Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:29 PM GMT

PDB ID	:	1B1Y
Title	:	SEVENFOLD MUTANT OF BARLEY BETA-AMYLASE
Authors	:	Mikami, B.; Yoon, H.J.; Yoshigi, N.
Deposited on	:	1998-11-25
Resolution	:	2.50 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 (i)) were used in the production of this report:

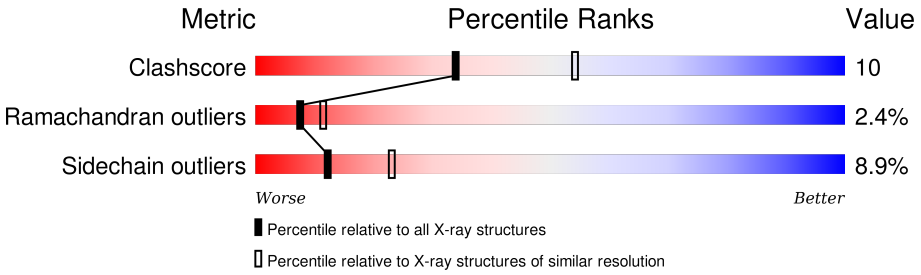
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	64% 30% 6% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4148 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 PROTEIN (BETA-AMYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3973	2532	690	732	19			

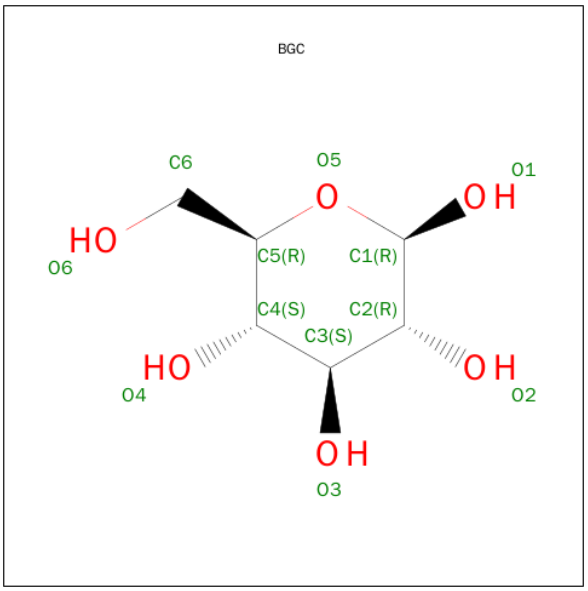
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	VAL	CONFLICT	UNP P16098
A	185	LEU	MET	ENGINEERED	UNP P16098
A	295	ALA	SER	ENGINEERED	UNP P16098
A	297	VAL	ILE	ENGINEERED	UNP P16098
A	350	PRO	SER	ENGINEERED	UNP P16098
A	351	PRO	SER	ENGINEERED	UNP P16098
A	352	ASP	GLN	ENGINEERED	UNP P16098
A	376	SER	ALA	ENGINEERED	UNP P16098
A	475	ILE	LEU	CONFLICT	UNP P16098

- 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 GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	140	Total O 140 140	0	0

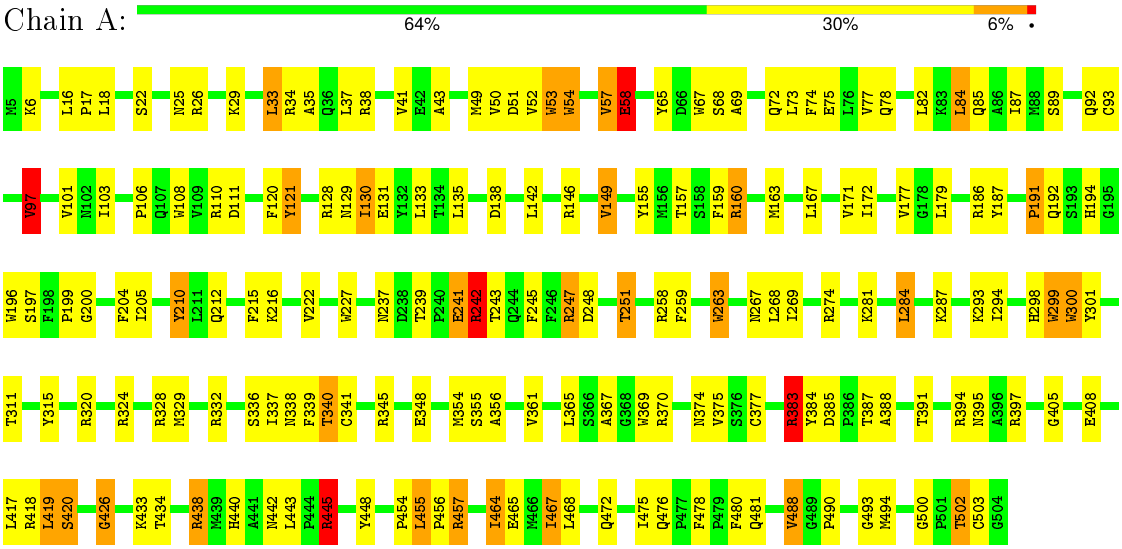
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: PROTEIN (BETA-AMYLASE)

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	72.11Å 72.11Å 250.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	79.9 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.187 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4148	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.85	0/4088	1.59	79/5554 (1.4%)

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	3

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	418	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	108	TRP	CD1-CG-CD2	9.41	113.83	106.30
1	A	146	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	A	300	TRP	CD1-CG-CD2	9.31	113.75	106.30
1	A	418	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	196	TRP	CD1-CG-CD2	8.38	113.01	106.30
1	A	300	TRP	CE2-CD2-CG	-8.33	100.64	107.30
1	A	383	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	67	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	299	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	227	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	369	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	A	263	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	A	108	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	369	TRP	CD1-CG-CD2	7.33	112.16	106.30
1	A	196	TRP	CE2-CD2-CG	-7.32	101.44	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	TRP	CD1-CG-CD2	7.23	112.08	106.30
1	A	67	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	370	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	315	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	A	179	LEU	CA-CB-CG	7.18	131.81	115.30
1	A	263	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	A	457	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	53	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	A	445	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	328	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	345	ARG	CA-CB-CG	-6.99	98.02	113.40
1	A	53	TRP	CD1-CG-CD2	6.84	111.78	106.30
1	A	457	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	54	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	54	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	A	369	TRP	CG-CD2-CE3	6.59	139.83	133.90
1	A	110	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	227	TRP	CE2-CD2-CG	-6.57	102.05	107.30
1	A	258	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	34	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	300	TRP	CG-CD2-CE3	6.41	139.67	133.90
1	A	110	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	146	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	370	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	57	VAL	CA-C-N	6.22	130.89	117.20
1	A	84	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	300	TRP	CB-CG-CD1	-6.13	119.03	127.00
1	A	108	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	A	121	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	A	57	VAL	O-C-N	-6.08	112.97	122.70
1	A	387	THR	CA-CB-OG1	-5.75	96.94	109.00
1	A	448	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	320	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	445	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	274	ARG	CB-CG-CD	-5.65	96.91	111.60
1	A	300	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	196	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	97	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	A	186	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	488	VAL	CG1-CB-CG2	-5.53	102.06	110.90
1	A	242	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	26	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	A	397	ARG	CB-CG-CD	-5.44	97.46	111.60
1	A	210	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	345	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	299	TRP	CB-CG-CD1	-5.41	119.96	127.00
1	A	417	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	58	GLU	CA-CB-CG	5.37	125.22	113.40
1	A	387	THR	CA-CB-CG2	5.36	119.91	112.40
1	A	369	TRP	CB-CG-CD1	-5.33	120.08	127.00
1	A	89	SER	N-CA-C	5.29	125.29	111.00
1	A	212	GLN	CA-CB-CG	-5.25	101.84	113.40
1	A	426	GLY	N-CA-C	5.18	126.05	113.10
1	A	160	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	74	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	A	340	THR	N-CA-C	5.14	124.88	111.00
1	A	274	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	247	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	52	VAL	N-CA-C	-5.07	97.32	111.00
1	A	196	TRP	N-CA-C	-5.06	97.35	111.00
1	A	384	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	281	LYS	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	TYR	Sidechain
1	A	405	GLY	Peptide
1	A	500	GLY	Peptide

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	3973	0	3814	79	0
2	A	23	0	21	0	0
3	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	140	0	0	1	0
All	All	4148	0	3847	79	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 (79) 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:VAL:HG22	1:A:82:LEU:HD21	1.56	0.88
1:A:197:SER:H	1:A:237:ASN:HD21	1.19	0.86
1:A:269:ILE:HD13	1:A:467:ILE:HD11	1.60	0.83
1:A:41:VAL:HG13	1:A:445:ARG:HH22	1.49	0.76
1:A:294:ILE:HD12	1:A:337:ILE:HG23	1.76	0.68
1:A:129:ASN:HD21	1:A:131:GLU:HG2	1.61	0.66
1:A:301:TYR:CD2	1:A:356:ALA:HB3	2.33	0.63
1:A:239:THR:HG23	1:A:241:GLU:HG2	1.82	0.62
1:A:129:ASN:ND2	1:A:131:GLU:HG2	2.15	0.61
1:A:383:ARG:HG2	1:A:388:ALA:HB2	1.83	0.60
1:A:293:LYS:HG2	1:A:338:ASN:HD22	1.67	0.59
1:A:135:LEU:HD11	1:A:267:ASN:HB3	1.84	0.58
1:A:33:LEU:HD23	1:A:37:LEU:HD13	1.87	0.56
1:A:284:LEU:HD22	1:A:457:ARG:HD3	1.86	0.56
1:A:197:SER:N	1:A:237:ASN:HD21	1.97	0.55
1:A:58:GLU:HB2	1:A:65:TYR:CE1	2.41	0.55
1:A:53:TRP:CH2	1:A:93:CYS:HB2	2.41	0.55
1:A:167:LEU:HD23	1:A:172:ILE:HB	1.88	0.55
1:A:243:THR:O	1:A:247:ARG:HB2	2.06	0.54
1:A:49:MET:SD	1:A:87:ILE:HD11	2.48	0.54
1:A:121:TYR:HB3	1:A:205:ILE:CG2	2.37	0.54
1:A:25:ASN:O	1:A:69:ALA:HB2	2.08	0.54
1:A:120:PHE:HB3	1:A:129:ASN:O	2.09	0.53
1:A:329:MET:C	1:A:329:MET:SD	2.88	0.52
1:A:293:LYS:HE3	4:A:684:HOH:O	2.09	0.52
1:A:78:GLN:HG3	1:A:171:VAL:HG21	1.91	0.52
1:A:49:MET:HA	1:A:85:GLN:O	2.10	0.52
1:A:84:LEU:HD12	1:A:172:ILE:HG12	1.90	0.52
1:A:245:PHE:HA	1:A:251:THR:OG1	2.10	0.51
1:A:35:ALA:O	1:A:38:ARG:HB3	2.12	0.50
1:A:239:THR:HG22	1:A:242:ARG:HG3	1.94	0.49
1:A:69:ALA:HA	1:A:72:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HA	1:A:433:LYS:HG3	1.94	0.48
1:A:336:SER:HB2	1:A:374:ASN:O	2.13	0.48
1:A:300:TRP:CZ3	1:A:354:MET:HG3	2.48	0.48
1:A:339:PHE:O	1:A:377:CYS:HA	2.13	0.48
1:A:438:ARG:HD3	1:A:442:ASN:OD1	2.14	0.48
1:A:361:VAL:O	1:A:365:LEU:HG	2.13	0.47
1:A:191:PRO:HG2	1:A:194:HIS:HB2	1.95	0.47
1:A:391:THR:HG22	1:A:395:ASN:HD21	1.78	0.47
1:A:138:ASP:O	1:A:149:VAL:HG12	2.16	0.46
1:A:475:ILE:HG22	1:A:476:GLN:N	2.31	0.46
1:A:68:SER:O	1:A:72:GLN:HG3	2.15	0.46
1:A:121:TYR:HB3	1:A:205:ILE:HG22	1.96	0.46
1:A:54:TRP:HA	1:A:155:TYR:CE2	2.51	0.46
1:A:287:LYS:HD3	1:A:454:PRO:HG3	1.97	0.46
1:A:187:TYR:CE1	1:A:268:LEU:HG	2.51	0.45
1:A:17:PRO:HD3	1:A:419:LEU:HB3	1.99	0.45
1:A:50:VAL:HG22	1:A:51:ASP:O	2.17	0.44
1:A:324:ARG:HA	1:A:367:ALA:HB1	1.99	0.44
1:A:434:THR:HG23	1:A:488:VAL:HG13	1.99	0.44
1:A:97:VAL:HG23	1:A:192:GLN:HE22	1.81	0.44
1:A:92:GLN:HB3	1:A:131:GLU:HB2	2.00	0.44
1:A:18:LEU:HB3	1:A:101:VAL:CG1	2.48	0.44
1:A:419:LEU:HD23	1:A:420:SER:N	2.33	0.44
1:A:197:SER:H	1:A:237:ASN:ND2	2.00	0.43
1:A:215:PHE:HB2	1:A:263:TRP:CZ2	2.53	0.43
1:A:391:THR:O	1:A:394:ARG:HB3	2.19	0.43
1:A:121:TYR:HB3	1:A:205:ILE:HG21	2.01	0.42
1:A:455:LEU:HA	1:A:456:PRO:HD3	1.83	0.42
1:A:464:ILE:O	1:A:468:LEU:HB2	2.20	0.42
1:A:58:GLU:HB2	1:A:65:TYR:CD1	2.55	0.42
1:A:365:LEU:HD22	1:A:375:VAL:HG11	2.00	0.42
1:A:298:HIS:O	1:A:355:SER:HA	2.20	0.42
1:A:237:ASN:HD22	1:A:237:ASN:HA	1.72	0.42
1:A:77:VAL:HG13	1:A:82:LEU:HB2	2.01	0.42
1:A:478:PHE:O	1:A:480:PHE:HD1	2.02	0.42
1:A:222:VAL:HG11	1:A:259:PHE:HE1	1.84	0.42
1:A:394:ARG:HD3	1:A:481:GLN:O	2.20	0.41
1:A:157:THR:HG23	1:A:160:ARG:NH2	2.35	0.41
1:A:16:LEU:HD12	1:A:50:VAL:HB	2.03	0.41
1:A:204:PHE:CE1	1:A:311:THR:HA	2.55	0.41
1:A:93:CYS:HB3	1:A:103:ILE:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PHE:CE1	1:A:163:MET:HG3	2.56	0.41
1:A:383:ARG:CG	1:A:388:ALA:HB2	2.50	0.41
1:A:93:CYS:SG	1:A:101:VAL:HG13	2.60	0.41
1:A:120:PHE:CD1	1:A:130:ILE:HA	2.56	0.40
1:A:440:HIS:O	1:A:443:LEU:HD12	2.22	0.40
1:A:216:LYS:HD3	1:A:216:LYS:HA	1.92	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	498/500 (100%)	447 (90%)	39 (8%)	12 (2%)	7 11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	490	PRO
1	A	57	VAL
1	A	502	THR
1	A	29	LYS
1	A	58	GLU
1	A	200	GLY
1	A	493	GLY
1	A	503	CYS
1	A	284	LEU
1	A	191	PRO
1	A	426	GLY

5.3.2 Protein sidechains (i)

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	414/414 (100%)	377 (91%)	37 (9%)	12 23

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	33	LEU
1	A	73	LEU
1	A	75	GLU
1	A	97	VAL
1	A	106	PRO
1	A	111	ASP
1	A	128	ARG
1	A	130	ILE
1	A	133	LEU
1	A	142	LEU
1	A	149	VAL
1	A	177	VAL
1	A	199	PRO
1	A	241	GLU
1	A	242	ARG
1	A	248	ASP
1	A	251	THR
1	A	299	TRP
1	A	332	ARG
1	A	340	THR
1	A	341	CYS
1	A	348	GLU
1	A	383	ARG
1	A	385	ASP
1	A	408	GLU
1	A	419	LEU
1	A	420	SER
1	A	438	ARG
1	A	445	ARG

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Mol	Chain	Res	Type
1	A	455	LEU
1	A	464	ILE
1	A	465	GLU
1	A	467	ILE
1	A	472	GLN
1	A	494	MET
1	A	502	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	72	GLN
1	A	85	GLN
1	A	129	ASN
1	A	237	ASN
1	A	338	ASN
1	A	395	ASN
1	A	399	HIS
1	A	402	ASN
1	A	431	ASN

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)

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	GLC	A	550	2	11,11,12	0.92	0	14,15,17	1.11	2 (14%)
2	BGC	A	551	2	12,12,12	0.72	0	17,17,17	1.47	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	GLC	A	550	2	-	0/2/19/22	0/1/1/1
2	BGC	A	551	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	551	BGC	O4-C4-C3	-2.64	104.40	110.34
2	A	550	GLC	C6-C5-C4	2.23	118.53	113.02
2	A	550	GLC	C1-O5-C5	2.57	115.51	112.25
2	A	551	BGC	C6-C5-C4	4.12	123.17	113.02

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)

1 ligand is 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	$\#\|Z\| > 2$
3	BGC	A	552	-	12,12,12	0.89	0	17,17,17	0.68	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
3	BGC	A	552	-	-	0/2/22/22	0/1/1/1

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 (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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.