Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:40 PM GMT

PDB ID	:	1BYH
Title	:	MOLECULAR AND ACTIVE-SITE STRUCTURE OF A BACILLUS (1-3,1 -4)-BETA-GLUCANASE
Authors	:	Keitel, T.; Heinemann, U.
Deposited on	:	1992-12-31
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

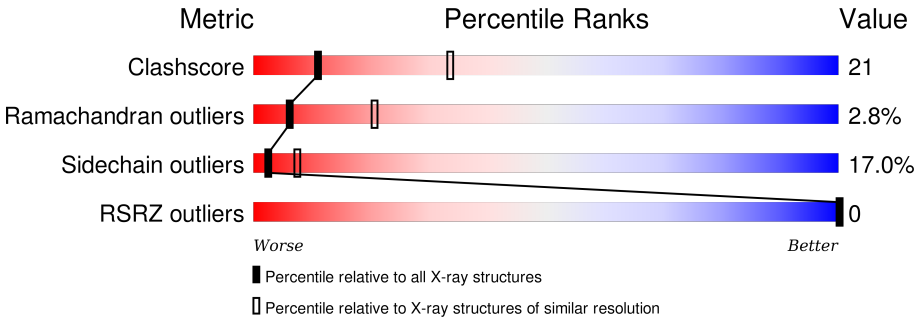
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	214	45% 36% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	218	-	-	-	X
4	NBU	A	215	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1797 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 HYBRID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1697	1090	273	329	5			

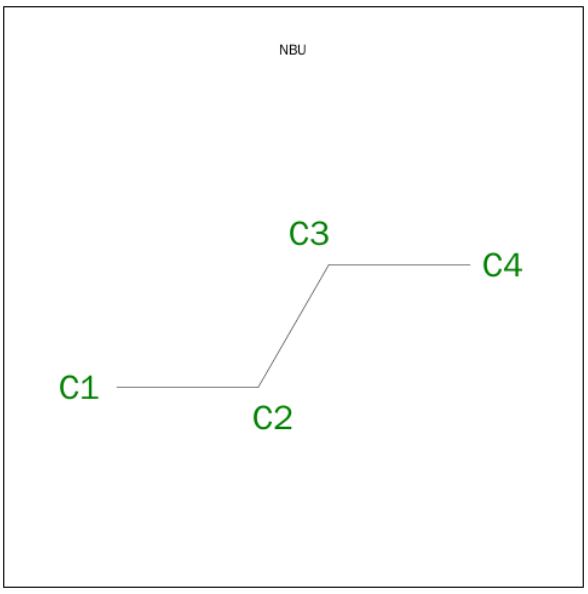
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			23	12	11		

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

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

- Molecule 4 is N-BUTANE (three-letter code: NBU) (formula: C_4H_{10}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 4 4	0	0

- Molecule 5 is water.

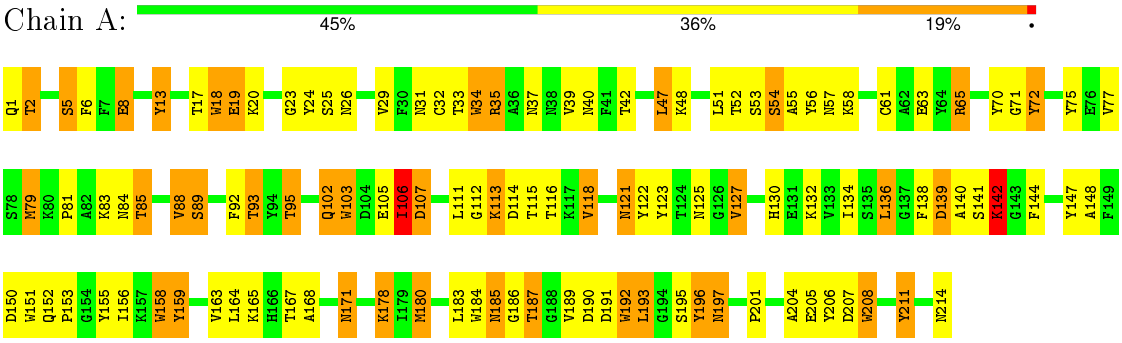
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	72	Total O 72 72	0	0

3 Residue-property plots (i)

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 (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: HYBRID

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.32Å 78.52Å 39.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 14.88 – 2.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 71.8 (14.88-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	14.87 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.168 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 80.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 4783 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	1797	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BGC, NBU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.25	6/1753 (0.3%)	2.13	69/2384 (2.9%)

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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLU	CD-OE2	17.24	1.44	1.25
1	A	106	ILE	CA-CB	6.62	1.70	1.54
1	A	103	TRP	CD1-NE1	-6.04	1.27	1.38
1	A	127	VAL	CA-CB	5.47	1.66	1.54
1	A	89	SER	CA-CB	-5.46	1.44	1.52
1	A	1	GLN	CA-CB	5.25	1.65	1.53

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	TYR	CB-CG-CD2	-13.15	113.11	121.00
1	A	34	TRP	CG-CD2-CE3	10.67	143.51	133.90
1	A	34	TRP	CB-CG-CD1	-9.98	114.03	127.00
1	A	13	TYR	CB-CG-CD2	-9.91	115.06	121.00
1	A	18	TRP	CD1-CG-CD2	9.37	113.80	106.30
1	A	158	TRP	CD1-CG-CD2	9.35	113.78	106.30
1	A	34	TRP	CE2-CD2-CG	-8.63	100.40	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	A	18	TRP	CE2-CD2-CG	-8.12	100.81	107.30
1	A	196	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	A	24	TYR	CB-CG-CD1	7.92	125.75	121.00
1	A	208	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	A	158	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	A	184	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	A	211	TYR	CB-CG-CD2	-7.64	116.42	121.00
1	A	35	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	105	GLU	OE1-CD-OE2	-7.43	114.38	123.30
1	A	70	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	A	184	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	151	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	A	118	VAL	CG1-CB-CG2	-7.37	99.11	110.90
1	A	65	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	208	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	95	THR	CA-CB-CG2	7.04	122.25	112.40
1	A	192	TRP	CD1-CG-CD2	7.03	111.92	106.30
1	A	79	MET	CA-CB-CG	6.84	124.93	113.30
1	A	151	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	A	122	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	A	208	TRP	CG-CD2-CE3	6.59	139.83	133.90
1	A	103	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	A	95	THR	CA-CB-OG1	-6.37	95.63	109.00
1	A	190	ASP	CA-C-N	-6.27	103.40	117.20
1	A	139	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	123	TYR	CB-CG-CD1	-6.25	117.25	121.00
1	A	142	LYS	CB-CG-CD	6.23	127.79	111.60
1	A	192	TRP	CE2-CD2-CG	-6.19	102.35	107.30
1	A	65	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	71	GLY	CA-C-O	6.16	131.68	120.60
1	A	103	TRP	CD1-CG-CD2	6.15	111.22	106.30
1	A	2	THR	N-CA-C	6.14	127.57	111.00
1	A	180	MET	CG-SD-CE	-6.05	90.52	100.20
1	A	102	GLN	CA-CB-CG	6.02	126.64	113.40
1	A	144	PHE	O-C-N	5.99	132.28	122.70
1	A	208	TRP	CB-CG-CD1	-5.99	119.22	127.00
1	A	106	ILE	O-C-N	-5.92	113.23	122.70
1	A	105	GLU	CA-CB-CG	5.92	126.42	113.40
1	A	72	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	19	GLU	CA-CB-CG	5.86	126.28	113.40
1	A	150	ASP	CB-CG-OD1	5.85	123.57	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	A	18	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	A	206	TYR	CB-CG-CD1	-5.69	117.58	121.00
1	A	88	VAL	CA-CB-CG2	-5.67	102.39	110.90
1	A	158	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	A	123	TYR	CD1-CG-CD2	5.58	124.03	117.90
1	A	70	TYR	CG-CD1-CE1	-5.54	116.87	121.30
1	A	47	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	207	ASP	CA-C-N	5.51	129.32	117.20
1	A	147	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	A	158	TRP	CB-CA-C	-5.42	99.56	110.40
1	A	72	TYR	N-CA-CB	-5.39	100.89	110.60
1	A	71	GLY	CA-C-N	-5.39	105.34	117.20
1	A	65	ARG	CA-CB-CG	5.31	125.08	113.40
1	A	122	TYR	CD1-CG-CD2	5.25	123.67	117.90
1	A	106	ILE	CG1-CB-CG2	-5.07	100.24	111.40
1	A	171	ASN	CA-CB-CG	5.05	124.51	113.40
1	A	103	TRP	CG-CD2-CE3	5.03	138.43	133.90
1	A	185	ASN	CB-CG-ND2	5.02	128.75	116.70
1	A	65	ARG	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	TYR	Sidechain
1	A	196	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1557	66	1
2	A	23	0	20	0	0
3	A	1	0	0	0	0
4	A	4	0	6	0	0
5	A	72	0	0	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1797	0	1583	66	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (66) 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:32:CYS:HB3	1:A:185:ASN:HD21	1.37	0.87
1:A:31:ASN:HB2	5:A:282:HOH:O	1.80	0.82
1:A:52:THR:HG22	1:A:201:PRO:HB3	1.63	0.81
1:A:197:ASN:H	1:A:197:ASN:HD22	1.36	0.73
1:A:187:THR:OG1	5:A:282:HOH:O	2.07	0.71
1:A:121:ASN:HD21	1:A:130:HIS:H	1.37	0.71
1:A:106:ILE:HD12	1:A:107:ASP:N	2.06	0.70
1:A:55:ALA:HB3	1:A:58:LYS:HD3	1.75	0.67
1:A:88:VAL:HG23	1:A:193:LEU:HD11	1.77	0.67
1:A:48:LYS:HG3	5:A:268:HOH:O	1.97	0.65
1:A:106:ILE:HD12	1:A:107:ASP:H	1.63	0.63
1:A:31:ASN:HB3	1:A:185:ASN:OD1	2.00	0.62
1:A:32:CYS:HB3	1:A:185:ASN:ND2	2.14	0.61
1:A:75:TYR:O	1:A:148:ALA:HA	2.02	0.59
1:A:197:ASN:H	1:A:197:ASN:ND2	1.99	0.58
1:A:51:LEU:O	1:A:201:PRO:HA	2.04	0.58
1:A:197:ASN:HD22	1:A:197:ASN:N	2.00	0.57
1:A:102:GLN:OE1	1:A:125:ASN:HB2	2.03	0.57
1:A:65:ARG:HH11	1:A:65:ARG:HB2	1.69	0.56
1:A:204:ALA:HB3	5:A:287:HOH:O	2.05	0.56
1:A:61:CYS:HB2	1:A:183:LEU:O	2.06	0.55
1:A:134:ILE:HD13	1:A:165:LYS:HG2	1.88	0.55
1:A:111:LEU:HD21	1:A:192:TRP:NE1	2.22	0.55
1:A:83:LYS:HG3	1:A:115:THR:OG1	2.07	0.55
1:A:88:VAL:CG2	1:A:193:LEU:HD11	2.37	0.53
1:A:136:LEU:HD13	1:A:138:PHE:CE1	2.44	0.53
1:A:65:ARG:HD3	1:A:180:MET:HE3	1.92	0.52
1:A:85:THR:HB	1:A:195:SER:O	2.11	0.51
1:A:106:ILE:HD13	1:A:158:TRP:CZ2	2.45	0.50
1:A:152:GLN:HE22	1:A:214:ASN:HD21	1.59	0.50
1:A:93:THR:HA	1:A:178:LYS:O	2.12	0.50
1:A:25:SER:HA	5:A:284:HOH:O	2.12	0.50
1:A:23:GLY:HA2	1:A:35:ARG:NH1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:HB3	1:A:58:LYS:HB3	1.95	0.49
1:A:63:GLU:OE1	5:A:264:HOH:O	2.19	0.49
1:A:92:PHE:HB3	1:A:107:ASP:HB3	1.95	0.48
1:A:17:THR:HB	1:A:18:TRP:CD1	2.49	0.47
1:A:18:TRP:HA	1:A:65:ARG:O	2.14	0.47
1:A:155:TYR:HA	1:A:168:ALA:O	2.14	0.47
1:A:29:VAL:O	1:A:186:GLY:HA2	2.15	0.47
1:A:65:ARG:HH11	1:A:65:ARG:CB	2.28	0.47
1:A:187:THR:N	5:A:282:HOH:O	2.48	0.47
1:A:72:TYR:CE2	1:A:153:PRO:HG3	2.50	0.46
1:A:113:LYS:HG2	1:A:193:LEU:O	2.17	0.44
1:A:42:THR:HG21	1:A:48:LYS:NZ	2.33	0.44
1:A:139:ASP:HB3	1:A:142:LYS:HG3	1.99	0.44
1:A:34:TRP:CE3	1:A:61:CYS:SG	3.11	0.43
1:A:5:SER:HA	1:A:211:TYR:O	2.18	0.43
1:A:26:ASN:HA	5:A:237:HOH:O	2.18	0.43
1:A:6:PHE:HE2	1:A:8:GLU:HB2	1.84	0.43
1:A:8:GLU:O	1:A:208:TRP:HB2	2.19	0.42
1:A:65:ARG:NH1	1:A:65:ARG:CB	2.83	0.42
1:A:183:LEU:HB2	5:A:287:HOH:O	2.20	0.42
1:A:81:PRO:HD2	1:A:140:ALA:O	2.20	0.42
1:A:116:THR:HA	1:A:138:PHE:O	2.20	0.42
1:A:118:VAL:HG23	1:A:136:LEU:HD21	2.00	0.42
1:A:159:TYR:HA	1:A:163:VAL:O	2.20	0.41
1:A:54:SER:OG	1:A:58:LYS:HG2	2.19	0.41
1:A:57:ASN:N	5:A:226:HOH:O	2.49	0.41
1:A:156:ILE:O	1:A:167:THR:HA	2.20	0.41
1:A:121:ASN:ND2	1:A:130:HIS:H	2.13	0.41
1:A:20:LYS:HD3	1:A:39:VAL:HB	2.03	0.41
1:A:79:MET:HB2	1:A:79:MET:HE3	1.89	0.41
1:A:111:LEU:N	1:A:111:LEU:HD12	2.35	0.41
1:A:95:THR:O	1:A:103:TRP:HA	2.21	0.41
1:A:54:SER:HB2	1:A:58:LYS:NZ	2.36	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:NE2	5:A:288:HOH:O[3_645]	2.12	0.08

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	212/214 (99%)	198 (93%)	8 (4%)	6 (3%)	6 21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	VAL
1	A	84	ASN
1	A	171	ASN
1	A	56	TYR
1	A	2	THR
1	A	112	GLY

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	176/176 (100%)	146 (83%)	30 (17%)	2 7

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	8	GLU
1	A	19	GLU
1	A	33	THR
1	A	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	ASN
1	A	47	LEU
1	A	53	SER
1	A	54	SER
1	A	77	VAL
1	A	85	THR
1	A	89	SER
1	A	93	THR
1	A	106	ILE
1	A	107	ASP
1	A	113	LYS
1	A	114	ASP
1	A	121	ASN
1	A	127	VAL
1	A	132	LYS
1	A	136	LEU
1	A	141	SER
1	A	142	LYS
1	A	164	LEU
1	A	178	LYS
1	A	187	THR
1	A	191	ASP
1	A	193	LEU
1	A	197	ASN
1	A	205	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	37	ASN
1	A	84	ASN
1	A	121	ASN
1	A	145	HIS
1	A	152	GLN
1	A	197	ASN
1	A	200	ASN

5.3.3 RNA

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)

2 carbohydrates 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	BGC	A	216	2,4	12,12,12	1.19	3 (25%)	17,17,17	1.90	4 (23%)
2	BGC	A	217	2	11,11,12	1.74	1 (9%)	14,15,17	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	216	2,4	-	0/2/22/22	0/1/1/1
2	BGC	A	217	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	216	BGC	C3-C2	2.04	1.57	1.52
2	A	216	BGC	C4-C3	2.13	1.58	1.52
2	A	216	BGC	O1-C1	2.15	1.47	1.39
2	A	217	BGC	C4-C5	4.68	1.63	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	216	BGC	O3-C3-C4	-4.01	101.31	110.34
2	A	216	BGC	O4-C4-C3	-2.40	104.93	110.34
2	A	216	BGC	C3-C4-C5	2.51	114.57	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	216	BGC	C4-C3-C2	4.41	119.03	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	NBU	A	215	1,2	3,3,3	0.53	0	2,2,2	0.40	0

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	NBU	A	215	1,2	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	214/214 (100%)	-0.62	0 100 100	7, 19, 26, 32	0

There are no RSRZ outliers to report.

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

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, 95^{th} 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(Å^2)	Q<0.9
2	BGC	A	216	12/12	0.93	0.16	0.28	18,28,32,32	0
2	BGC	A	217	11/12	0.93	0.13	-0.60	13,22,26,27	0

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
4	NBU	A	215	4/4	0.91	0.18	6.84	23,25,29,32	0
3	CA	A	218	1/1	0.79	0.27	2.44	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.