



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:37 AM UTC

PDB ID : 2XM2 / pdb_00002xm2
Title : BtGH84 in complex with LOGNAc
Authors : He, Y.; Davies, G.J.
Deposited on : 2010-07-22
Resolution : 1.95 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

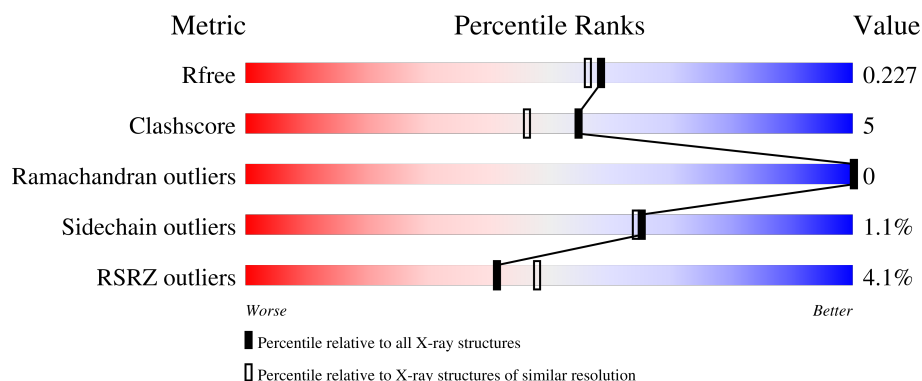
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	5% 79% 10% 11%
1	B	716	2% 79% 9% 10%

2 Entry composition [i](#)

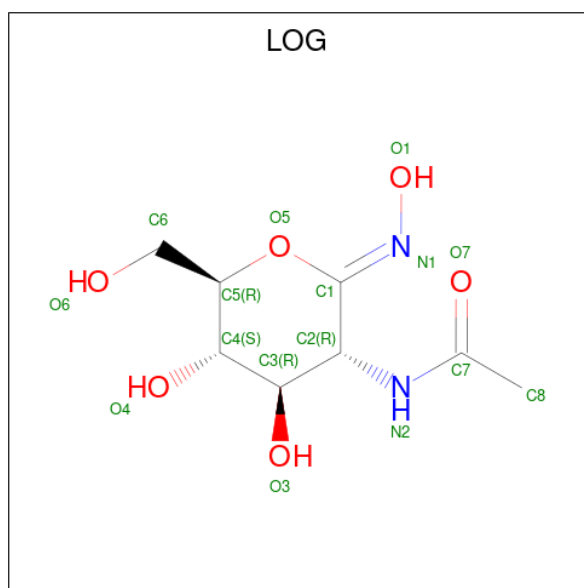
There are 4 unique types of molecules in this entry. The entry contains 11232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	635	Total	C	N	O	S	0	3	0
			5184	3329	870	967	18			
1	B	641	Total	C	N	O	S	0	2	0
			5217	3350	876	973	18			

- Molecule 2 is N-acetylglucosaminono-1,5-lactone (Z)-oxime (CCD ID: LOG) (formula: $C_8H_{14}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	8	2	6		
2	B	1	Total	C	N	O	0	0
			16	8	2	6		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	356	Total	O	0	0
			356	356		
4	B	419	Total	O	0	0
			419	419		

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.

Chain A:

5% 79% 10% 11%

Residue	Category
GLN	Green
ASN	Green
VAL	Green
SER	Green
L5	Green
V14	Green
K17	Green
T18	Green
I19	Green
P22	Green
A23	Green
V24	Green
Y25	Green
L41	Green
L45	Green
K48	Green
GLN	Green
SER	Green
SER	Green
LYS	Green
LYS	Green
GLY	Green
M55	Green
L63	Green
E87	Green
K88	Green
E89	Green
L104	Green
G114	Green
P125	Green
Y129	Green
Y170	Green
P174	Green
Y180	Green
S236	Green
F237	Green
A238	Green
D243	Green
N250	Green
Q254	Green
K269	Green
I272	Green
N273	Green
Q274	Green
L275	Green
V276	Green
Y293	Green
M308	Green
V314	Green
I315	Green
Y335	Green
I336	Green
W337	Green
P341	Green
V342	Green
G368	Green
T371	Green
N372	Green
P373	Green
E378	Green
L605	Green
P606	Green
W392	Green
A406	Green
I410	Green
M423	Green
M441	Green
Q444	Green
P445	Green
F448	Green
A453	Green
P454	Green
P490	Green
E517	Green
GLY	Green
R519	Green
Y523	Green
Q536	Green
F539	Green
Y540	Green
Q543	Green
A557	Green
I561	Green
T568	Green
V572	Green
A582	Green
Y590	Green
M591	Green
P592	Green
H593	Green
K594	Green
M595	Green
ILE	Green
SER	Green
ASN	Green
VAL	Green
GLU	Green
GLN	Green
ILE	Green
LYS	Green
ASN	Green
L605	Green
P606	Green
W392	Green
A406	Green
K610	Green
A611	Green
V614	Green
L615	Green
S617	Green
P618	Green
ALA	Green
ASN	Green
GLU	Green
VAL	Green
VAL	Green
LYS	Green
TRP	Green
ALA	Green
ALA	Green
GLY	Green
ASN	Green
SER	Green
VAL	Green
E632	Green
D636	Green
A637	Green
F638	Green
Y639	Green
P640	Green
G641	Green
E642	Green
N643	Green
I644	Green
Q645	Green
I646	Green
N647	Green
PHE	Green
GLY	Green
LYS	Green
ASP	Green
ALA	Green
PRO	Green
CYS	Green
THR	Green
TRP	Green
GLY	Green
ARG	Green
GLU	Green
GLU	Green
ILE	Green
SER	Green
THR	Green
ASP	Green
GLY	Green
LYS	Green
GLU	Green
TRP	Green
LYS	Green
GLN	Green
LEU	Green
LYS	Green
S681	Green
A682	Green
G683	Green
L684	Green
A687	Green
F688	Green
V689	Green
K690	Green
F691	Green
V692	Green
R693	Green
F694	Green
THR	Green
ASN	Green
VAL	Green
SER	Green
ASP	Green
GLU	Green
GLN	Green
TYR	Green
LEU	Green
ARG	Green
GLN	Green
F709	Green
K715	Green
LYS	Green
GLN	Grey

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.51Å 93.44Å 98.92Å 104.12° 94.26° 102.92°	Depositor
Resolution (Å)	43.70 – 1.95 43.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.1 (43.70-1.95) 94.6 (43.70-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.221 0.187 , 0.227	Depositor DCC
R_{free} test set	6015 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.8	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	0.95	EDS
Total number of atoms	11232	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.96	0/5323	0.95	1/7212 (0.0%)
1	B	1.00	0/5354	0.98	3/7253 (0.0%)
All	All	0.98	0/10677	0.97	4/14465 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	560	VAL	CB-CA-C	-5.99	105.72	111.05
1	A	89	GLU	N-CA-C	5.63	117.09	108.42
1	B	399	THR	CB-CA-C	-5.32	102.46	110.92
1	B	49	GLN	N-CA-C	5.18	117.84	109.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	540[B]	TYR	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5184	0	5098	44	0
1	B	5217	0	5138	55	0
2	A	16	0	14	0	0
2	B	16	0	14	1	0
3	A	6	0	8	0	0
3	B	18	0	24	3	0
4	A	356	0	0	4	0
4	B	419	0	0	8	0
All	All	11232	0	10296	99	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 5.

All (99) 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:52:LYS:N	1:B:52:LYS:HD3	1.96	0.79
1:A:536:GLN:HG2	1:A:590:TYR:CD1	2.24	0.73
1:A:593:HIS:HD2	1:A:636:ASP:H	1.42	0.68
1:B:693:ARG:NH2	4:B:2414:HOH:O	2.28	0.65
1:B:26:GLN:HE21	1:B:52:LYS:HA	1.61	0.65
1:B:593:HIS:HE1	4:B:2397:HOH:O	1.79	0.65
1:B:454:PHE:HZ	1:B:572:VAL:HG12	1.62	0.64
1:B:536:GLN:HG2	1:B:590:TYR:CD1	2.33	0.63
1:B:462:LYS:HE3	1:B:466:GLU:OE2	2.00	0.62
1:B:228:LYS:HE3	4:B:2187:HOH:O	1.99	0.61
1:B:286:TRP:HE1	3:B:1716:GOL:H32	1.66	0.61
1:A:519:ARG:NH1	1:A:523:TYR:CZ	2.69	0.60
1:B:111:LEU:C	1:B:112:LYS:HG2	2.25	0.60
1:A:519:ARG:NH1	1:A:523:TYR:CE2	2.70	0.59
1:B:55:MET:HE2	1:B:90:ILE:HG13	1.85	0.58
1:B:189:GLN:CD	4:B:2148:HOH:O	2.46	0.58
1:A:83:LEU:C	1:A:83:LEU:HD23	2.29	0.58
1:B:593:HIS:HD2	1:B:636:ASP:H	1.52	0.57
1:B:308:MET:HA	1:B:335:TYR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:PHE:HZ	1:B:572:VAL:CG1	2.19	0.56
1:A:236:SER:HB3	1:A:274:GLN:HB2	1.87	0.55
1:B:313:ARG:NH1	4:B:2234:HOH:O	2.27	0.54
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.88	0.54
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.89	0.54
1:A:25:TYR:HE1	1:A:48:LYS:HB2	1.73	0.53
1:A:19:ILE:CD1	1:A:55:MET:HE1	2.38	0.53
1:A:174:PRO:HD2	4:A:2101:HOH:O	2.08	0.53
1:B:639:TYR:CE1	1:B:715:LYS:HD3	2.44	0.52
1:B:454:PHE:CZ	1:B:572:VAL:CG1	2.93	0.52
1:B:15:GLN:HB2	1:B:118:GLU:HB3	1.92	0.52
1:B:606:PRO:O	1:B:617:SER:OG	2.28	0.52
1:A:423:MET:O	1:A:423:MET:HE3	2.10	0.51
1:A:632:GLU:HB2	1:A:693:ARG:HG3	1.93	0.51
1:A:269:LYS:HB2	1:A:272:ILE:HD12	1.92	0.50
1:B:289:PRO:O	1:B:290:ASN:HB2	2.11	0.50
1:B:617:SER:O	1:B:618:PRO:C	2.54	0.50
1:B:536:GLN:HG2	1:B:590:TYR:CE1	2.46	0.50
1:B:536:GLN:HG2	1:B:590:TYR:CG	2.47	0.49
1:A:170:TYR:HB2	1:A:180:TYR:CE1	2.47	0.49
1:B:50:SER:O	1:B:51:SER:HB3	2.11	0.49
1:B:433:HIS:HA	3:B:1716:GOL:H11	1.94	0.49
1:B:172:SER:OG	1:B:173:ALA:N	2.44	0.49
1:A:539:PHE:O	1:A:543:GLN:HG2	2.13	0.48
1:A:308:MET:HA	1:A:335:TYR:O	2.13	0.48
1:B:536:GLN:CG	1:B:590:TYR:CD1	2.96	0.48
1:A:41:LEU:HB2	1:A:104:LEU:HD11	1.93	0.48
1:B:341:PRO:O	1:B:342:VAL:C	2.56	0.48
1:A:250:ASN:O	1:A:254:GLN:HG3	2.14	0.48
1:A:591:MET:HG3	1:A:593:HIS:O	2.14	0.48
1:A:238:ALA:HA	1:A:276:VAL:O	2.14	0.47
1:A:423:MET:HE1	4:A:2280:HOH:O	2.13	0.47
1:B:355:VAL:O	1:B:399:THR:HG23	2.14	0.47
1:B:591:MET:HG3	1:B:593:HIS:O	2.14	0.47
1:B:434:GLY:HA2	3:B:1717:GOL:H12	1.97	0.47
1:B:454:PHE:CZ	1:B:572:VAL:HG12	2.47	0.46
1:A:536:GLN:HG2	1:A:590:TYR:CG	2.49	0.46
1:B:282:TYR:OH	2:B:1000:LOG:N1	2.47	0.46
1:B:489:LYS:HB2	1:B:490:PRO:HD3	1.97	0.46
1:B:562:LYS:HB3	1:B:563:PRO:HD3	1.97	0.46
1:A:341:PRO:O	1:A:342:VAL:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:HG12	1:A:315:ILE:HD13	1.97	0.45
1:B:269:LYS:HB2	1:B:272:ILE:HG12	1.98	0.45
1:A:378:GLU:HG3	1:A:490:PRO:HB2	1.99	0.45
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.53	0.44
1:A:372:ASN:HA	1:A:373:PRO:HD3	1.87	0.44
1:B:81:TYR:CE2	1:B:123:ASP:HB3	2.53	0.43
1:B:189:GLN:NE2	4:B:2148:HOH:O	2.52	0.43
1:A:543:GLN:NE2	1:A:609:VAL:HG12	2.33	0.43
1:B:454:PHE:CZ	1:B:572:VAL:HG13	2.53	0.43
1:A:441:MET:HB2	4:A:2280:HOH:O	2.17	0.43
1:B:532:LYS:HA	1:B:532:LYS:HD2	1.86	0.43
1:B:173:ALA:HA	1:B:174:PRO:HA	1.78	0.43
1:B:231:GLN:NE2	4:B:2190:HOH:O	2.44	0.43
1:B:489:LYS:N	1:B:490:PRO:CD	2.82	0.43
1:A:568:THR:O	1:A:572:VAL:HG22	2.18	0.42
1:A:644:ILE:O	1:A:681:SER:HA	2.19	0.42
1:A:337:TRP:C	1:A:337:TRP:CD1	2.97	0.42
1:A:582:ALA:HB1	4:A:2341:HOH:O	2.19	0.42
1:B:141:TRP:CD1	1:B:377:ALA:HB2	2.54	0.42
1:B:262:ASP:HA	1:B:266:ALA:HB3	2.00	0.42
1:B:378:GLU:HG3	1:B:490:PRO:HB2	2.02	0.42
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.55	0.42
1:A:605:LEU:HA	1:A:606:PRO:HD3	1.94	0.41
1:A:644:ILE:HD12	1:A:684:LEU:HD21	2.02	0.41
1:B:644:ILE:O	1:B:681:SER:HA	2.20	0.41
1:A:385:TYR:CD2	1:A:406:ALA:HB2	2.56	0.41
1:B:23:ALA:HA	1:B:48:LYS:HD2	2.03	0.41
1:B:292:ASN:HD22	1:B:292:ASN:N	2.19	0.41
1:A:454:PHE:HZ	1:A:572:VAL:CG1	2.32	0.41
1:B:385:TYR:CD2	1:B:406:ALA:HB2	2.55	0.41
1:A:454:PHE:CZ	1:A:572:VAL:HG13	2.55	0.41
1:B:26:GLN:NE2	1:B:52:LYS:O	2.54	0.41
1:A:454:PHE:HZ	1:A:572:VAL:HG12	1.85	0.41
1:A:293:TYR:CD2	1:A:293:TYR:C	2.99	0.41
1:B:396:LYS:HE2	4:B:2290:HOH:O	2.21	0.40
1:A:129:TYR:O	1:A:368:GLY:HA2	2.22	0.40
1:A:406:ALA:O	1:A:410:ILE:HD12	2.20	0.40
1:B:356:TYR:HB3	1:B:399:THR:HG21	2.04	0.40
1:A:22:PRO:HB2	1:A:25:TYR:HB3	2.02	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	624/716 (87%)	605 (97%)	19 (3%)	0	100	100
1	B	631/716 (88%)	610 (97%)	21 (3%)	0	100	100
All	All	1255/1432 (88%)	1215 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	562/630 (89%)	556 (99%)	6 (1%)	65	64
1	B	566/630 (90%)	560 (99%)	6 (1%)	65	64
All	All	1128/1260 (90%)	1116 (99%)	12 (1%)	65	64

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

Mol	Chain	Res	Type
1	A	45	LEU
1	A	87	GLU
1	A	272	ILE
1	A	337	TRP
1	A	371	THR
1	A	642	GLU
1	B	112	LYS
1	B	292	ASN

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Mol	Chain	Res	Type
1	B	371	THR
1	B	496	THR
1	B	615	LEU
1	B	617	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	144	GLN
1	A	189	GLN
1	A	292	ASN
1	A	349	HIS
1	A	537	GLN
1	A	543	GLN
1	A	593	HIS
1	B	15	GLN
1	B	26	GLN
1	B	28	ASN
1	B	73	GLN
1	B	105	GLN
1	B	187	GLN
1	B	274	GLN
1	B	290	ASN
1	B	292	ASN
1	B	349	HIS
1	B	401	GLN
1	B	444	GLN
1	B	459	ASN
1	B	537	GLN
1	B	543	GLN
1	B	593	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	LOG	A	1000	-	13,16,16	1.11	1 (7%)	14,22,22	1.39	3 (21%)
3	GOL	B	1716	-	5,5,5	0.24	0	5,5,5	0.56	0
3	GOL	B	1717	-	5,5,5	0.66	0	5,5,5	1.09	0
3	GOL	A	1716	-	5,5,5	0.37	0	5,5,5	0.79	0
3	GOL	B	1718	-	5,5,5	0.40	0	5,5,5	0.64	0
2	LOG	B	1000	-	13,16,16	1.09	0	14,22,22	1.77	4 (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
2	LOG	A	1000	-	-	1/6/28/28	0/1/1/1
3	GOL	B	1716	-	-	2/4/4/4	-
3	GOL	B	1717	-	-	3/4/4/4	-
3	GOL	A	1716	-	-	4/4/4/4	-
3	GOL	B	1718	-	-	0/4/4/4	-
2	LOG	B	1000	-	-	1/6/28/28	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	LOG	C2-N2	2.05	1.50	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	LOG	C2-N2-C7	-3.54	115.75	121.82
2	A	1000	LOG	O5-C1-C2	3.13	126.87	118.37
2	B	1000	LOG	O5-C1-C2	2.85	126.12	118.37
2	B	1000	LOG	O3-C3-C2	-2.63	103.65	108.98
2	A	1000	LOG	C3-C2-N2	2.10	115.64	112.26
2	A	1000	LOG	C2-N2-C7	-2.01	118.37	121.82
2	B	1000	LOG	C8-C7-N2	-2.01	112.79	116.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1716	GOL	O1-C1-C2-C3
3	B	1717	GOL	O1-C1-C2-C3
3	B	1717	GOL	O1-C1-C2-O2
3	A	1716	GOL	C1-C2-C3-O3
3	B	1716	GOL	C1-C2-C3-O3
3	B	1717	GOL	C1-C2-C3-O3
3	B	1716	GOL	O2-C2-C3-O3
3	A	1716	GOL	O2-C2-C3-O3
2	A	1000	LOG	C1-C2-N2-C7
2	B	1000	LOG	C1-C2-N2-C7
3	A	1716	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1716	GOL	2	0
3	B	1717	GOL	1	0
2	B	1000	LOG	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	635/716 (88%)	0.11	35 (5%)	30 36	13, 27, 66, 86	3 (0%)
1	B	641/716 (89%)	-0.07	17 (2%)	56 62	12, 24, 57, 89	2 (0%)
All	All	1276/1432 (89%)	0.02	52 (4%)	41 48	12, 25, 62, 89	5 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	PHE	4.7
1	A	605	LEU	4.2
1	B	680	LEU	4.2
1	A	618	PRO	4.1
1	A	454	PHE	4.0
1	A	682	ALA	3.9
1	B	605	LEU	3.9
1	A	709	PHE	3.8
1	B	648	PHE	3.5
1	B	286	TRP	3.4
1	A	646	ILE	3.3
1	A	17	LYS	3.3
1	A	638	ILE	3.3
1	A	683	GLY	3.3
1	A	540[A]	TYR	3.2
1	A	691	PHE	3.1
1	A	453	ALA	3.1
1	B	454	PHE	3.1
1	A	616	ILE	3.0
1	A	647	ASN	3.0
1	B	709	PHE	2.9
1	B	453	ALA	2.8
1	B	618	PRO	2.8
1	B	694	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	18	THR	2.7
1	B	693	ARG	2.7
1	A	23	ALA	2.6
1	B	16	ASN	2.6
1	B	457	GLY	2.4
1	A	640	PRO	2.3
1	B	594	LYS	2.3
1	A	14	VAL	2.3
1	A	632	GLU	2.3
1	A	684	LEU	2.3
1	B	23	ALA	2.3
1	B	646	ILE	2.3
1	A	637	ALA	2.3
1	A	19	ILE	2.3
1	A	614	VAL	2.3
1	B	632	GLU	2.2
1	B	292	ASN	2.2
1	A	594	LYS	2.2
1	A	687	ALA	2.2
1	A	689	VAL	2.2
1	A	114	GLY	2.1
1	A	644	ILE	2.1
1	A	243	ASP	2.1
1	A	693	ARG	2.1
1	A	519	ARG	2.1
1	A	692	VAL	2.1
1	A	611	ALA	2.0
1	A	448	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
3	GOL	B	1717	6/6	0.91	0.11	31,32,34,37	0
3	GOL	A	1716	6/6	0.92	0.14	27,32,33,34	0
2	LOG	A	1000	16/16	0.94	0.07	14,17,21,32	1
3	GOL	B	1716	6/6	0.94	0.12	25,27,32,33	0
2	LOG	B	1000	16/16	0.94	0.07	14,17,21,32	1
3	GOL	B	1718	6/6	0.94	0.10	27,33,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.