



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:58 PM UTC

PDB ID : 2W66 / pdb_00002w66
Title : BtGH84 in complex with HQ602
Authors : He, Y.; Davies, G.J.
Deposited on : 2008-12-17
Resolution : 2.27 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

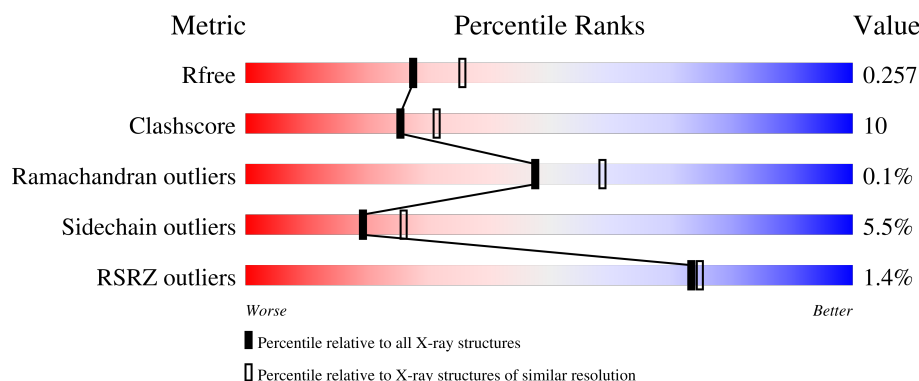
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

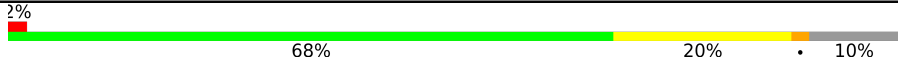
The reported resolution of this entry is 2.27 Å.

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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	716	
1	B	716	

2 Entry composition [i](#)

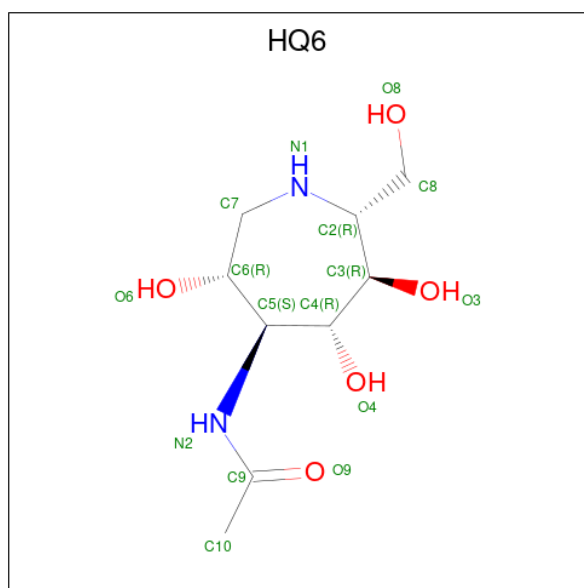
There are 5 unique types of molecules in this entry. The entry contains 11119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O-GLCNACASE BT_4395.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	S	0	2	0
			5259	3374	886	981	18			
1	B	648	Total	C	N	O	S	0	1	0
			5264	3375	888	983	18			

- Molecule 2 is N-[(3R,4S,5R,6R,7R)-3,5,6-trihydroxy-7-(hydroxymethyl)azepan-4-yl]acetamide (CCD ID: HQ6) (formula: C₉H₁₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	9	2	5		
2	B	1	Total	C	N	O	0	0
			16	9	2	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

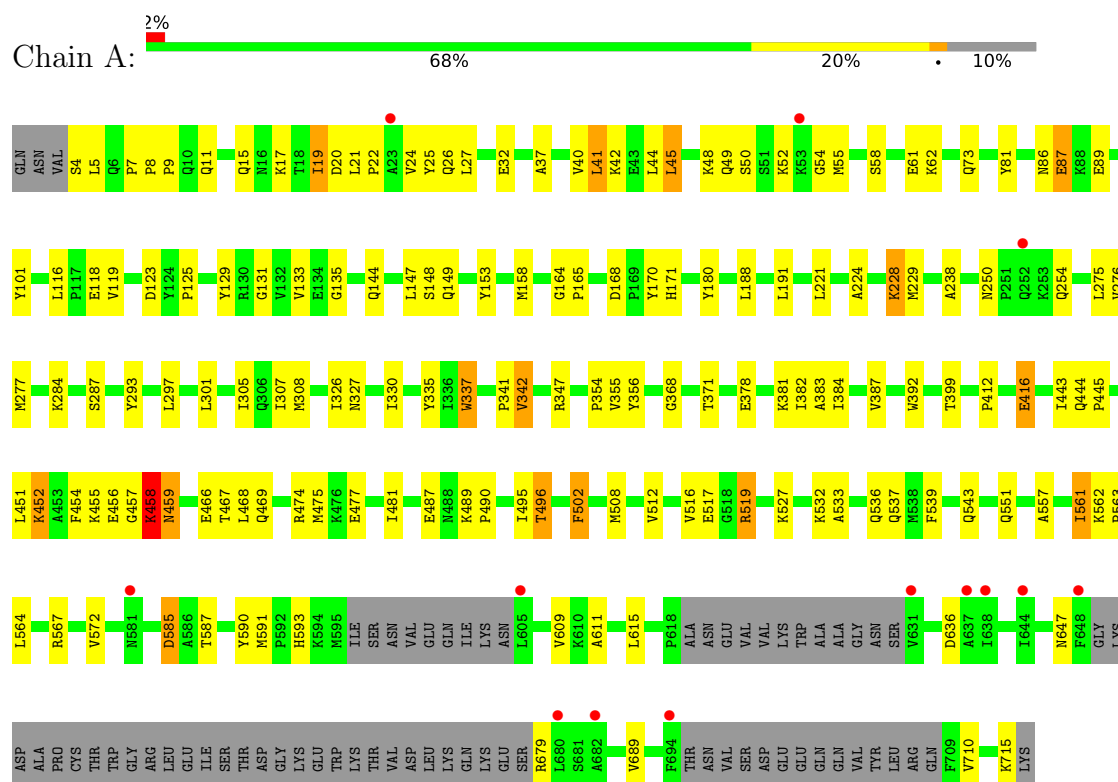
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	262	Total	O	0	0
			262	262		
5	B	288	Total	O	0	0
			288	288		

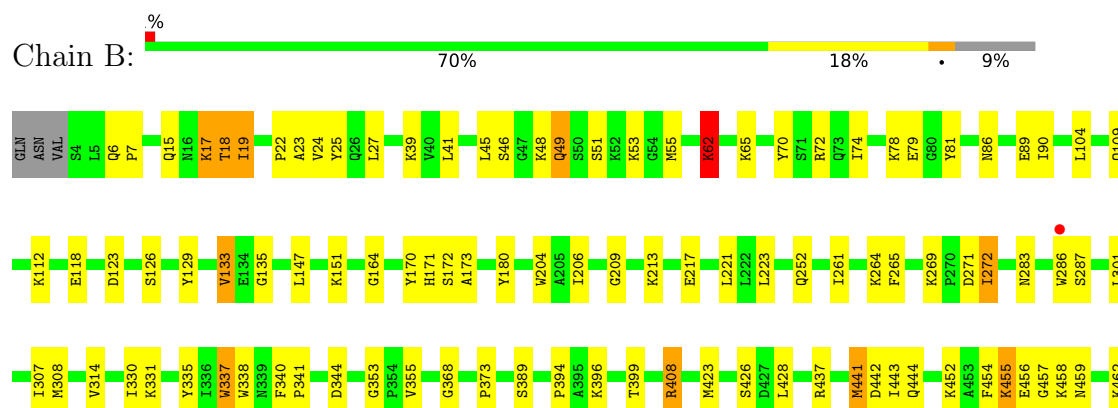
3 Residue-property plots [i](#)

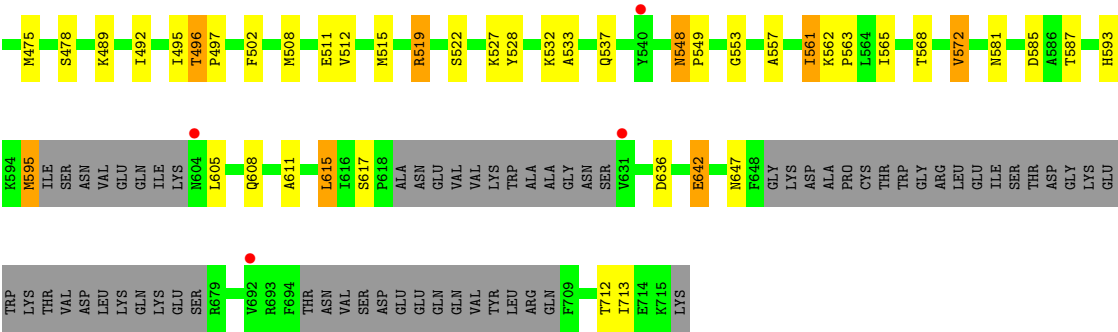
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: O-GLCNACASE BT_4395



• Molecule 1: O-GLCNACASE BT_4395





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.20Å 93.47Å 99.01Å 104.16° 94.01° 103.02°	Depositor
Resolution (Å)	95.35 – 2.27 95.16 – 2.27	Depositor EDS
% Data completeness (in resolution range)	95.9 (95.35-2.27) 95.9 (95.16-2.27)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.188 , 0.236 0.211 , 0.257	Depositor DCC
R_{free} test set	3781 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11119	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: CA, HQ6, GOL

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	0.89	1/5397 (0.0%)	1.05	12/7312 (0.2%)
1	B	0.90	1/5396 (0.0%)	1.09	20/7311 (0.3%)
All	All	0.89	2/10793 (0.0%)	1.07	32/14623 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	496	THR	CA-C	5.96	1.59	1.52
1	A	382	ILE	CA-CB	5.18	1.60	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	ILE	N-CA-C	8.03	118.09	110.30
1	B	62	LYS	CA-C-N	-7.96	113.97	123.44
1	B	62	LYS	C-N-CA	-7.96	113.97	123.44
1	A	517	GLU	N-CA-C	-7.84	102.43	110.97
1	B	553	GLY	N-CA-C	7.55	122.56	111.76
1	B	548	ASN	CA-C-N	6.97	127.12	119.87
1	B	548	ASN	C-N-CA	6.97	127.12	119.87
1	B	89	GLU	N-CA-C	6.94	118.73	108.60
1	B	489	LYS	CA-C-N	-6.32	112.49	119.19
1	B	489	LYS	C-N-CA	-6.32	112.49	119.19
1	B	611	ALA	CB-CA-C	-6.27	109.33	116.54
1	A	458	LYS	N-CA-C	-6.25	100.59	109.96
1	B	51	SER	N-CA-C	6.21	118.28	108.79
1	A	54	GLY	N-CA-C	5.89	119.45	112.33
1	B	495	ILE	N-CA-C	5.80	121.02	113.07
1	B	171	HIS	N-CA-C	-5.80	106.34	113.41
1	B	209	GLY	N-CA-C	5.79	121.17	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	496	THR	CA-C-N	-5.69	112.73	119.05
1	B	496	THR	C-N-CA	-5.69	112.73	119.05
1	B	478	SER	N-CA-C	-5.47	105.34	112.23
1	B	492	ILE	N-CA-CB	5.45	116.92	110.55
1	A	502	PHE	N-CA-C	-5.43	105.44	111.36
1	A	611	ALA	CB-CA-C	-5.36	110.38	116.54
1	A	457	GLY	N-CA-C	-5.35	108.47	115.47
1	A	89	GLU	N-CA-C	5.34	116.96	108.79
1	A	7	PRO	CA-C-N	5.32	125.86	120.38
1	A	7	PRO	C-N-CA	5.32	125.86	120.38
1	B	561	ILE	N-CA-C	5.26	116.73	111.00
1	B	353	GLY	CA-C-N	5.12	125.40	119.92
1	B	353	GLY	C-N-CA	5.12	125.40	119.92
1	A	496	THR	CA-C-N	-5.07	113.70	118.97
1	A	496	THR	C-N-CA	-5.07	113.70	118.97

There are no chirality outliers.

There are no planarity outliers.

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	5259	0	5179	115	0
1	B	5264	0	5176	85	0
2	A	16	0	18	1	0
2	B	16	0	18	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	12	0	16	1	0
5	A	262	0	0	8	0
5	B	288	0	0	5	0
All	All	11119	0	10407	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (201) 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:22:PRO:HG3	1:A:55:MET:SD	2.07	0.93
1:A:593:HIS:HD2	1:A:636:ASP:H	1.16	0.92
1:A:19:ILE:HD12	1:A:20:ASP:O	1.70	0.92
1:A:19:ILE:HG13	1:A:19:ILE:O	1.82	0.80
1:B:337:TRP:CD2	2:B:1716:HQ6:H103	2.18	0.79
1:A:4:SER:HA	5:A:2001:HOH:O	1.84	0.78
1:B:337:TRP:CE2	2:B:1716:HQ6:H103	2.24	0.72
1:B:508:MET:O	1:B:512:VAL:HG23	1.90	0.72
1:A:593:HIS:CD2	1:A:636:ASP:H	2.06	0.72
1:B:408:ARG:HD2	5:B:2191:HOH:O	1.89	0.71
1:A:22:PRO:CG	1:A:55:MET:SD	2.79	0.71
1:A:508:MET:O	1:A:512:VAL:HG23	1.90	0.71
1:B:308:MET:HA	1:B:335:TYR:O	1.91	0.71
1:A:615:LEU:HB3	1:A:710:VAL:HG22	1.75	0.69
1:B:527:LYS:HA	1:B:527:LYS:HE2	1.75	0.68
1:B:23:ALA:HA	1:B:48:LYS:HD2	1.77	0.65
1:A:452:LYS:HB3	1:A:452:LYS:NZ	2.11	0.65
1:B:6:GLN:H	1:B:109:GLN:HE22	1.45	0.65
1:B:593:HIS:HD2	1:B:636:ASP:H	1.42	0.65
1:B:217:GLU:O	1:B:221:LEU:HD23	1.97	0.64
1:A:337:TRP:CD2	2:A:1716:HQ6:H103	2.33	0.64
1:B:585:ASP:OD1	1:B:587:THR:HG23	1.98	0.64
1:B:6:GLN:NE2	1:B:389:SER:OG	2.30	0.64
1:A:41:LEU:HD12	1:A:41:LEU:O	1.98	0.63
1:A:355:VAL:O	1:A:399:THR:HG23	1.98	0.63
1:B:55:MET:HE2	1:B:90:ILE:HG13	1.81	0.62
1:B:355:VAL:O	1:B:399:THR:HG23	1.99	0.62
1:B:533:ALA:O	1:B:537:GLN:HG3	2.01	0.61
1:B:170:TYR:HB2	1:B:180:TYR:CE1	2.36	0.60
1:A:308:MET:HA	1:A:335:TYR:O	2.02	0.60
1:B:72:ARG:HB2	5:B:2028:HOH:O	2.02	0.59
1:B:78:LYS:O	1:B:79:GLU:HB2	2.02	0.59
1:A:354:PRO:HB2	1:A:399:THR:HG22	1.84	0.58
1:B:454:PHE:CZ	1:B:572:VAL:HG13	2.39	0.58
1:B:301:LEU:HD12	1:B:307:ILE:HD11	1.85	0.58
1:A:452:LYS:HB3	1:A:452:LYS:HZ2	1.67	0.56
1:A:165:PRO:HG2	1:A:168:ASP:HB2	1.87	0.56
1:A:148:SER:HB3	5:A:2162:HOH:O	2.05	0.56
1:A:562:LYS:HE3	5:A:2246:HOH:O	2.06	0.55
1:A:689:VAL:HG13	1:A:689:VAL:O	2.07	0.54
1:A:527:LYS:HE2	1:A:527:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:CA	5:A:2001:HOH:O	2.51	0.54
1:B:423:MET:SD	1:B:441:MET:HE1	2.47	0.54
1:B:454:PHE:HZ	1:B:572:VAL:CG1	2.20	0.54
1:A:454:PHE:HZ	1:A:572:VAL:HG12	1.73	0.54
1:B:70:TYR:O	1:B:74:ILE:HG13	2.07	0.54
2:B:1716:HQ6:H71C	2:B:1716:HQ6:O9	2.06	0.54
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.90	0.54
1:A:615:LEU:CB	1:A:710:VAL:HG22	2.38	0.54
1:A:26:GLN:OE1	1:A:52:LYS:HD2	2.08	0.53
1:A:585:ASP:OD1	1:A:587:THR:HG23	2.08	0.53
1:B:81:TYR:CE2	1:B:123:ASP:HB3	2.44	0.53
1:A:86:ASN:HB2	1:A:87:GLU:OE1	2.09	0.53
1:A:536:GLN:HG2	1:A:590:TYR:CD1	2.43	0.53
1:A:25:TYR:HE1	1:A:48:LYS:HB2	1.73	0.53
1:A:133:VAL:HG13	1:A:133:VAL:O	2.08	0.53
1:A:170:TYR:HB2	1:A:180:TYR:CE1	2.44	0.53
1:A:456:GLU:OE1	1:A:458:LYS:HD3	2.09	0.52
1:A:26:GLN:OE1	1:A:52:LYS:CD	2.58	0.52
1:B:25:TYR:CD2	1:B:25:TYR:C	2.87	0.52
1:A:477:GLU:O	1:A:481:ILE:HG13	2.09	0.51
1:B:454:PHE:HZ	1:B:572:VAL:HG13	1.72	0.51
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.92	0.51
1:A:131:GLY:HA2	1:A:158:MET:HE2	1.92	0.51
1:A:543:GLN:OE1	1:A:609:VAL:HG12	2.10	0.51
1:B:17:LYS:HD2	1:B:118:GLU:OE1	2.11	0.51
1:B:568:THR:O	1:B:572:VAL:HG22	2.11	0.50
1:B:41:LEU:HB2	1:B:104:LEU:HD11	1.93	0.50
1:B:269:LYS:HB2	1:B:272:ILE:HG13	1.94	0.50
1:A:459:ASN:OD1	1:A:459:ASN:N	2.38	0.50
1:B:45:LEU:O	1:B:48:LYS:HB2	2.12	0.50
1:B:475:MET:HE3	1:B:502:PHE:CE1	2.48	0.49
1:A:19:ILE:CD1	1:A:20:ASP:O	2.53	0.49
1:B:133:VAL:O	1:B:133:VAL:HG13	2.13	0.48
1:A:468:LEU:HD13	1:A:564:LEU:HD21	1.95	0.48
1:A:456:GLU:C	1:A:458:LYS:H	2.21	0.48
1:A:17:LYS:HD3	1:A:118:GLU:OE1	2.13	0.48
1:B:223:LEU:HD11	1:B:265:PHE:HB2	1.95	0.48
1:A:444:GLN:N	1:A:445:PRO:CD	2.77	0.47
1:B:22:PRO:HB2	1:B:25:TYR:HB3	1.96	0.47
1:B:147:LEU:O	1:B:151:LYS:HE3	2.14	0.47
1:B:496:THR:O	1:B:497:PRO:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LYS:HA	1:A:532:LYS:HD2	1.62	0.47
1:B:454:PHE:C	1:B:456:GLU:H	2.23	0.47
1:A:516:VAL:HG22	1:A:572:VAL:HG11	1.94	0.47
1:B:338:TRP:CH2	1:B:355:VAL:HG13	2.49	0.47
1:B:39:LYS:HD2	5:B:2030:HOH:O	2.14	0.47
1:A:15:GLN:C	1:A:17:LYS:H	2.21	0.47
1:A:354:PRO:HB2	1:A:399:THR:CG2	2.44	0.47
1:B:443:ILE:C	1:B:443:ILE:HD12	2.39	0.47
1:A:297:LEU:O	1:A:301:LEU:HB2	2.15	0.47
1:B:24:VAL:HG22	1:B:49:GLN:HB2	1.96	0.47
1:A:61:GLU:O	1:A:62:LYS:C	2.57	0.46
1:B:261:ILE:O	1:B:265:PHE:HB3	2.15	0.46
1:B:562:LYS:HB3	1:B:563:PRO:HD3	1.97	0.46
1:A:144:GLN:HG2	5:A:2048:HOH:O	2.15	0.46
1:B:172:SER:OG	1:B:173:ALA:N	2.45	0.46
1:A:228:LYS:HB3	1:A:228:LYS:HE2	1.72	0.46
1:A:25:TYR:CE2	1:A:50:SER:HB3	2.50	0.46
1:A:131:GLY:HA2	1:A:158:MET:HG2	1.98	0.46
1:B:511:GLU:O	1:B:515:MET:HG3	2.16	0.46
1:B:519:ARG:H	1:B:519:ARG:HG2	1.41	0.46
1:A:168:ASP:HB3	1:A:171:HIS:HB3	1.96	0.46
1:A:277:MET:HG2	1:A:301:LEU:HD11	1.98	0.46
1:A:536:GLN:HG2	1:A:590:TYR:CG	2.50	0.46
1:A:15:GLN:OE1	1:A:15:GLN:HA	2.16	0.45
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.51	0.45
1:A:443:ILE:C	1:A:443:ILE:HD12	2.41	0.45
1:B:548:ASN:HB2	1:B:549:PRO:HD2	1.96	0.45
1:A:238:ALA:HA	1:A:276:VAL:O	2.16	0.45
1:A:412:PRO:HD2	1:A:487:GLU:OE1	2.17	0.45
1:A:378:GLU:OE1	1:A:381:LYS:NZ	2.42	0.45
1:B:204:TRP:CZ3	1:B:206:ILE:HB	2.51	0.45
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.98	0.45
1:A:41:LEU:HD11	1:A:45:LEU:HD21	1.97	0.45
1:A:41:LEU:HD11	1:A:45:LEU:CD2	2.46	0.45
1:A:451:LEU:HD21	1:A:567:ARG:HD3	1.99	0.45
1:B:562:LYS:HB3	5:B:2265:HOH:O	2.17	0.45
1:A:326:ILE:HG23	1:A:327:ASN:H	1.80	0.45
1:A:519:ARG:H	1:A:519:ARG:HG2	1.26	0.45
1:B:135:GLY:HA2	1:B:164:GLY:O	2.16	0.45
1:B:86:ASN:HA	1:B:118:GLU:HG3	1.98	0.45
1:B:341:PRO:HD2	1:B:373:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426[B]:SER:O	1:B:437:ARG:HB2	2.17	0.45
1:A:149:GLN:HE22	1:A:384:ILE:HD13	1.82	0.45
1:A:475:MET:HE3	1:A:502:PHE:CE1	2.51	0.45
1:A:41:LEU:CD1	1:A:45:LEU:HD22	2.46	0.45
1:A:539:PHE:O	1:A:543:GLN:HG2	2.17	0.44
1:A:562:LYS:HB3	1:A:563:PRO:HD3	2.00	0.44
1:B:62:LYS:HG3	1:B:62:LYS:O	2.16	0.44
1:A:135:GLY:HA2	1:A:164:GLY:O	2.18	0.44
1:A:489:LYS:N	1:A:490:PRO:CD	2.80	0.44
1:B:428:LEU:HD12	1:B:428:LEU:N	2.33	0.44
1:A:454:PHE:C	1:A:456:GLU:H	2.26	0.44
1:B:452:LYS:O	1:B:455:LYS:HG3	2.18	0.44
1:A:250:ASN:O	1:A:254:GLN:HG3	2.17	0.44
1:A:416:GLU:HB3	1:A:474:ARG:HH21	1.82	0.44
1:A:81:TYR:CE2	1:A:123:ASP:HB3	2.53	0.44
1:A:41:LEU:HD12	1:A:41:LEU:C	2.40	0.44
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.52	0.43
1:A:679:ARG:N	5:A:2259:HOH:O	2.51	0.43
1:B:515:MET:HG2	1:B:527:LYS:HB2	2.00	0.43
1:A:37:ALA:HB2	1:A:101:TYR:HA	1.99	0.43
1:A:40:VAL:O	1:A:44:LEU:HG	2.18	0.43
1:A:533:ALA:O	1:A:537:GLN:HG3	2.18	0.43
1:A:8:PRO:HA	1:A:9:PRO:HD3	1.89	0.43
1:A:224:ALA:O	1:A:228:LYS:HG2	2.18	0.43
1:A:527:LYS:HE2	1:A:527:LYS:CA	2.47	0.43
1:A:149:GLN:HB3	1:A:153:TYR:CZ	2.53	0.43
1:A:293:TYR:CD2	1:A:293:TYR:C	2.97	0.43
1:A:326:ILE:HG23	1:A:327:ASN:N	2.34	0.43
1:A:21:LEU:HD23	1:A:48:LYS:HE3	2.00	0.43
1:A:26:GLN:CD	1:A:52:LYS:HD2	2.44	0.43
1:A:188:LEU:HD13	1:A:229:MET:HE1	2.00	0.42
1:A:591:MET:HG3	1:A:593:HIS:O	2.18	0.42
1:B:330:ILE:O	1:B:331:LYS:HB2	2.19	0.42
1:A:21:LEU:HD12	1:A:22:PRO:HD2	2.02	0.42
1:A:519:ARG:NE	5:A:2222:HOH:O	2.48	0.42
1:B:17:LYS:C	1:B:18:THR:CG2	2.92	0.42
1:B:512:VAL:HG21	1:B:565:ILE:HG23	2.01	0.42
1:A:147:LEU:HD23	1:A:191:LEU:HD23	2.01	0.42
1:A:495:ILE:O	1:A:496:THR:C	2.60	0.42
1:A:562:LYS:CE	5:A:2246:HOH:O	2.67	0.42
1:B:22:PRO:C	1:B:24:VAL:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:SER:HB2	1:B:394:PRO:HD2	2.02	0.42
1:A:21:LEU:HD23	1:A:48:LYS:CE	2.50	0.42
1:B:527:LYS:HE2	1:B:527:LYS:CA	2.46	0.42
1:A:341:PRO:O	1:A:342:VAL:C	2.63	0.42
1:B:340:PHE:CG	1:B:341:PRO:HA	2.55	0.42
1:B:396:LYS:HD3	1:B:396:LYS:HA	1.81	0.42
1:A:45:LEU:O	1:A:48:LYS:HG2	2.20	0.42
1:A:347:ARG:HG3	1:A:551:GLN:OE1	2.20	0.42
1:A:356:TYR:HB3	1:A:399:THR:HG21	2.02	0.42
1:B:271:ASP:OD1	1:B:271:ASP:N	2.52	0.42
1:A:15:GLN:O	1:A:17:LYS:N	2.46	0.41
1:A:147:LEU:CD2	1:A:191:LEU:HD23	2.50	0.41
1:A:383:ALA:O	1:A:387:VAL:HG23	2.20	0.41
1:B:86:ASN:HB2	5:B:2036:HOH:O	2.19	0.41
1:B:129:TYR:O	1:B:368:GLY:HA2	2.19	0.41
1:B:528:TYR:O	1:B:532:LYS:HG2	2.20	0.41
1:B:19:ILE:O	1:B:19:ILE:HG13	2.16	0.41
1:A:275:LEU:HD23	1:A:305:ILE:HG12	2.02	0.41
1:B:459:ASN:HD22	1:B:459:ASN:HA	1.71	0.41
1:B:462:LYS:HE2	1:B:462:LYS:HB3	1.73	0.41
1:B:642:GLU:HB2	1:B:712:THR:O	2.19	0.41
1:B:283:ASN:HD21	1:B:286:TRP:CG	2.38	0.41
1:B:456:GLU:O	1:B:457:GLY:C	2.63	0.41
1:A:19:ILE:HD11	1:A:116:LEU:HD12	2.01	0.41
1:B:6:GLN:HA	1:B:7:PRO:HA	1.91	0.41
1:A:129:TYR:O	1:A:368:GLY:HA2	2.20	0.41
1:A:307:ILE:HD12	1:A:330:ILE:HB	2.03	0.41
1:B:314:VAL:HG13	2:B:1716:HQ6:H72C	2.01	0.41
1:B:454:PHE:C	1:B:456:GLU:N	2.79	0.41
1:B:608:GLN:HB2	1:B:615:LEU:HD22	2.01	0.41
1:B:344:ASP:O	4:B:1718:GOL:H32	2.21	0.41
1:A:444:GLN:N	1:A:445:PRO:HD2	2.37	0.40
1:A:474:ARG:HH11	1:A:474:ARG:HD2	1.74	0.40
1:B:264:LYS:HA	1:B:264:LYS:HD3	1.88	0.40
1:A:284:LYS:O	1:A:287:SER:HB2	2.21	0.40
1:B:46:SER:C	1:B:48:LYS:H	2.30	0.40
1:B:595:MET:HE2	1:B:595:MET:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	639/716 (89%)	605 (95%)	33 (5%)	1 (0%)	43	53
1	B	639/716 (89%)	607 (95%)	32 (5%)	0	100	100
All	All	1278/1432 (89%)	1212 (95%)	65 (5%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	VAL

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	570/630 (90%)	540 (95%)	30 (5%)	20	28
1	B	570/630 (90%)	537 (94%)	33 (6%)	18	24
All	All	1140/1260 (90%)	1077 (94%)	63 (6%)	19	26

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	GLN
1	A	19	ILE
1	A	24	VAL
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	32	GLU
1	A	41	LEU
1	A	42	LYS
1	A	45	LEU
1	A	49	GLN
1	A	58	SER
1	A	73	GLN
1	A	87	GLU
1	A	119	VAL
1	A	221	LEU
1	A	228	LYS
1	A	337	TRP
1	A	371	THR
1	A	416	GLU
1	A	452	LYS
1	A	455	LYS
1	A	458	LYS
1	A	459	ASN
1	A	466	GLU
1	A	467	THR
1	A	469	GLN
1	A	519	ARG
1	A	585	ASP
1	A	647	ASN
1	A	715	LYS
1	B	15	GLN
1	B	17	LYS
1	B	18	THR
1	B	19	ILE
1	B	27	LEU
1	B	49	GLN
1	B	53	LYS
1	B	62	LYS
1	B	65	LYS
1	B	112	LYS
1	B	133	VAL
1	B	213	LYS
1	B	252	GLN
1	B	272	ILE
1	B	287	SER
1	B	337	TRP
1	B	408	ARG

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Mol	Chain	Res	Type
1	B	441	MET
1	B	442	ASP
1	B	444	GLN
1	B	455	LYS
1	B	458	LYS
1	B	519	ARG
1	B	522	SER
1	B	572	VAL
1	B	581	ASN
1	B	595	MET
1	B	605	LEU
1	B	615	LEU
1	B	617	SER
1	B	642	GLU
1	B	647	ASN
1	B	713	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	49	GLN
1	A	149	GLN
1	A	189	GLN
1	A	273	ASN
1	A	292	ASN
1	A	349	HIS
1	A	401	GLN
1	A	547	GLN
1	A	581	ASN
1	A	593	HIS
1	B	6	GLN
1	B	109	GLN
1	B	254	GLN
1	B	306	GLN
1	B	444	GLN
1	B	459	ASN
1	B	469	GLN
1	B	547	GLN
1	B	583	HIS
1	B	593	HIS
1	B	643	ASN

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Mol	Chain	Res	Type
1	B	647	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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$
4	GOL	B	1718	-	5,5,5	0.44	0	5,5,5	0.74	0
4	GOL	B	1717	-	5,5,5	0.43	0	5,5,5	0.55	0
2	HQ6	A	1716	-	13,16,16	1.48	2 (15%)	13,22,22	1.26	2 (15%)
2	HQ6	B	1716	-	13,16,16	1.91	5 (38%)	13,22,22	2.19	3 (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
4	GOL	B	1718	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	1717	-	-	4/4/4/4	-
2	HQ6	A	1716	-	-	0/5/27/27	0/1/1/1
2	HQ6	B	1716	-	-	0/5/27/27	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1716	HQ6	C9-N2	3.50	1.45	1.34
2	A	1716	HQ6	C9-N2	3.36	1.45	1.34
2	B	1716	HQ6	C3-C2	3.08	1.58	1.53
2	B	1716	HQ6	C4-C5	2.91	1.57	1.53
2	B	1716	HQ6	C3-C4	2.57	1.57	1.53
2	B	1716	HQ6	C10-C9	2.29	1.55	1.50
2	A	1716	HQ6	C7-N1	-2.16	1.44	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1716	HQ6	C3-C4-C5	5.56	122.90	114.67
2	A	1716	HQ6	C3-C4-C5	2.98	119.08	114.67
2	B	1716	HQ6	O9-C9-N2	-2.60	117.39	121.98
2	B	1716	HQ6	C10-C9-N2	2.57	120.38	116.12
2	A	1716	HQ6	O3-C3-C2	2.18	112.97	107.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1717	GOL	C1-C2-C3-O3
4	B	1718	GOL	C1-C2-C3-O3
4	B	1717	GOL	O1-C1-C2-C3
4	B	1717	GOL	O2-C2-C3-O3
4	B	1718	GOL	O2-C2-C3-O3
4	B	1717	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1718	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1716	HQ6	1	0
2	B	1716	HQ6	4	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	647/716 (90%)	-0.11	13 (2%) 65 66	2, 6, 33, 42	2 (0%)
1	B	648/716 (90%)	-0.26	5 (0%) 82 84	1, 6, 32, 42	1 (0%)
All	All	1295/1432 (90%)	-0.19	18 (1%) 73 75	1, 6, 33, 42	3 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	631	VAL	4.7
1	A	631	VAL	4.3
1	A	682	ALA	3.7
1	A	605	LEU	2.9
1	A	680	LEU	2.6
1	A	23	ALA	2.6
1	B	286	TRP	2.5
1	B	604	ASN	2.4
1	A	53	LYS	2.4
1	A	694	PHE	2.3
1	A	648	PHE	2.2
1	B	692	VAL	2.1
1	A	644	ILE	2.1
1	A	252	GLN	2.1
1	A	638	ILE	2.1
1	A	637	ALA	2.0
1	B	540	TYR	2.0
1	A	581	ASN	2.0

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

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

6.3 Carbohydrates [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
4	GOL	B	1717	6/6	0.87	0.13	31,33,33,34	0
3	CA	B	1719	1/1	0.92	0.21	25,25,25,25	0
4	GOL	B	1718	6/6	0.92	0.13	11,16,16,19	0
2	HQ6	B	1716	16/16	0.94	0.06	2,5,8,9	0
2	HQ6	A	1716	16/16	0.95	0.06	2,4,6,8	0
3	CA	A	1717	1/1	0.96	0.18	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.