



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 1B1Y / pdb_00001b1y
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

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

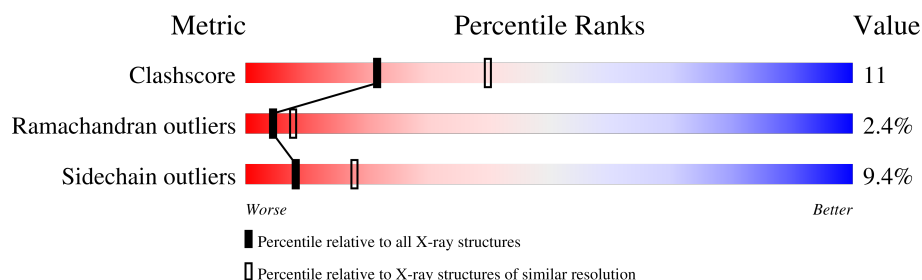
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	 56% 33% 11%
2	B	2	 100%

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:

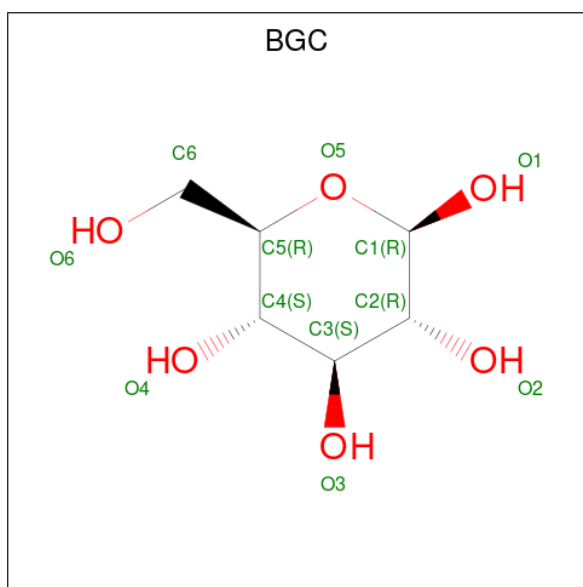
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	VAL	conflict	UNP P16098
A	185	LEU	MET	engineered mutation	UNP P16098
A	295	ALA	SER	engineered mutation	UNP P16098
A	297	VAL	ILE	engineered mutation	UNP P16098
A	350	PRO	SER	engineered mutation	UNP P16098
A	351	PRO	SER	engineered mutation	UNP P16098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

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



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

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



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

- Molecule 4 is water.

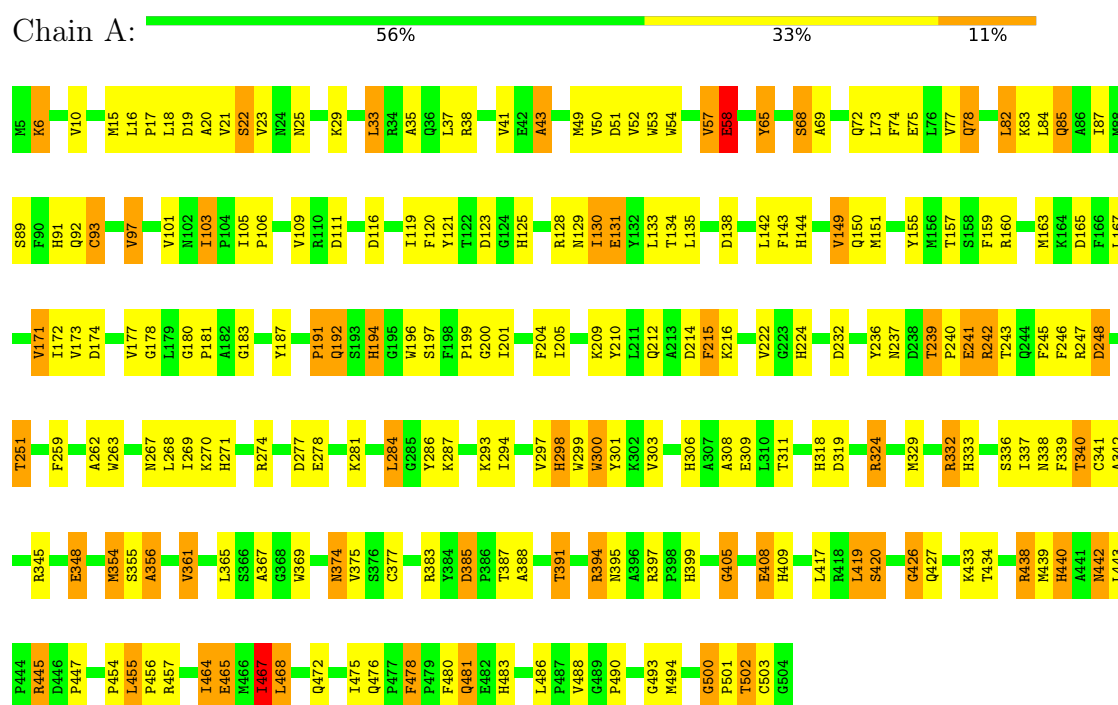
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		

3 Residue-property plots

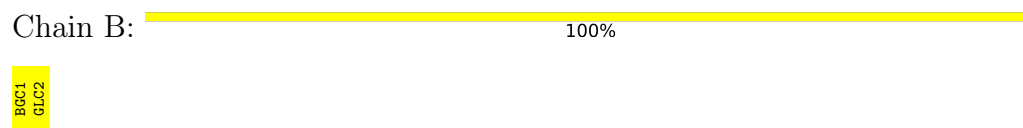
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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)



• Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [i](#)

5.1 Standard geometry [i](#)

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	1.09	19/4088 (0.5%)	1.89	113/5554 (2.0%)

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	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	HIS	CD2-NE2	-7.38	1.29	1.37
1	A	333	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	91	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	125	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	409	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	306	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	271	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	224	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	483	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	467	ILE	CA-CB	6.12	1.62	1.54
1	A	298	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	399	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	144	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	194	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	306	HIS	CG-ND1	-5.88	1.31	1.38
1	A	318	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	271	HIS	CG-ND1	-5.32	1.32	1.38
1	A	333	HIS	CG-ND1	-5.23	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	HIS	CG-ND1	-5.14	1.32	1.38

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	VAL	N-CA-C	-10.56	101.63	111.45
1	A	165	ASP	CA-CB-CG	10.53	123.13	112.60
1	A	340	THR	N-CA-C	10.07	124.88	112.59
1	A	89	SER	N-CA-C	9.64	125.29	108.52
1	A	131	GLU	N-CA-C	9.11	124.20	113.18
1	A	214	ASP	N-CA-C	-8.71	101.75	111.07
1	A	143	PHE	CA-CB-CG	-8.67	105.13	113.80
1	A	319	ASP	CA-CB-CG	8.50	121.10	112.60
1	A	387	THR	CA-CB-OG1	-8.44	96.94	109.60
1	A	19	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	345	ARG	CA-CB-CG	-8.04	98.02	114.10
1	A	20	ALA	N-CA-C	-8.00	102.51	111.07
1	A	196	TRP	N-CA-C	-7.93	97.35	109.95
1	A	57	VAL	O-C-N	-7.68	112.97	122.57
1	A	68	SER	N-CA-C	7.66	120.37	111.02
1	A	123	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	21	VAL	N-CA-C	-7.16	98.15	108.17
1	A	248	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	277	ASP	O-C-N	6.92	129.19	122.07
1	A	324	ARG	N-CA-C	-6.91	104.66	113.23
1	A	417	LEU	O-C-N	-6.91	115.12	123.27
1	A	478	PHE	N-CA-C	-6.77	101.26	109.72
1	A	239	THR	CA-C-N	6.73	126.24	119.24
1	A	239	THR	C-N-CA	6.73	126.24	119.24
1	A	236	TYR	N-CA-C	6.69	119.14	111.11
1	A	394	ARG	N-CA-C	-6.66	103.64	111.03
1	A	150	GLN	N-CA-C	-6.54	104.23	111.36
1	A	374	ASN	N-CA-C	-6.53	98.98	109.96
1	A	103	ILE	N-CA-CB	-6.50	104.67	111.36
1	A	391	THR	N-CA-C	-6.49	104.13	111.14
1	A	215	PHE	CA-C-O	-6.27	114.24	120.82
1	A	274	ARG	CB-CG-CD	-6.26	96.91	111.30
1	A	116	ASP	CA-C-N	6.24	126.15	119.28
1	A	116	ASP	C-N-CA	6.24	126.15	119.28
1	A	85	GLN	N-CA-C	-6.23	98.36	108.52
1	A	332	ARG	CB-CA-C	-6.15	100.58	110.79
1	A	212	GLN	CA-CB-CG	-6.13	101.84	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	HIS	CB-CG-CD2	-6.11	123.25	131.20
1	A	397	ARG	CB-CG-CD	-6.02	97.46	111.30
1	A	500	GLY	CA-C-N	6.01	127.36	119.84
1	A	500	GLY	C-N-CA	6.01	127.36	119.84
1	A	43	ALA	N-CA-C	-5.97	105.49	112.89
1	A	369	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	A	240	PRO	O-C-N	5.90	128.55	122.18
1	A	180	GLY	CA-C-N	5.90	125.92	119.90
1	A	180	GLY	C-N-CA	5.90	125.92	119.90
1	A	194	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	A	178	GLY	CA-C-O	-5.87	116.30	121.58
1	A	209	LYS	N-CA-C	5.87	119.54	112.38
1	A	348	GLU	N-CA-C	5.86	120.29	113.20
1	A	298	HIS	N-CA-C	5.84	119.66	112.54
1	A	356	ALA	CA-C-N	5.83	127.13	119.84
1	A	356	ALA	C-N-CA	5.83	127.13	119.84
1	A	385	ASP	CA-C-N	5.80	125.66	119.28
1	A	385	ASP	C-N-CA	5.80	125.66	119.28
1	A	52	VAL	N-CA-C	-5.78	97.32	109.34
1	A	91	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	300	TRP	CG-CD2-CE3	5.77	139.67	133.90
1	A	478	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	65	TYR	N-CA-C	5.71	118.83	109.76
1	A	82	LEU	N-CA-C	5.64	119.29	110.32
1	A	6	LYS	N-CA-C	5.62	118.95	111.75
1	A	286	TYR	N-CA-C	5.62	119.22	110.17
1	A	481	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	A	486	LEU	O-C-N	-5.61	116.69	121.23
1	A	58	GLU	CA-CB-CG	5.56	125.22	114.10
1	A	405	GLY	CA-C-N	5.55	126.09	120.38
1	A	405	GLY	C-N-CA	5.55	126.09	120.38
1	A	93	CYS	N-CA-C	-5.54	100.16	108.96
1	A	387	THR	CA-CB-CG2	5.54	119.91	110.50
1	A	22	SER	N-CA-C	5.52	122.55	110.80
1	A	300	TRP	CE2-CD2-CG	-5.47	100.64	107.20
1	A	91	HIS	N-CA-C	5.44	117.46	109.24
1	A	23	VAL	N-CA-C	5.44	120.66	109.34
1	A	232	ASP	N-CA-C	5.43	118.92	112.72
1	A	426	GLY	N-CA-C	5.43	126.05	113.18
1	A	74	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	303	VAL	CA-C-N	5.40	125.05	119.05
1	A	303	VAL	C-N-CA	5.40	125.05	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	VAL	N-CA-C	-5.39	105.12	111.00
1	A	270	LYS	CB-CG-CD	-5.38	98.93	111.30
1	A	354	MET	N-CA-C	-5.36	103.90	111.56
1	A	271	HIS	N-CA-C	-5.34	105.15	110.97
1	A	342	ALA	N-CA-C	5.32	122.14	110.80
1	A	297	VAL	N-CA-CB	-5.29	102.50	111.23
1	A	173	VAL	CB-CA-C	-5.28	104.24	110.84
1	A	300	TRP	CB-CG-CD1	-5.25	119.03	126.90
1	A	309	GLU	N-CA-C	-5.24	105.01	111.40
1	A	271	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	A	105	ILE	CA-C-N	5.17	126.31	119.84
1	A	105	ILE	C-N-CA	5.17	126.31	119.84
1	A	128	ARG	N-CA-C	5.17	116.74	108.41
1	A	442	ASN	N-CA-C	5.17	119.43	113.38
1	A	308	ALA	N-CA-C	5.17	117.65	111.71
1	A	271	HIS	CA-CB-CG	5.16	118.96	113.80
1	A	281	LYS	CA-CB-CG	5.15	124.40	114.10
1	A	361	VAL	N-CA-C	-5.12	105.50	110.42
1	A	278	GLU	CA-C-O	-5.12	115.63	120.90
1	A	78	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	174	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	465	GLU	CA-CB-CG	5.08	124.27	114.10
1	A	409	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	A	501	PRO	N-CA-C	5.06	122.89	112.47
1	A	408	GLU	CA-CB-CG	5.05	124.21	114.10
1	A	262	ALA	N-CA-C	-5.05	105.68	111.14
1	A	68	SER	CA-C-O	-5.04	115.53	121.07
1	A	57	VAL	N-CA-CB	-5.03	102.93	111.23
1	A	240	PRO	CA-C-N	5.03	127.27	120.38
1	A	240	PRO	C-N-CA	5.03	127.27	120.38
1	A	318	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	A	192	GLN	CA-C-N	5.01	126.95	120.44
1	A	192	GLN	C-N-CA	5.01	126.95	120.44
1	A	246	PHE	N-CA-C	5.00	119.47	113.17

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	85	0
2	B	23	0	21	0	0
3	A	12	0	12	0	0
4	A	140	0	0	1	0
All	All	4148	0	3847	85	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 11.

All (85) 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:329:MET:SD	1:A:329:MET:C	2.88	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PHE:HB3	1:A:129:ASN:O	2.09	0.53
1:A:78:GLN:HG3	1:A:171:VAL:HG21	1.91	0.52
1:A:293:LYS:HE3	4:A:684:HOH:O	2.09	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:10:VAL:HG11	1:A:439:MET:HE3	1.92	0.51
1:A:354:MET:HE2	1:A:354:MET:HA	1.93	0.50
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:43:ALA:HA	1:A:433:LYS:HG3	1.94	0.48
1:A:69:ALA:HA	1:A:72:GLN:HE21	1.78	0.48
1:A:336:SER:HB2	1:A:374:ASN:O	2.13	0.48
1:A:15:MET:HE2	1:A:49:MET:SD	2.53	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:54:TRP:HA	1:A:155:TYR:CE2	2.51	0.46
1:A:121:TYR:HB3	1:A:205:ILE:HG22	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:HB2	1:A:65:TYR:CD1	2.55	0.42
1:A:298:HIS:O	1:A:355:SER:HA	2.20	0.42
1:A:365:LEU:HD22	1:A:375:VAL:HG11	2.00	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:83:LYS:HZ1	1:A:447:PRO:HA	1.86	0.41
1:A:16:LEU:HD12	1:A:50:VAL:HB	2.03	0.41
1:A:119:ILE:C	1:A:134:THR:HG22	2.46	0.41
1:A:181:PRO:C	1:A:183:GLY:H	2.28	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
1:A:159:PHE:CE1	1:A:163:MET:HG3	2.56	0.41
1:A:93:CYS:SG	1:A:101:VAL:HG13	2.60	0.41
1:A:383:ARG:CG	1:A:388:ALA:HB2	2.50	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%)	4 8

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 ⓘ

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%)	375 (91%)	39 (9%)	8 18

All (39) 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	130	ILE
1	A	133	LEU
1	A	142	LEU
1	A	149	VAL
1	A	151	MET
1	A	177	VAL
1	A	199	PRO
1	A	201	ILE

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Mol	Chain	Res	Type
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	385	ASP
1	A	408	GLU
1	A	419	LEU
1	A	420	SER
1	A	427	GLN
1	A	438	ARG
1	A	445	ARG
1	A	455	LEU
1	A	464	ILE
1	A	465	GLU
1	A	467	ILE
1	A	468	LEU
1	A	472	GLN
1	A	494	MET
1	A	502	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	194	HIS
1	A	212	GLN
1	A	235	GLN
1	A	237	ASN
1	A	249	ASN
1	A	266	ASN
1	A	338	ASN
1	A	395	ASN
1	A	399	HIS
1	A	402	ASN

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Mol	Chain	Res	Type
1	A	427	GLN

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 ⓘ

2 monosaccharides 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	B	1	2	12,12,12	0.72	0	17,17,17	1.44	2 (11%)
2	GLC	B	2	2	11,11,12	0.89	0	15,15,17	1.09	2 (13%)

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	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	2/2/19/22	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(°)	Ideal(°)
2	B	1	BGC	C6-C5-C4	4.13	123.17	113.02
2	B	1	BGC	O4-C4-C3	-2.54	104.40	110.38
2	B	2	GLC	C1-O5-C5	2.48	115.51	112.19
2	B	2	GLC	C6-C5-C4	2.24	118.53	113.02

There are no chirality outliers.

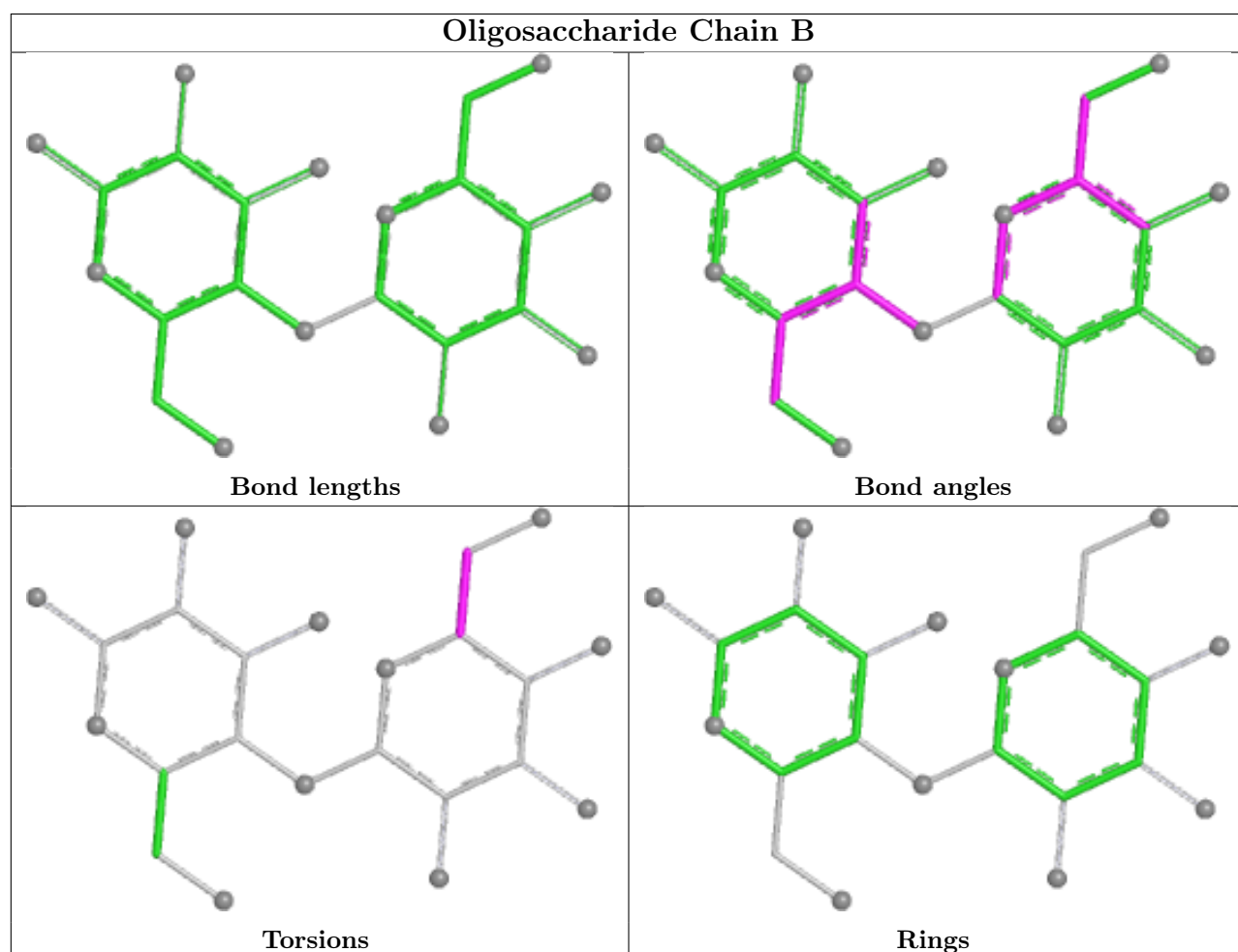
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	GLC	C4-C5-C6-O6
2	B	2	GLC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

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	0.90	0	17,17,17	0.65	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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.