



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:06 AM UTC

PDB ID : 2XJ7 / pdb_00002xj7
Title : BtGH84 in complex with 6-acetamido-6-deoxy-castanospermine
Authors : He, Y.; Davies, G.J.
Deposited on : 2010-07-02
Resolution : 2.00 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

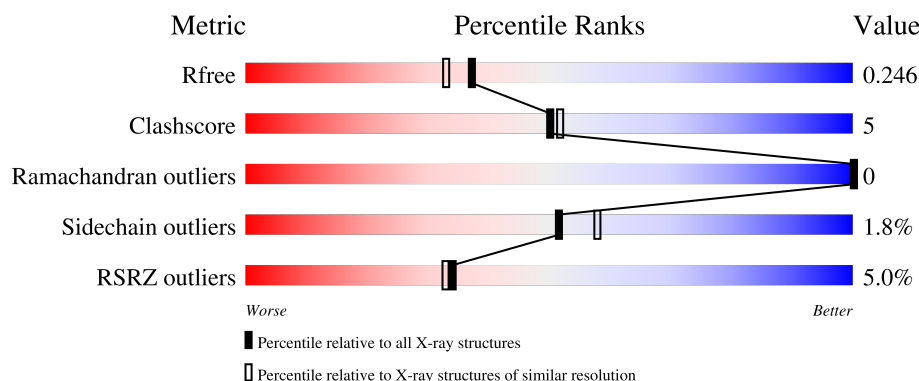
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	4% 74% 14% • 11%
1	B	716	5% 77% 11% • 12%

2 Entry composition [i](#)

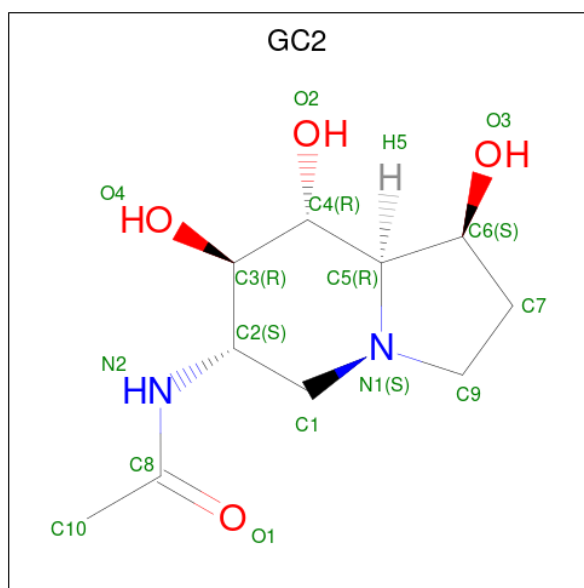
There are 4 unique types of molecules in this entry. The entry contains 10749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	639	Total	C	N	O	S	0	2	0
			5184	3323	870	972	19			
1	B	633	Total	C	N	O	S	0	1	0
			5139	3296	865	960	18			

- Molecule 2 is 6-ACETAMIDO-6-DEOXY-CASTANOSPERMINE (CCD ID: GC2) (formula: $C_{10}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	10	2	4		
2	B	1	Total	C	N	O	0	0
			16	10	2	4		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total 190	O 190	0	0
4	B	202	Total 202	O 202	0	0

GLN	K686	A687	P688	V689	K690	F691	F692	ARG	PHE	THR	ASN	VAL	SER	ASP	GLU	GLU	GLN	GLN	VAL	TYR	LEU	ARG	ARG	GLN	F709	V710	L711	K715	LYS
-----	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.49Å 93.98Å 98.81Å 104.13° 93.88° 103.13°	Depositor
Resolution (Å)	47.50 – 2.00 47.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.50-2.00) 97.6 (47.50-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.239 0.209 , 0.246	Depositor DCC
R_{free} test set	5654 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10749	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: GC2, CA

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	0.99	5/5318 (0.1%)	1.01	11/7205 (0.2%)
1	B	1.02	5/5268 (0.1%)	1.01	7/7132 (0.1%)
All	All	1.01	10/10586 (0.1%)	1.01	18/14337 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ALA	CA-CB	6.50	1.63	1.53
1	A	125	PRO	CA-C	-6.24	1.45	1.52
1	B	236	SER	N-CA	5.68	1.53	1.45
1	A	41	LEU	N-CA	-5.55	1.39	1.46
1	B	133	VAL	CA-CB	5.54	1.60	1.54
1	B	489	LYS	C-O	-5.39	1.19	1.24
1	B	149	GLN	N-CA	-5.35	1.39	1.46
1	A	376	HIS	CA-CB	5.33	1.59	1.52
1	A	315	ILE	CA-CB	5.29	1.61	1.54
1	B	203	VAL	N-CA	-5.00	1.40	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	PHE	N-CA-C	7.19	119.80	111.02
1	A	149	GLN	N-CA-C	6.36	118.22	111.28
1	B	380	SER	N-CA-C	-6.19	105.69	113.18
1	A	467	THR	N-CA-C	-6.15	104.49	111.07
1	A	291	GLY	N-CA-C	-6.05	103.34	112.89
1	B	499	VAL	N-CA-C	5.92	116.10	110.42
1	A	62	LYS	CA-C-N	-5.83	114.16	123.31
1	A	62	LYS	C-N-CA	-5.83	114.16	123.31
1	B	336	ILE	N-CA-C	5.71	116.44	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	ILE	N-CA-C	5.66	115.85	110.42
1	A	432	GLY	N-CA-C	-5.50	107.50	114.16
1	B	296	THR	N-CA-C	-5.28	105.64	111.71
1	A	209	GLY	N-CA-C	5.24	120.11	113.24
1	B	455	LYS	N-CA-C	-5.15	104.93	111.11
1	A	611	ALA	CB-CA-C	-5.12	110.65	116.54
1	B	561	ILE	N-CA-C	5.10	115.31	110.42
1	A	683	GLY	N-CA-C	-5.07	104.64	111.54
1	A	690	LYS	N-CA-C	-5.02	107.22	113.55

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	5184	0	5089	61	0
1	B	5139	0	5057	50	0
2	A	16	0	18	0	0
2	B	16	0	18	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	190	0	0	0	0
4	B	202	0	0	3	0
All	All	10749	0	10182	109	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 (109) 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:41:LEU:HB2	1:A:104:LEU:HD21	1.30	1.07
1:A:41:LEU:HB2	1:A:104:LEU:CD2	1.99	0.91
1:B:41:LEU:HB2	1:B:104:LEU:HD21	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:HE2	1:A:90:ILE:HG13	1.57	0.84
1:B:451:LEU:HG	1:B:455:LYS:HE2	1.67	0.75
1:A:19:ILE:CD1	1:A:118:GLU:HG2	2.19	0.71
1:A:19:ILE:HD11	1:A:118:GLU:HG2	1.72	0.70
1:B:462:LYS:HG2	1:B:466:GLU:OE2	1.93	0.68
1:B:593:HIS:HD2	1:B:636:ASP:H	1.43	0.67
1:B:454:PHE:HZ	1:B:516:VAL:HG13	1.64	0.62
1:A:643:ASN:HB2	1:A:682:ALA:O	1.99	0.61
1:B:490:PRO:O	1:B:494:GLU:HG3	1.99	0.61
1:A:283:ASN:HD21	1:A:286:TRP:CG	2.19	0.60
1:A:444:GLN:NE2	1:A:448:GLU:OE2	2.31	0.60
1:A:81:TYR:CE2	1:A:123:ASP:HB3	2.37	0.59
1:A:15:GLN:HB2	1:A:118:GLU:HB2	1.85	0.58
1:A:34:ASN:O	1:A:38:VAL:HG23	2.03	0.58
1:B:362:ILE:HD12	1:B:366:MET:HE3	1.85	0.58
1:A:37:ALA:O	1:A:104:LEU:HD22	2.04	0.57
1:B:462:LYS:CG	1:B:466:GLU:OE2	2.52	0.57
1:B:616:ILE:HD11	1:B:633:ILE:HD11	1.87	0.57
1:A:19:ILE:HD11	1:A:118:GLU:CG	2.34	0.57
1:A:308:MET:HA	1:A:335:TYR:O	2.05	0.56
1:A:593:HIS:HD2	1:A:636:ASP:H	1.55	0.54
1:B:238:ALA:HA	1:B:276:VAL:O	2.07	0.54
1:B:543:GLN:NE2	1:B:609:VAL:HG12	2.22	0.54
1:B:454:PHE:CZ	1:B:516:VAL:HG13	2.43	0.53
1:A:385:TYR:CD2	1:A:406:ALA:HB2	2.43	0.53
1:A:423[B]:MET:SD	1:A:442[B]:ASP:OD2	2.66	0.53
1:B:451:LEU:HG	1:B:455:LYS:CE	2.38	0.53
1:B:308:MET:HA	1:B:335:TYR:O	2.10	0.52
1:A:451:LEU:HG	1:A:564:LEU:HD12	1.92	0.52
1:A:489:LYS:HB2	1:A:490:PRO:HD3	1.92	0.52
1:A:164:GLY:N	1:A:165:PRO:HD3	2.25	0.52
1:B:536:GLN:HG3	1:B:590:TYR:CD1	2.44	0.52
1:A:19:ILE:CD1	1:A:118:GLU:CG	2.88	0.52
1:A:188:LEU:HD13	1:A:229:MET:HE1	1.91	0.51
1:A:562:LYS:HB3	1:A:563:PRO:HD3	1.93	0.51
1:B:37:ALA:O	1:B:104:LEU:HD22	2.10	0.50
1:B:133:VAL:O	1:B:133:VAL:HG13	2.11	0.50
1:B:536:GLN:CG	1:B:590:TYR:CD1	2.94	0.50
1:A:568:THR:O	1:A:572:VAL:HG22	2.13	0.48
1:A:153:TYR:O	1:A:154:GLY:C	2.55	0.48
1:B:254:GLN:O	1:B:258:LEU:HD23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:GLU:O	1:B:477:GLU:HG3	2.13	0.48
1:A:26:GLN:HG2	1:A:56:LEU:HD12	1.96	0.47
1:B:97:GLU:HG3	4:B:2020:HOH:O	2.13	0.47
1:B:341:PRO:O	1:B:342:VAL:C	2.57	0.47
1:A:26:GLN:HE21	1:A:56:LEU:HD13	1.79	0.47
1:A:474:ARG:HA	1:A:474:ARG:HD2	1.70	0.47
1:B:454:PHE:O	1:B:455:LYS:C	2.57	0.47
1:A:64:ASP:O	1:A:65:LYS:C	2.58	0.47
1:B:444:GLN:NE2	1:B:448:GLU:OE2	2.48	0.47
1:B:170:TYR:HB2	1:B:180:TYR:CE1	2.50	0.47
1:B:239:VAL:HG12	1:B:241:PHE:CE2	2.50	0.47
1:B:288:ASN:C	1:B:288:ASN:OD1	2.57	0.47
1:A:616:ILE:HG13	1:A:709:PHE:HB3	1.97	0.46
1:A:644:ILE:O	1:A:681:SER:HA	2.16	0.46
1:A:324:SER:O	1:A:328:GLU:HG2	2.16	0.46
1:B:315:ILE:HD11	2:B:1000:GC2:C7	2.46	0.45
1:A:301:LEU:HD12	1:A:307:ILE:HD11	1.98	0.45
1:A:262:ASP:O	1:A:267:GLN:HG2	2.15	0.45
1:B:423:MET:HE3	1:B:423:MET:HB3	1.73	0.45
1:B:314:VAL:HG23	4:B:2112:HOH:O	2.16	0.44
1:A:484:MET:HB3	1:B:536:GLN:NE2	2.32	0.44
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.99	0.44
1:A:26:GLN:NE2	1:A:56:LEU:HD13	2.33	0.44
1:B:129:TYR:O	1:B:368:GLY:HA2	2.18	0.44
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.99	0.44
1:A:26:GLN:HE21	1:A:56:LEU:CD1	2.30	0.43
1:B:261:ILE:O	1:B:265:PHE:HB3	2.18	0.43
1:B:250:ASN:O	1:B:254:GLN:HG3	2.19	0.43
1:B:56:LEU:HD23	1:B:89:GLU:OE1	2.18	0.43
1:B:610:LYS:O	1:B:611:ALA:C	2.61	0.43
1:B:595:MET:HE1	1:B:605:LEU:HB3	2.01	0.43
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.53	0.43
1:A:461:ASP:O	1:A:463:ALA:N	2.51	0.43
1:B:385:TYR:CD2	1:B:406:ALA:HB2	2.54	0.43
1:A:271:ASP:OD1	1:A:271:ASP:N	2.51	0.43
1:A:323:ILE:HG13	1:A:323:ILE:O	2.18	0.43
1:B:609:VAL:O	1:B:610:LYS:HD3	2.19	0.43
1:A:646:ILE:O	1:A:680:LEU:HB2	2.19	0.43
1:A:187:GLN:O	1:A:190:GLU:HB3	2.19	0.42
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.53	0.42
1:A:133:VAL:HG13	1:A:133:VAL:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:VAL:HG22	1:A:572:VAL:HG11	2.01	0.42
1:A:532:LYS:HA	1:A:532:LYS:HD2	1.95	0.42
1:A:453:ALA:HB1	1:A:459:ASN:O	2.20	0.41
1:A:461:ASP:O	1:A:462:LYS:C	2.63	0.41
1:B:170:TYR:CZ	1:B:181:PRO:HD3	2.55	0.41
1:A:26:GLN:HB2	1:A:51:SER:O	2.20	0.41
1:A:484:MET:HE3	1:B:537:GLN:HG2	2.02	0.41
1:B:143:HIS:NE2	1:B:190:GLU:OE1	2.40	0.41
1:B:451:LEU:HA	1:B:451:LEU:HD12	1.85	0.41
1:A:55:MET:CE	1:A:90:ILE:HG13	2.40	0.41
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.55	0.41
1:A:341:PRO:O	1:A:342:VAL:C	2.64	0.41
1:A:606:PRO:HG2	1:A:617:SER:HB2	2.03	0.41
1:B:174:PRO:HD2	4:B:2062:HOH:O	2.21	0.41
1:B:293:TYR:CD2	1:B:293:TYR:C	2.99	0.41
1:B:443:ILE:C	1:B:443:ILE:HD12	2.45	0.41
1:A:451:LEU:HG	1:A:564:LEU:CD1	2.50	0.41
1:A:126:SER:HB2	1:A:394:PRO:HD2	2.03	0.40
1:A:288:ASN:HA	1:A:289:PRO:HD2	1.94	0.40
1:A:461:ASP:C	1:A:463:ALA:N	2.77	0.40
1:B:21:LEU:HD12	1:B:22:PRO:HD2	2.04	0.40
1:B:22:PRO:HB2	1:B:25:TYR:HB3	2.02	0.40
1:A:14:VAL:HG22	1:A:15:GLN:O	2.22	0.40
1:A:131:GLY:HA3	1:A:160:THR:O	2.22	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	627/716 (88%)	602 (96%)	25 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	618/716 (86%)	593 (96%)	25 (4%)	0	100	100
All	All	1245/1432 (87%)	1195 (96%)	50 (4%)	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%)	550 (98%)	12 (2%)	47	52
1	B	557/630 (88%)	549 (99%)	8 (1%)	59	66
All	All	1119/1260 (89%)	1099 (98%)	20 (2%)	51	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	26	GLN
1	A	39	LYS
1	A	46	SER
1	A	151	LYS
1	A	371	THR
1	A	461	ASP
1	A	519	ARG
1	A	613	ARG
1	A	615	LEU
1	A	616	ILE
1	A	689	VAL
1	B	14	VAL
1	B	24	VAL
1	B	104	LEU
1	B	423	MET
1	B	452	LYS
1	B	454	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	615	LEU
1	B	715	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	73	GLN
1	A	187	GLN
1	A	267	GLN
1	A	306	GLN
1	A	339	ASN
1	A	372	ASN
1	A	433	HIS
1	A	593	HIS
1	B	10	GLN
1	B	26	GLN
1	B	28	ASN
1	B	349	HIS
1	B	372	ASN
1	B	469	GLN
1	B	536	GLN
1	B	543	GLN
1	B	547	GLN
1	B	578	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GC2	B	1000	-	16,17,17	0.96	0	18,25,25	2.10	6 (33%)
2	GC2	A	1000	-	16,17,17	0.90	0	18,25,25	1.55	2 (11%)

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	GC2	B	1000	-	-	1/4/33/33	1/2/2/2
2	GC2	A	1000	-	-	2/4/33/33	1/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	GC2	C2-N2-C8	5.98	130.92	122.90
2	A	1000	GC2	C1-C2-N2	4.61	116.37	109.71
2	A	1000	GC2	C2-N2-C8	3.74	127.91	122.90
2	B	1000	GC2	C10-C8-N2	2.71	120.62	116.12
2	B	1000	GC2	O4-C3-C2	-2.69	103.81	109.40
2	B	1000	GC2	O3-C6-C7	-2.52	105.52	111.43
2	B	1000	GC2	C1-C2-N2	2.50	113.32	109.71
2	B	1000	GC2	O1-C8-C10	-2.06	118.38	122.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	GC2	C1-C2-N2-C8
2	B	1000	GC2	C1-C2-N2-C8
2	A	1000	GC2	C3-C2-N2-C8

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	GC2	C1-C2-C3-C4-C5-N1
2	B	1000	GC2	C1-C2-C3-C4-C5-N1

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	GC2	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	639/716 (89%)	0.40	29 (4%) 38 37	24, 38, 75, 94	2 (0%)
1	B	633/716 (88%)	0.39	35 (5%) 30 29	20, 40, 81, 101	1 (0%)
All	All	1272/1432 (88%)	0.39	64 (5%) 34 33	20, 39, 79, 101	3 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	605	LEU	7.4
1	A	631	VAL	7.3
1	A	457	GLY	4.9
1	A	680	LEU	4.7
1	B	641	GLY	4.7
1	A	459	ASN	4.5
1	A	606	PRO	4.5
1	B	683	GLY	4.1
1	B	684	LEU	4.0
1	B	617	SER	4.0
1	B	691	PHE	3.9
1	A	646	ILE	3.9
1	B	709	PHE	3.9
1	B	614	VAL	3.8
1	A	53	LYS	3.6
1	B	687	ALA	3.6
1	A	715	LYS	3.5
1	A	454	PHE	3.4
1	B	454	PHE	3.3
1	A	709	PHE	3.2
1	B	688	PRO	3.1
1	A	453	ALA	3.1
1	B	23	ALA	3.1
1	B	638	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	595	MET	3.0
1	A	23	ALA	3.0
1	B	616	ILE	2.9
1	B	644	ILE	2.9
1	B	643	ASN	2.8
1	B	692	VAL	2.7
1	B	686	LYS	2.7
1	B	690	LYS	2.7
1	B	637	ALA	2.6
1	A	451	LEU	2.6
1	B	689	VAL	2.6
1	A	687	ALA	2.6
1	B	640	PRO	2.6
1	B	711	LEU	2.6
1	B	645	GLN	2.6
1	A	455	LYS	2.6
1	B	587	THR	2.5
1	A	691	PHE	2.5
1	A	689	VAL	2.4
1	A	710	VAL	2.4
1	B	19	ILE	2.4
1	A	289	PRO	2.4
1	A	618	PRO	2.4
1	B	21	LEU	2.4
1	B	533	ALA	2.3
1	B	4	SER	2.3
1	B	54	GLY	2.3
1	B	470	TYR	2.3
1	A	52	LYS	2.3
1	A	63	GLY	2.3
1	A	452	LYS	2.2
1	A	712	THR	2.2
1	A	441	MET	2.2
1	B	710	VAL	2.2
1	A	683	GLY	2.1
1	B	32	GLU	2.1
1	A	682	ALA	2.1
1	B	453	ALA	2.1
1	A	633	ILE	2.1
1	B	609	VAL	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	GC2	A	1000	16/16	0.93	0.09	26,28,31,33	0
2	GC2	B	1000	16/16	0.93	0.08	26,29,32,32	0
3	CA	A	1716	1/1	0.94	0.12	54,54,54,54	0
3	CA	B	1716	1/1	0.97	0.18	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.