



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 6R5O / pdb_00006r5o
Title : The crystal structure the Glycoside Hydrolase BglX inactive mutant D286N from *P. aeruginosa* in complex with two glucose molecules
Authors : Batuecas, M.T.; Hermoso, J.A.
Deposited on : 2019-03-25
Resolution : 2.40 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

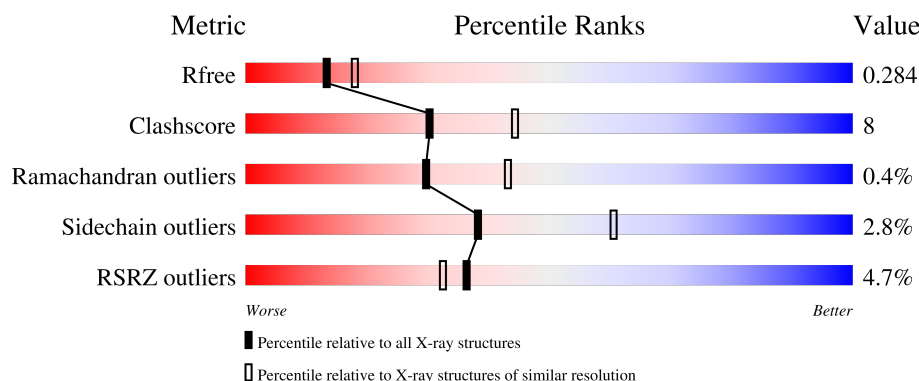
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	733	
1	B	733	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11721 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.

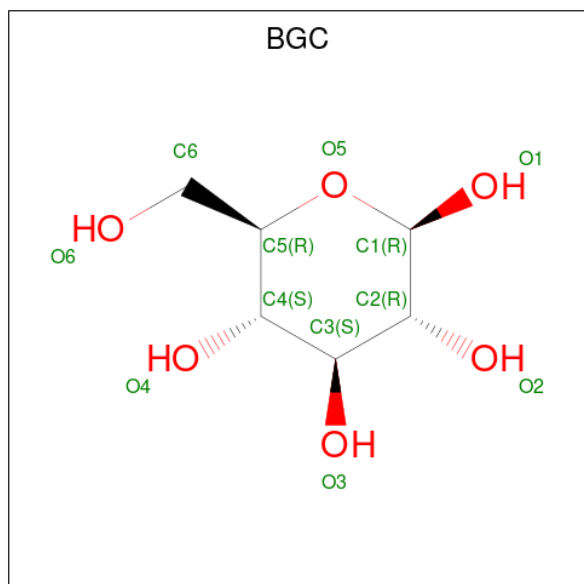
- Molecule 1 is a protein called Periplasmic beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	730	Total	C	N	O	S	0	5	0
			5631	3538	1011	1061	21			
1	A	730	Total	C	N	O	S	0	4	0
			5626	3534	1011	1061	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	286	ASN	ASP	engineered mutation	UNP Q9I311
A	286	ASN	ASP	engineered mutation	UNP Q9I311

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



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

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

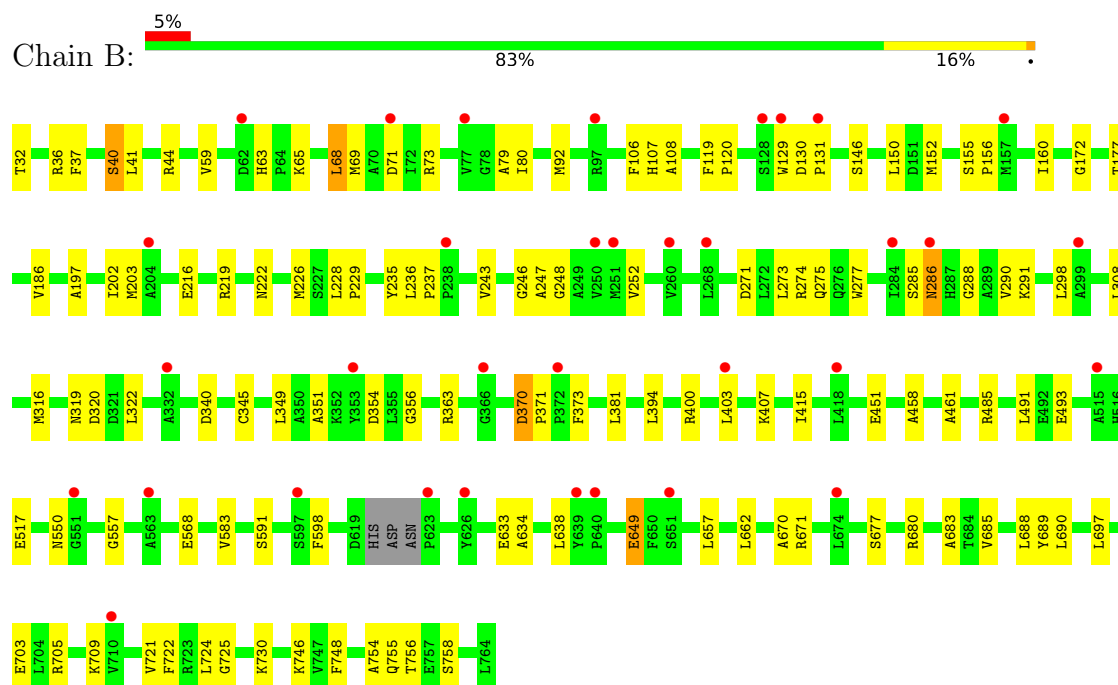
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	205	Total	O	0	0
			205	205		
4	A	209	Total	O	0	0
			209	209		

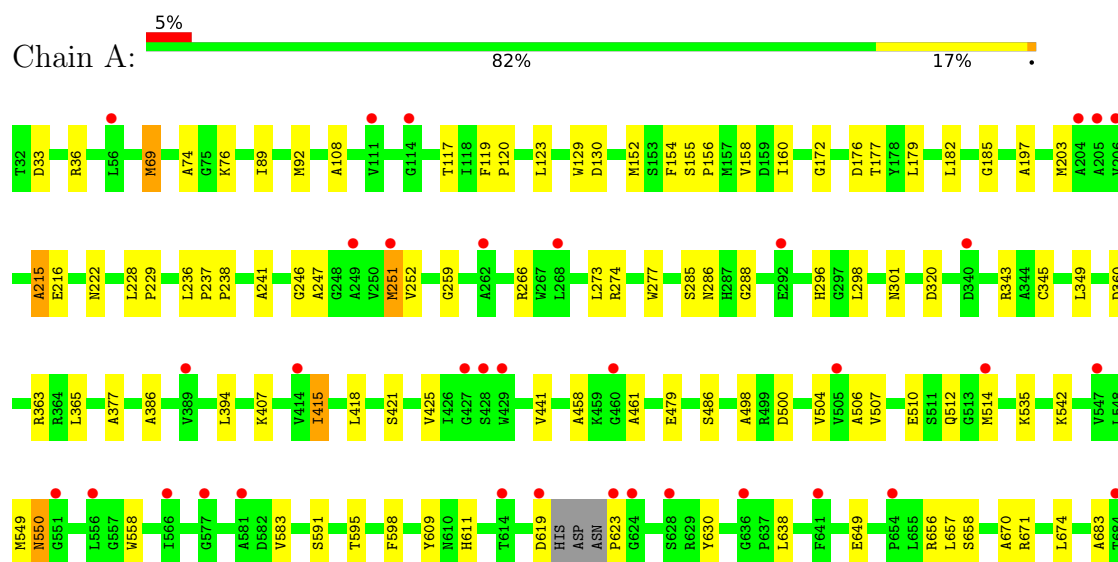
3 Residue-property plots [i](#)

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: Periplasmic beta-glucosidase



• Molecule 1: Periplasmic beta-glucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.50Å 74.91Å 82.10Å 65.64° 74.18° 68.90°	Depositor
Resolution (Å)	46.72 – 2.40 46.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.9 (46.72-2.40) 83.9 (46.72-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.238 , 0.276 0.242 , 0.284	Depositor DCC
R_{free} test set	1960 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 20.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11721	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: MG, 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	1.08	0/5747	1.44	1/7785 (0.0%)
1	B	1.07	0/5755	1.44	3/7794 (0.0%)
All	All	1.08	0/11502	1.44	4/15579 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	GLY	CA-C-O	-6.38	115.90	122.28
1	A	172	GLY	CA-C-O	-6.02	116.26	122.28
1	B	657	LEU	CA-C-N	5.67	128.19	120.54
1	B	657	LEU	C-N-CA	5.67	128.19	120.54

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	5626	0	5622	99	0
1	B	5631	0	5631	93	0
2	A	24	0	24	0	0
2	B	24	0	24	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	209	0	0	32	1
4	B	205	0	0	28	1
All	All	11721	0	11301	190	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (190) 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:152:MET:HA	4:A:904:HOH:O	1.26	1.23
1:B:63:HIS:O	4:B:901:HOH:O	1.55	1.22
1:B:59:VAL:HA	4:B:901:HOH:O	1.56	1.00
1:B:150:LEU:O	4:B:902:HOH:O	1.80	0.97
1:A:479:GLU:OE1	1:A:512:GLN:NE2	2.02	0.92
1:A:595:THR:OG1	4:A:901:HOH:O	1.89	0.89
1:A:252:VAL:O	1:A:286:ASN:ND2	2.07	0.88
1:A:415:ILE:HD12	1:A:504:VAL:HG13	1.57	0.84
1:A:251:MET:HE2	1:A:286:ASN:ND2	1.92	0.84
1:A:394:LEU:O	4:A:902:HOH:O	1.98	0.82
1:A:708:ARG:NE	4:A:905:HOH:O	2.14	0.80
1:B:59:VAL:HG11	1:B:65:LYS:CE	2.12	0.79
1:A:203:MET:N	4:A:904:HOH:O	2.17	0.78
1:B:59:VAL:HG11	1:B:65:LYS:CG	2.17	0.75
1:A:742:PRO:HB2	4:A:1043:HOH:O	1.88	0.74
1:B:356:GLY:O	4:B:904:HOH:O	2.06	0.74
1:A:415:ILE:CD1	1:A:504:VAL:HG13	2.17	0.74
1:B:152:MET:HE2	1:B:203:MET:HE3	1.70	0.73
1:B:59:VAL:CG1	1:B:65:LYS:HG3	2.19	0.72
1:A:251:MET:CE	1:A:286:ASN:ND2	2.52	0.72
1:B:649:GLU:OE2	1:B:677:SER:OG	2.07	0.72
1:B:690:LEU:HD12	1:B:705:ARG:HG3	1.73	0.69
1:A:176:ASP:OD1	4:A:903:HOH:O	2.10	0.69
1:B:130:ASP:HB2	1:B:709:LYS:CE	2.23	0.68
1:A:619:ASP:C	1:A:623:PRO:HD2	2.19	0.68
1:A:203:MET:O	4:A:904:HOH:O	2.11	0.68
1:B:286:ASN:OD1	2:B:801:BGC:C1	2.42	0.68
1:B:290:VAL:HG12	1:B:322:LEU:HD12	1.76	0.67
1:B:41:LEU:O	1:B:44:ARG:HB3	1.94	0.67
1:A:185:GLY:N	4:A:911:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LYS:HA	1:B:68:LEU:HD23	1.78	0.66
1:A:251:MET:HE2	1:A:286:ASN:HD21	1.61	0.65
1:B:662:LEU:HD21	4:B:1006:HOH:O	1.96	0.65
1:B:725:GLY:C	4:B:1006:HOH:O	2.40	0.65
1:B:59:VAL:CG1	1:B:65:LYS:CG	2.74	0.65
1:A:701:VAL:HG22	4:A:906:HOH:O	1.98	0.64
1:B:36:ARG:O	1:B:40:SER:OG	2.15	0.64
1:B:59:VAL:HG11	1:B:65:LYS:HG3	1.79	0.64
1:A:638:LEU:HD23	4:A:982:HOH:O	1.97	0.63
1:B:286:ASN:OD1	2:B:801:BGC:H1	1.99	0.63
1:B:363:ARG:HD2	4:B:904:HOH:O	1.99	0.62
1:B:146:SER:HA	4:B:902:HOH:O	1.98	0.62
1:A:535:LYS:HD3	1:A:558:TRP:CZ2	2.36	0.61
1:B:755:GLN:O	1:B:756:THR:HG23	1.99	0.61
1:A:611:HIS:O	4:A:906:HOH:O	2.17	0.60
1:B:59:VAL:HG11	1:B:65:LYS:HE3	1.84	0.60
1:B:152:MET:CE	1:B:203:MET:HE3	2.31	0.59
1:B:662:LEU:CD2	4:B:1006:HOH:O	2.49	0.59
1:B:203:MET:HE1	1:B:351:ALA:HB1	1.83	0.59
1:B:721:VAL:HA	4:B:1037:HOH:O	2.03	0.58
1:A:500:ASP:OD1	4:A:907:HOH:O	2.17	0.58
1:A:747:VAL:HG22	1:A:759:ARG:O	2.03	0.58
1:B:370:ASP:CG	1:B:371:PRO:HD2	2.28	0.58
1:A:158:VAL:O	1:A:158:VAL:HG12	2.03	0.58
1:B:146:SER:CA	4:B:902:HOH:O	2.52	0.58
1:A:708:ARG:NH1	1:A:721:VAL:O	2.32	0.57
1:B:130:ASP:HB2	1:B:709:LYS:HE3	1.84	0.57
1:B:108:ALA:HA	1:B:152:MET:O	2.04	0.57
1:B:79:ALA:HB2	1:B:106:PHE:CE1	2.39	0.56
1:A:108:ALA:HA	1:A:152:MET:O	2.05	0.56
1:B:649:GLU:CD	1:B:677:SER:HG	2.11	0.56
1:A:712:LEU:HD22	1:A:716:GLU:HG2	1.87	0.56
1:B:59:VAL:HG11	1:B:65:LYS:HE2	1.86	0.55
1:A:689:TYR:HB2	1:A:748:PHE:HB2	1.87	0.55
1:A:156:PRO:HG2	4:A:931:HOH:O	2.06	0.55
1:A:657:LEU:HD21	1:A:747:VAL:HG21	1.89	0.54
1:A:498:ALA:O	1:A:542:LYS:HE3	2.08	0.53
1:B:557:GLY:O	4:B:905:HOH:O	2.19	0.53
1:A:158:VAL:CG1	1:A:238:PRO:HB3	2.39	0.53
1:A:421:SER:O	1:A:425:VAL:HG23	2.09	0.53
1:A:216:GLU:HB3	1:A:222:ASN:ND2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:SER:N	4:B:902:HOH:O	2.42	0.53
1:B:400:ARG:HD3	4:B:1011:HOH:O	2.08	0.52
1:A:69:MET:SD	1:A:92:MET:HG2	2.50	0.52
1:B:155:SER:OG	1:B:156:PRO:HA	2.10	0.52
1:B:671:ARG:HA	4:B:1037:HOH:O	2.09	0.52
1:A:69:MET:SD	1:A:92:MET:CG	2.98	0.51
1:A:415:ILE:HG23	1:A:458:ALA:O	2.08	0.51
1:B:274:ARG:NH2	4:B:936:HOH:O	2.43	0.51
4:B:1051:HOH:O	1:A:296:HIS:HD2	1.92	0.51
1:A:215:ALA:HB2	4:A:1033:HOH:O	2.10	0.51
1:A:155[A]:SER:OG	1:A:156:PRO:HA	2.10	0.51
1:B:340:ASP:HA	4:B:932:HOH:O	2.11	0.51
1:B:216:GLU:HB3	1:B:222:ASN:ND2	2.26	0.51
1:A:123:LEU:CD1	4:A:901:HOH:O	2.59	0.51
1:B:59:VAL:HG13	1:B:65:LYS:HG3	1.91	0.50
1:A:708:ARG:NH2	4:A:905:HOH:O	2.44	0.50
1:A:708:ARG:CZ	4:A:905:HOH:O	2.54	0.50
1:A:92:MET:HB2	4:A:964:HOH:O	2.12	0.50
1:B:689:TYR:HB2	1:B:748:PHE:HB2	1.94	0.50
1:A:266:ARG:NE	4:A:909:HOH:O	2.24	0.49
1:B:202:ILE:CG2	4:B:902:HOH:O	2.60	0.49
1:B:219:ARG:HD3	1:A:630:TYR:CE2	2.46	0.49
1:B:291:LYS:HB2	1:B:322:LEU:HD11	1.95	0.49
1:A:739:THR:HG22	1:A:740:ALA:O	2.13	0.48
1:B:591:SER:CB	1:B:683:ALA:HB3	2.43	0.48
1:B:203:MET:SD	1:B:248:GLY:HA3	2.53	0.48
1:B:197:ALA:O	1:B:363:ARG:NE	2.45	0.48
1:B:394:LEU:HD12	1:B:583:VAL:HG21	1.95	0.48
1:A:386:ALA:HB2	4:A:994:HOH:O	2.13	0.48
1:A:418:LEU:HD13	1:A:549:MET:HB2	1.95	0.47
1:B:415:ILE:HA	1:B:458:ALA:O	2.15	0.47
1:A:591:SER:CB	1:A:683:ALA:HB3	2.44	0.47
1:A:598:PHE:O	1:A:638:LEU:N	2.46	0.47
1:B:129:TRP:CE3	1:B:685:VAL:HG11	2.50	0.47
1:B:598:PHE:O	1:B:638:LEU:N	2.45	0.47
1:A:241:ALA:CB	4:A:911:HOH:O	2.63	0.47
1:A:671:ARG:HD2	4:A:1076:HOH:O	2.13	0.47
1:B:730:LYS:NZ	4:B:924:HOH:O	2.36	0.47
1:B:243:VAL:HA	4:B:989:HOH:O	2.14	0.47
1:A:301:ASN:HB2	4:A:1053:HOH:O	2.14	0.46
1:A:158:VAL:O	1:A:158:VAL:CG1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLY:HA2	1:A:320:ASP:OD2	2.16	0.46
1:A:129:TRP:CE3	1:A:685:VAL:HG11	2.50	0.46
1:A:197:ALA:O	1:A:363:ARG:NE	2.46	0.46
1:A:656:ARG:NH1	4:A:934:HOH:O	2.48	0.46
1:B:288:GLY:HA2	1:B:320:ASP:OD2	2.16	0.46
1:B:485:ARG:NH1	1:B:493:GLU:OE1	2.43	0.46
1:B:517:GLU:OE2	2:B:802:BGC:O2	2.27	0.46
1:B:69:MET:HE1	1:B:92:MET:HG3	1.98	0.46
1:A:713:GLU:O	1:A:716:GLU:HB3	2.15	0.46
1:A:394:LEU:HD12	1:A:583:VAL:HG21	1.97	0.46
1:A:236:LEU:N	1:A:237:PRO:CD	2.79	0.45
1:B:236:LEU:N	1:B:237:PRO:CD	2.79	0.45
1:B:670:ALA:HB3	1:B:722:PHE:HB2	1.99	0.45
1:B:73:ARG:HG2	4:B:959:HOH:O	2.17	0.45
1:B:228:LEU:N	1:B:229:PRO:CD	2.80	0.45
1:B:271:ASP:O	1:B:275:GLN:HG2	2.17	0.44
1:B:689:TYR:HA	1:B:703:GLU:O	2.17	0.44
1:A:158:VAL:HG12	1:A:238:PRO:CB	2.47	0.44
1:A:117:THR:HG23	4:A:994:HOH:O	2.17	0.44
1:A:702:LYS:NZ	1:A:755:GLN:O	2.46	0.44
1:B:286:ASN:OD1	2:B:801:BGC:O1	2.30	0.44
1:A:670:ALA:HB3	1:A:722:PHE:HB2	2.00	0.44
1:B:226[B]:MET:HE1	1:B:235:TYR:CD1	2.53	0.44
1:A:130:ASP:HA	4:A:990:HOH:O	2.18	0.44
1:A:158:VAL:HG12	1:A:238:PRO:HB2	2.00	0.44
1:B:131:PRO:HB3	1:B:186:VAL:HG21	2.00	0.44
1:A:689:TYR:HA	1:A:703:GLU:O	2.17	0.44
1:B:697:LEU:HD22	1:A:259:GLY:HA3	1.99	0.43
1:A:119:PHE:HB3	1:A:120:PRO:HD2	2.00	0.43
1:B:721:VAL:HG22	4:B:1037:HOH:O	2.18	0.43
1:A:345:CYS:O	1:A:349:LEU:HG	2.19	0.43
1:A:415:ILE:HA	1:A:458:ALA:O	2.19	0.43
1:B:59:VAL:CG1	1:B:65:LYS:HG2	2.48	0.43
1:A:123:LEU:HD11	4:A:901:HOH:O	2.17	0.43
1:B:633[B]:GLU:HG3	1:B:634:ALA:O	2.19	0.43
1:A:160:ILE:HD11	1:A:177:THR:HA	2.00	0.43
1:B:246:GLY:O	1:B:247:ALA:C	2.62	0.42
1:A:182:LEU:C	1:A:182:LEU:HD13	2.44	0.42
1:A:274:ARG:NE	4:A:922:HOH:O	2.41	0.42
1:B:345:CYS:O	1:B:349:LEU:HG	2.19	0.42
1:A:74:ALA:HB3	1:A:76:LYS:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ASP:OD1	1:A:609:TYR:OH	2.28	0.42
1:A:743:GLY:N	4:A:945:HOH:O	2.52	0.42
1:A:418:LEU:HB2	1:A:507:VAL:HG12	2.00	0.42
1:A:89:ILE:CG2	1:A:365:LEU:HD21	2.50	0.42
1:A:156:PRO:CG	4:A:931:HOH:O	2.67	0.42
1:B:37:PHE:CE1	4:B:1004:HOH:O	2.71	0.42
1:B:65:LYS:O	1:B:69:MET:HG2	2.19	0.42
1:A:591:SER:HB3	1:A:683:ALA:HB3	2.02	0.42
1:A:228:LEU:N	1:A:229:PRO:CD	2.83	0.41
1:A:273:LEU:O	1:A:277:TRP:HB2	2.20	0.41
1:B:119:PHE:O	1:B:120:PRO:C	2.64	0.41
1:B:591:SER:HB2	1:B:683:ALA:HB3	2.02	0.41
1:A:441:VAL:HG11	1:A:507:VAL:HG11	2.01	0.41
1:A:549:MET:C	1:A:550:ASN:HD22	2.28	0.41
1:B:71:ASP:HA	4:B:949:HOH:O	2.20	0.41
1:B:381:LEU:C	4:B:1000:HOH:O	2.63	0.41
1:B:59:VAL:HG13	1:B:65:LYS:CG	2.48	0.41
1:A:158:VAL:CG1	1:A:238:PRO:CB	2.99	0.41
1:B:160:ILE:HD11	1:B:177:THR:HA	2.02	0.41
1:B:273:LEU:O	1:B:277:TRP:HB2	2.21	0.41
1:A:69:MET:SD	1:A:92:MET:HG3	2.60	0.41
1:A:510:GLU:HB3	1:A:514:MET:HB2	2.03	0.41
1:A:649:GLU:CD	1:A:649:GLU:N	2.79	0.41
1:B:80:ILE:O	1:B:107:HIS:HA	2.21	0.41
1:B:688:LEU:HD21	1:B:724:LEU:HD21	2.03	0.41
1:B:748:PHE:CD2	1:B:758:SER:HB3	2.56	0.41
1:A:360:ASP:HB3	1:A:363:ARG:HB3	2.03	0.41
1:A:748:PHE:CD2	1:A:758:SER:HB3	2.56	0.41
1:B:65:LYS:HG3	4:B:1078:HOH:O	2.20	0.40
1:A:377:ALA:HA	4:A:938:HOH:O	2.21	0.40
1:A:688:LEU:HD21	1:A:724:LEU:HD21	2.03	0.40
1:B:550:ASN:HD21	1:B:568:GLU:CD	2.29	0.40
1:A:246:GLY:O	1:A:247:ALA:C	2.63	0.40
1:B:69:MET:SD	1:B:92:MET:HG2	2.61	0.40
1:B:252:VAL:HB	4:B:986:HOH:O	2.21	0.40
1:A:415:ILE:O	1:A:506:ALA:HA	2.21	0.40
1:A:674:LEU:HD23	1:A:710:VAL:HG11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1101:HOH:O	4:A:1072:HOH:O[1_546]	2.13	0.07

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	730/733 (100%)	678 (93%)	49 (7%)	3 (0%)	30	43
1	B	731/733 (100%)	671 (92%)	57 (8%)	3 (0%)	30	43
All	All	1461/1466 (100%)	1349 (92%)	106 (7%)	6 (0%)	30	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	373	PHE
1	B	461	ALA
1	B	754	ALA
1	A	154	PHE
1	A	461	ALA
1	A	215	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	587/586 (100%)	572 (97%)	15 (3%)	40	63
1	B	588/586 (100%)	570 (97%)	18 (3%)	35	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1175/1172 (100%)	1142 (97%)	33 (3%)	38 60

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

Mol	Chain	Res	Type
1	B	32	THR
1	B	40	SER
1	B	68	LEU
1	B	285	SER
1	B	286	ASN
1	B	298	LEU
1	B	308	LEU
1	B	316	MET
1	B	319	ASN
1	B	354	ASP
1	B	370	ASP
1	B	403	LEU
1	B	407	LYS
1	B	451	GLU
1	B	491	LEU
1	B	649	GLU
1	B	680	ARG
1	B	746	LYS
1	A	33	ASP
1	A	36	ARG
1	A	69	MET
1	A	179	LEU
1	A	251	MET
1	A	285	SER
1	A	298	LEU
1	A	343	ARG
1	A	407	LYS
1	A	415	ILE
1	A	486	SER
1	A	550	ASN
1	A	658	SER
1	A	726	GLU
1	A	757	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	317	ASN
1	B	422	GLN
1	B	560	GLN
1	B	562	ASN
1	B	738	HIS
1	A	107	HIS
1	A	296	HIS
1	A	376	ASN
1	A	550	ASN
1	A	560	GLN
1	A	562	ASN
1	A	738	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	BGC	A	801	-	12,12,12	0.87	0	17,17,17	1.08	1 (5%)
2	BGC	B	802	-	12,12,12	0.86	1 (8%)	17,17,17	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	B	801	-	12,12,12	0.87	0	17,17,17	1.86	5 (29%)
2	BGC	A	802	-	12,12,12	0.60	0	17,17,17	1.54	4 (23%)

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	802	-	-	2/2/22/22	0/1/1/1
2	BGC	B	801	-	-	0/2/22/22	0/1/1/1
2	BGC	A	802	-	-	2/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	BGC	O1-C1	2.03	1.46	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BGC	O2-C2-C1	4.29	119.16	109.25
2	B	801	BGC	C1-O5-C5	-3.04	107.78	113.65
2	A	802	BGC	C1-C2-C3	-2.88	104.49	110.36
2	B	801	BGC	C1-C2-C3	-2.69	104.86	110.36
2	B	802	BGC	O5-C5-C6	2.66	113.04	106.44
2	A	802	BGC	C6-C5-C4	-2.56	106.72	113.02
2	A	801	BGC	C3-C4-C5	2.52	114.81	110.23
2	B	801	BGC	O3-C3-C2	-2.43	104.65	110.38
2	B	802	BGC	C3-C4-C5	2.41	114.59	110.23
2	A	802	BGC	O5-C5-C4	2.31	113.86	109.70
2	B	801	BGC	O4-C4-C3	-2.27	105.03	110.38
2	A	802	BGC	C4-C3-C2	-2.04	107.25	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	802	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	802	BGC	O5-C5-C6-O6
2	A	802	BGC	C4-C5-C6-O6
2	A	802	BGC	O5-C5-C6-O6
2	A	801	BGC	C4-C5-C6-O6
2	A	801	BGC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	802	BGC	1	0
2	B	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	730/733 (99%)	0.65	35 (4%)	35 32	26, 51, 75, 96	4 (0%)
1	B	730/733 (99%)	0.66	34 (4%)	36 32	23, 51, 72, 120	5 (0%)
All	All	1460/1466 (99%)	0.66	69 (4%)	36 32	23, 51, 74, 120	9 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	LEU	4.4
1	B	204	ALA	4.0
1	A	623	PRO	3.6
1	B	515	ALA	3.6
1	A	205	ALA	3.4
1	A	556	LEU	3.4
1	B	551	GLY	3.4
1	B	251	MET	3.3
1	B	651	SER	3.3
1	B	129	TRP	3.2
1	A	619	ASP	3.1
1	A	268	LEU	3.1
1	B	238	PRO	3.0
1	B	640	PRO	3.0
1	B	284	ILE	3.0
1	A	460	GLY	2.9
1	A	427	GLY	2.9
1	B	623	PRO	2.8
1	A	566	ILE	2.8
1	A	414	VAL	2.8
1	B	62	ASP	2.8
1	A	429	TRP	2.7
1	B	597	SER	2.7
1	B	77	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	710	VAL	2.6
1	B	366	GLY	2.6
1	B	353	TYR	2.5
1	A	636	GLY	2.5
1	A	684	THR	2.5
1	A	204	ALA	2.4
1	B	639	TYR	2.4
1	A	641	PHE	2.4
1	A	111	VAL	2.4
1	B	71	ASP	2.4
1	B	403	LEU	2.3
1	B	260	VAL	2.3
1	B	97	ARG	2.3
1	A	249	ALA	2.3
1	A	654	PRO	2.3
1	B	128	SER	2.3
1	B	332	ALA	2.2
1	A	251	MET	2.2
1	B	250	VAL	2.2
1	A	614	THR	2.2
1	A	581	ALA	2.2
1	B	268	LEU	2.2
1	A	206	VAL	2.2
1	B	157	MET	2.1
1	B	286	ASN	2.1
1	A	389	VAL	2.1
1	A	514	MET	2.1
1	A	56	LEU	2.1
1	A	114	GLY	2.1
1	A	292	GLU	2.1
1	B	563	ALA	2.1
1	A	340	ASP	2.1
1	A	262	ALA	2.1
1	A	628	SER	2.1
1	B	131	PRO	2.1
1	A	547	VAL	2.0
1	A	551	GLY	2.0
1	A	577	GLY	2.0
1	A	624	GLY	2.0
1	A	505	VAL	2.0
1	B	299	ALA	2.0
1	B	674	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	372	PRO	2.0
1	B	626	TYR	2.0
1	A	428	SER	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(Å ²)	Q<0.9
2	BGC	A	802	12/12	0.87	0.09	41,50,55,56	0
2	BGC	B	801	12/12	0.88	0.09	32,36,39,44	0
2	BGC	B	802	12/12	0.89	0.08	34,41,44,44	0
2	BGC	A	801	12/12	0.92	0.07	32,36,40,42	0
3	MG	B	803	1/1	0.95	0.09	61,61,61,61	0
3	MG	A	803	1/1	0.98	0.09	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.