12	2.03	0.41
1:B:407:VAL:O	1:B:460:TYR:HA	2.21	0.41
1:A:408:VAL:HA	1:A:461:SER:O	2.21	0.41
1:A:445:LEU:O	1:A:450:GLN:HG3	2.21	0.41
1:B:189:GLY:HA3	1:B:190:GLU:HA	1.79	0.41
1:A:404:ARG:HA	1:A:457:GLU:O	2.21	0.41
1:B:402:VAL:C	1:B:403:LYS:HD2	2.45	0.41
1:A:617:SER:HA	3:A:935:HOH:O	2.20	0.40
1:B:149:LEU:HD23	1:B:233:PRO:HB2	2.02	0.40
1:B:319:PHE:O	1:B:323:ALA:N	2.48	0.40
1:B:478:TYR:O	1:B:480:ASP:HA	2.20	0.40
1:A:269:ARG:NH2	1:A:278:LEU:HG	2.37	0.40
1:B:446:ASP:C	1:B:448:LEU:N	2.80	0.40
1:A:681:ASP:HB2	1:A:682:GLY:HA3	2.03	0.40
1:A:443:THR:HG23	1:A:445:LEU:N	2.36	0.40
1:A:466:VAL:HG12	1:A:467:ILE:HG23	2.01	0.40
1:B:194:LYS:NZ	3:B:949:HOH:O	2.54	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	763/796 (96%)	727 (95%)	34 (4%)	2 (0%)	36	46
1	B	761/796 (96%)	727 (96%)	31 (4%)	3 (0%)	30	38
All	All	1524/1592 (96%)	1454 (95%)	65 (4%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	TYR
1	B	188	ALA
1	B	320	TYR
1	B	479	PRO
1	A	596	PRO

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	610/637 (96%)	605 (99%)	5 (1%)	73	86
1	B	610/637 (96%)	603 (99%)	7 (1%)	65	81
All	All	1220/1274 (96%)	1208 (99%)	12 (1%)	68	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	423	THR
1	A	445	LEU
1	A	448	LEU
1	A	456	CYS
1	B	37	LEU
1	B	39	GLU
1	B	155	THR
1	B	451	LEU
1	B	456	CYS
1	B	457	GLU
1	B	522	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	211	GLN

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Mol	Chain	Res	Type
1	A	223	HIS
1	A	450	GLN
1	A	691	HIS
1	A	759	ASN
1	B	46	GLN
1	B	292	GLN
1	B	450	GLN
1	B	482	GLN
1	B	641	GLN
1	B	651	GLN
1	B	759	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](#)

2 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	$\# Z > 2$
2	BGC	A	801	-	12,12,12	1.19	1 (8%)	17,17,17	1.00	0
2	BGC	B	801	-	12,12,12	1.17	1 (8%)	17,17,17	0.87	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
2	BGC	A	801	-	-	2/2/22/22	0/1/1/1
2	BGC	B	801	-	-	2/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BGC	O5-C1	3.08	1.50	1.42
2	A	801	BGC	O5-C1	3.08	1.50	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BGC	O5-C5-C6-O6
2	A	801	BGC	C4-C5-C6-O6
2	B	801	BGC	C4-C5-C6-O6
2	B	801	BGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BGC	3	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	765/796 (96%)	0.44	45 (5%) 28 30	22, 31, 43, 54	0
1	B	763/796 (95%)	0.51	60 (7%) 18 20	22, 32, 45, 56	0
All	All	1528/1592 (95%)	0.47	105 (6%) 23 25	22, 32, 44, 56	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	THR	8.2
1	B	453	ALA	7.5
1	B	479	PRO	7.3
1	B	452	THR	6.8
1	B	31	LEU	6.5
1	B	480	ASP	6.5
1	A	448	LEU	6.1
1	A	53	ASP	6.0
1	B	36	THR	5.3
1	A	51	GLY	5.2
1	B	478	TYR	5.1
1	B	451	LEU	5.1
1	B	424	GLY	4.9
1	B	40	LYS	4.9
1	A	440	MET	4.8
1	B	189	GLY	4.4
1	A	30	ASP	4.4
1	A	35	MET	4.3
1	B	30	ASP	4.3
1	B	454	ASP	4.3
1	B	474	ALA	4.1
1	A	424	GLY	4.0
1	A	439	ASP	3.9
1	A	60	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	37	LEU	3.9
1	B	41	VAL	3.8
1	A	452	THR	3.7
1	A	188	ALA	3.7
1	B	34	ARG	3.6
1	A	450	GLN	3.6
1	A	31	LEU	3.6
1	B	789	LEU	3.5
1	B	60	ASN	3.5
1	A	682	GLY	3.5
1	B	52	GLY	3.5
1	B	455	ASP	3.5
1	A	44	MET	3.4
1	B	35	MET	3.4
1	B	44	MET	3.4
1	B	473	PRO	3.3
1	B	188	ALA	3.3
1	A	178	MET	3.3
1	A	62	HIS	3.2
1	B	53	ASP	3.2
1	B	448	LEU	3.2
1	B	477	PHE	3.2
1	B	482	GLN	3.0
1	A	474	ALA	3.0
1	A	455	ASP	3.0
1	B	32	LEU	3.0
1	B	397	PHE	3.0
1	A	48	ASP	3.0
1	A	34	ARG	2.9
1	B	447	GLY	2.9
1	B	42	GLY	2.9
1	B	187	LYS	2.8
1	A	41	VAL	2.8
1	A	61	LYS	2.8
1	B	481	GLY	2.8
1	B	190	GLU	2.8
1	A	680	ALA	2.8
1	A	681	ASP	2.7
1	B	680	ALA	2.7
1	B	439	ASP	2.7
1	A	45	MET	2.7
1	A	55	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	28	ILE	2.7
1	B	43	GLN	2.6
1	A	398	ALA	2.6
1	B	39	GLU	2.6
1	A	578	PHE	2.6
1	B	27	ARG	2.6
1	B	55	GLU	2.6
1	B	483	PRO	2.6
1	B	56	ASP	2.5
1	A	683	THR	2.5
1	B	402	VAL	2.5
1	B	476	GLU	2.5
1	B	28	ILE	2.5
1	B	469	LEU	2.5
1	A	27	ARG	2.5
1	A	453	ALA	2.5
1	B	475	GLY	2.5
1	A	318	GLN	2.4
1	B	596	PRO	2.4
1	B	550	GLU	2.4
1	B	399	ALA	2.4
1	A	485	PRO	2.3
1	A	596	PRO	2.3
1	A	32	LEU	2.3
1	B	54	LEU	2.3
1	A	399	ALA	2.2
1	B	400	ASN	2.2
1	B	456	CYS	2.2
1	A	50	ARG	2.2
1	B	47	LEU	2.2
1	A	76	ARG	2.1
1	B	48	ASP	2.1
1	A	59	VAL	2.1
1	B	485	PRO	2.1
1	B	364	ARG	2.1
1	B	430	SER	2.1
1	A	454	ASP	2.1
1	A	47	LEU	2.0
1	A	26	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 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($\text{\AA}^2$)	Q<0.9
2	BGC	A	801	12/12	0.88	0.11	25,26,27,27	0
2	BGC	B	801	12/12	0.92	0.08	26,27,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.