



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:33 AM GMT

PDB ID : 2XJ7
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

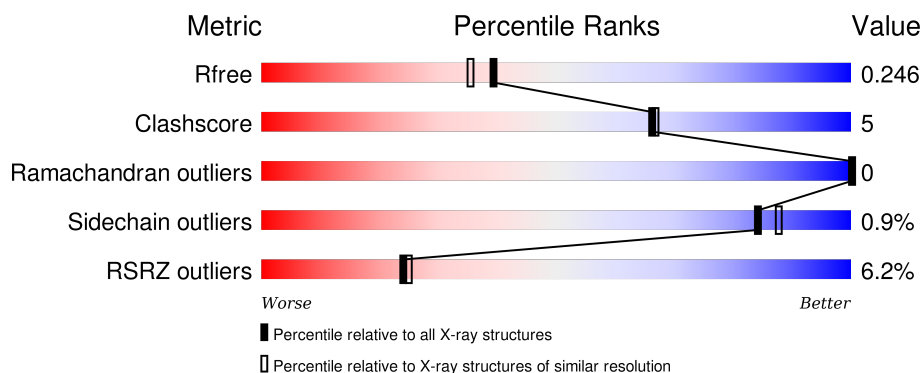
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

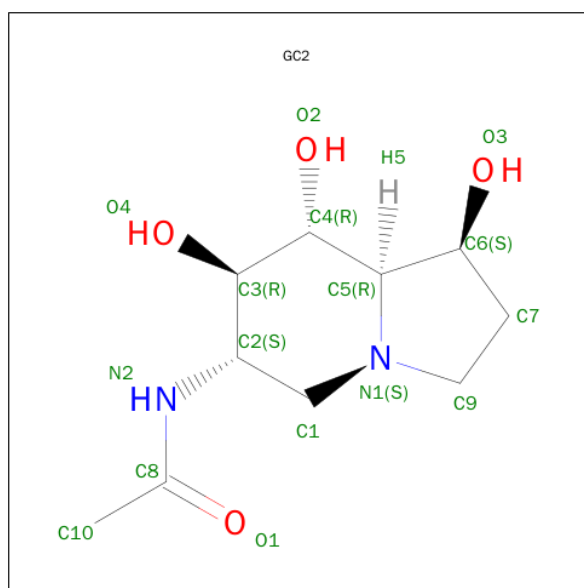
Mol	Chain	Length	Quality of chain
1	A	716	<div> <div>4%</div> <div>77%</div> <div>11%</div> <div>11%</div> </div>
1	B	716	<div> <div>7%</div> <div>79%</div> <div>9%</div> <div>12%</div> </div>

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 (three-letter code: GC2) (formula: $C_{10}H_{18}N_2O_4$).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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:

Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.15). The x-axis lists amino acids. A bar chart at the top shows the percentage of each amino acid: 4% (red), 77% (green), 11% (yellow), and 11% (grey). Red dots indicate positions with high conservation (bits > 0.05).

Position	Amino Acid	Information Content (bits)
1	ALA	0.02
2	GLY	0.02
3	ASN	0.02
4	VAL	0.02
5	ASN	0.02
6	VAL	0.02
7	ASP	0.02
8	GLU	0.02
9	GLU	0.02
10	GLN	0.02
11	GLN	0.02
12	VAL	0.02
13	TYR	0.02
14	LEU	0.02
15	ARG	0.02
16	F709	0.02
17	L711	0.02
18	T712	0.02
19	K715	0.02
20	LYS	0.02
21	ALA	0.02
22	GLY	0.02
23	ASN	0.02
24	VAL	0.02
25	SER	0.02
26	ASP	0.02
27	GLY	0.02
28	LYS	0.02
29	GLU	0.02
30	TRP	0.02
31	ALA	0.02
32	GLY	0.02
33	ASN	0.02
34	VAL	0.02
35	ASP	0.02
36	GLU	0.02
37	LEU	0.02
38	LYS	0.02
39	GLN	0.02
40	GLU	0.02
41	LEU	0.02
42	SER	0.02
43	ARG	0.02
44	L680	0.02
45	S681	0.02
46	A682	0.02
47	G683	0.02
48	L684	0.02
49	A687	0.02
50	F688	0.02
51	F691	0.02
52	V692	0.02
53	ARG	0.02
54	THR	0.02
55	ALA	0.02
56	TRP	0.02
57	LYS	0.02
58	VAL	0.02
59	GLU	0.02
60	VAL	0.02
61	ASN	0.02
62	ALA	0.02
63	K452	0.02
64	L451	0.02
65	E448	0.02
66	Q444	0.02
67	I443	0.02
68	D442	0.02
69	M423	0.02
70	LYS	0.02
71	ILE	0.02
72	GLN	0.02
73	GLU	0.02
74	GLN	0.02
75	VAL	0.02
76	ASN	0.02
77	SER	0.02
78	ILE	0.02
79	N595	0.02
80	K594	0.02
81	H581	0.02
82	THR	0.02
83	SER	0.02
84	ILE	0.02
85	LEU	0.02
86	LEU	0.02
87	ARG	0.02
88	GLY	0.02
89	ASP	0.02
90	THR	0.02
91	E532	0.02
92	S324	0.02
93	I323	0.02
94	M308	0.02
95	I307	0.02
96	L301	0.02
97	K39	0.02
98	V38	0.02
99	A37	0.02
100	N34	0.02
101	Q26	0.02
102	Y25	0.02
103	V24	0.02
104	D262	0.02
105	D242	0.02
106	E190	0.02
107	Q187	0.02
108	V14	0.02
109	M16	0.02
110	I19	0.02
111	D20	0.02
112	L21	0.02
113	Q165	0.02
114	G164	0.02
115	T160	0.02
116	K166	0.02
117	VAL	0.02
118	ASN	0.02
119	GLN	0.02
120	GLU	0.02
121	ASP	0.02
122	ASP	0.02
123	ASP	0.02
124	ASP	0.02
125	ASP	0.02
126	ASP	0.02
127	ASP	0.02
128	ASP	0.02
129	ASP	0.02
130	ASP	0.02
131	ASP	0.02
132	ASP	0.02
133	ASP	0.02
134	ASP	0.02
135	ASP	0.02
136	ASP	0.02
137	ASP	0.02
138	ASP	0.02
139	ASP	0.02
140	ASP	0.02
141	ASP	0.02
142	ASP	0.02
143	ASP	0.02
144	ASP	0.02
145	ASP	0.02
146	ASP	0.02
147	ASP	0.02
148	ASP	0.02
149	ASP	0.02

[illegible]

[illegible]

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) 88.8 (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	5649 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 114487 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, GC2

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	0.84	1/5318 (0.0%)	0.73	0/7205
1	B	0.85	1/5268 (0.0%)	0.73	0/7132
All	All	0.85	2/10586 (0.0%)	0.73	0/14337

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	GLU	CD-OE2	7.91	1.34	1.25
1	A	145	ALA	CA-CB	5.24	1.63	1.52

There are no bond angle outliers.

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	56	0
1	B	5139	0	5057	46	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	202	0	0	4	0
All	All	10749	0	10182	101	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 (101) 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
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: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: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:543:GLN:NE2	1:B:609:VAL:HG12	2.22	0.54
1:B:238:ALA:HA	1:B:276:VAL:O	2.07	0.54
1:A:55:MET:HE2	1:A:90:ILE:HG13	1.90	0.54
1:B:454:PHE:CZ	1:B:516:VAL:HG13	2.43	0.53
1:A:423[B]:MET:SD	1:A:442[B]:ASP:OD2	2.66	0.53
1:A:385:TYR:CD2	1:A:406:ALA:HB2	2.43	0.53
1:B:451:LEU:HG	1:B:455:LYS:CE	2.38	0.53
1:A:55:MET:CE	1:A:90:ILE:HG13	2.40	0.52
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLY:N	1:A:165:PRO:HD3	2.25	0.52
1:B:715:LYS:NZ	4:B:2202:HOH:O	2.42	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: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:HG13	1:B:133:VAL:O	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:B:254:GLN:O	1:B:258:LEU:HD23	2.13	0.48
1:B:473:GLU:O	1:B:477:GLU:HG3	2.13	0.48
1:B:97:GLU:HG3	4:B:2020:HOH:O	2.13	0.47
1:A:26:GLN:HG2	1:A:56:LEU:HD12	1.96	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: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: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:A:153:TYR:O	1:A:154:GLY:C	2.55	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: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:B:609:VAL:O	1:B:610:LYS:HD3	2.19	0.43
1:A:323:ILE:HG13	1:A:323:ILE:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:OD1	1:A:271:ASP:N	2.51	0.43
1:B:341:PRO:O	1:B:342:VAL:C	2.57	0.43
1:A:646:ILE:O	1:A:680:LEU:HB2	2.19	0.43
1:B:454:PHE:O	1:B:455:LYS:C	2.57	0.42
1:A:187:GLN:O	1:A:190:GLU:HB3	2.19	0.42
1:A:64:ASP:O	1:A:65:LYS:C	2.58	0.42
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.53	0.42
1:B:288:ASN:C	1:B:288:ASN:OD1	2.57	0.42
1:A:516:VAL:HG22	1:A:572:VAL:HG11	2.01	0.42
1:A:133:VAL:HG13	1:A:133:VAL:O	2.20	0.42
1:A:532:LYS:HD2	1:A:532:LYS:HA	1.95	0.42
1:B:170:TYR:CZ	1:B:181:PRO:HD3	2.55	0.41
1:A:453:ALA:HB1	1:A:459:ASN:O	2.20	0.41
1:B:451:LEU:HA	1:B:451:LEU:HD12	1.85	0.41
1:A:26:GLN:HB2	1:A:51:SER:O	2.20	0.41
1:B:143:HIS:NE2	1:B:190:GLU:OE1	2.40	0.41
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.55	0.41
1:B:174:PRO:HD2	4:B:2062:HOH:O	2.21	0.41
1:A:606:PRO:HG2	1:A:617:SER:HB2	2.03	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:B:282:TYR:OH	1:B:286:TRP:CZ3	2.72	0.40
1:B:22:PRO:HB2	1:B:25:TYR:HB3	2.02	0.40
1:B:21:LEU:HD12	1:B:22:PRO:HD2	2.04	0.40
1:A:14:VAL:HG22	1:A:15:GLN:O	2.22	0.40
1:A:166:LYS:NZ	1:A:242:ASP:OD2	2.52	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
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%)	556 (99%)	6 (1%)	80	83
1	B	557/630 (88%)	553 (99%)	4 (1%)	88	91
All	All	1119/1260 (89%)	1109 (99%)	10 (1%)	84	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	39	LYS
1	A	371	THR
1	A	461	ASP
1	A	613	ARG
1	A	616	ILE
1	B	104	LEU
1	B	423	MET
1	B	454	PHE
1	B	615	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	HIS
1	A	433	HIS
1	A	547	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	593	HIS
1	B	10	GLN
1	B	26	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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	1000	-	17,17,17	1.01	1 (5%)	16,25,25	1.23	2 (12%)
2	GC2	B	1000	-	17,17,17	1.07	1 (5%)	16,25,25	2.11	5 (31%)

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	A	1000	-	-	0/4/33/33	1/2/2/2
2	GC2	B	1000	-	-	0/4/33/33	1/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	GC2	C1-C2	2.40	1.55	1.52
2	B	1000	GC2	C1-C2	2.65	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	GC2	O3-C6-C7	-2.71	105.52	111.71
2	B	1000	GC2	O4-C3-C2	-2.68	103.81	109.11
2	A	1000	GC2	C3-C2-N2	-2.27	105.12	110.56
2	B	1000	GC2	O1-C8-C10	-2.01	118.38	122.06
2	B	1000	GC2	C10-C8-N2	2.36	120.62	116.11
2	A	1000	GC2	C2-N2-C8	3.79	127.91	123.04
2	B	1000	GC2	C2-N2-C8	6.13	130.92	123.04

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.00	32 (5%) 32 34	25, 38, 75, 94	0
1	B	633/716 (88%)	0.09	47 (7%) 17 18	25, 40, 81, 101	0
All	All	1272/1432 (88%)	0.04	79 (6%) 24 25	25, 39, 79, 101	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	709	PHE	7.5
1	B	691	PHE	5.9
1	B	689	VAL	5.9
1	B	638	ILE	5.8
1	B	692	VAL	5.7
1	A	633	ILE	5.5
1	A	692	VAL	5.4
1	B	710	VAL	5.3
1	B	684	LEU	5.2
1	B	24	VAL	5.2
1	A	646	ILE	5.0
1	B	614	VAL	4.7
1	A	680	LEU	4.6
1	B	53	LYS	4.5
1	B	47	GLY	4.3
1	A	710	VAL	4.3
1	B	21	LEU	4.2
1	A	709	PHE	4.1
1	B	711	LEU	3.9
1	B	52	LYS	3.8
1	A	644	ILE	3.8
1	B	23	ALA	3.7
1	B	643	ASN	3.7
1	B	595	MET	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	691	PHE	3.6
1	B	644	ILE	3.6
1	A	455	LYS	3.6
1	B	51	SER	3.6
1	B	637	ALA	3.5
1	B	48	LYS	3.5
1	A	687	ALA	3.4
1	B	686	LYS	3.3
1	A	47	GLY	3.3
1	B	690	LYS	3.2
1	A	682	ALA	3.2
1	B	594	LYS	3.2
1	B	616	ILE	3.2
1	A	49	GLN	3.2
1	B	617	SER	3.1
1	B	49	GLN	3.0
1	A	688	PRO	3.0
1	B	633	ILE	3.0
1	A	631	VAL	2.9
1	B	688	PRO	2.9
1	A	52	LYS	2.9
1	A	459	ASN	2.9
1	B	16	ASN	2.8
1	A	452	LYS	2.8
1	B	641	GLY	2.8
1	B	45	LEU	2.8
1	B	640	PRO	2.7
1	A	684	LEU	2.7
1	B	54	GLY	2.7
1	B	683	GLY	2.7
1	B	451	LEU	2.6
1	B	713	ILE	2.6
1	B	687	ALA	2.6
1	A	681	SER	2.6
1	A	581	ASN	2.6
1	A	616	ILE	2.6
1	B	25	TYR	2.5
1	B	46	SER	2.4
1	B	455	LYS	2.4
1	A	24	VAL	2.4
1	A	712	THR	2.4
1	A	21	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	715	LYS	2.3
1	B	19	ILE	2.3
1	A	594	LYS	2.3
1	A	595	MET	2.3
1	B	22	PRO	2.3
1	B	50	SER	2.2
1	A	25	TYR	2.2
1	B	645	GLN	2.2
1	A	16	ASN	2.2
1	A	645	GLN	2.2
1	A	632	GLU	2.1
1	B	88	LYS	2.0
1	B	632	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	GC2	A	1000	16/16	0.94	0.10	0.63	26,28,31,33	0
2	GC2	B	1000	16/16	0.94	0.09	-0.29	26,29,32,32	0
3	CA	A	1716	1/1	0.85	0.08	-0.73	54,54,54,54	0
3	CA	B	1716	1/1	0.95	0.16	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.