



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:08 PM UTC

PDB ID : 1BYB / pdb_00001byb
Title : CRYSTAL STRUCTURES OF SOYBEAN BETA-AMYLASE REACTED WITH BETA-MALTOSE AND MALTAL: ACTIVE SITE COMPONENTS AND THEIR APPARENT ROLE IN CATALYSIS
Authors : Mikami, B.; Degano, M.; Hehre, E.J.; Sacchettini, J.C.
Deposited on : 1994-01-25
Resolution : 1.90 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

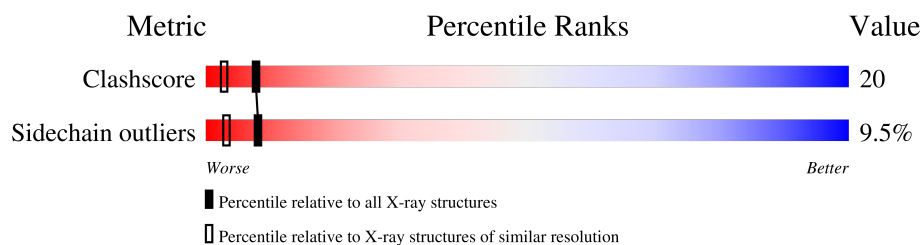
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	495	 70% 23% 5% ..
2	B	4	 25% 75%

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
2	GLC	B	1	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4307 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 BETA-AMYLASE.

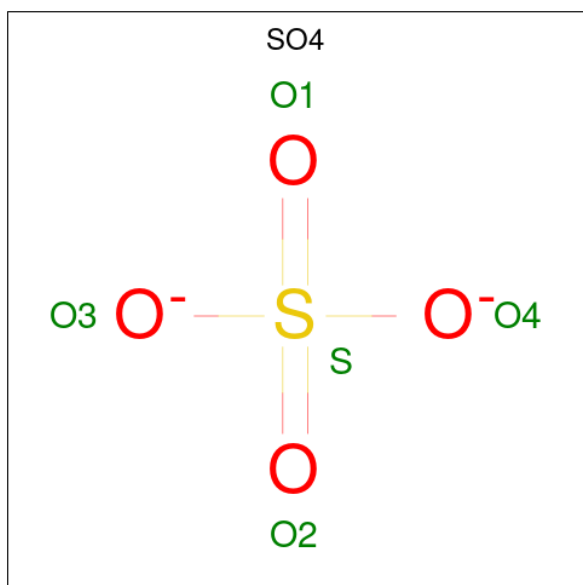
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	3925	2518	662	728	17	0	0	1

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	4	45	24	21	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

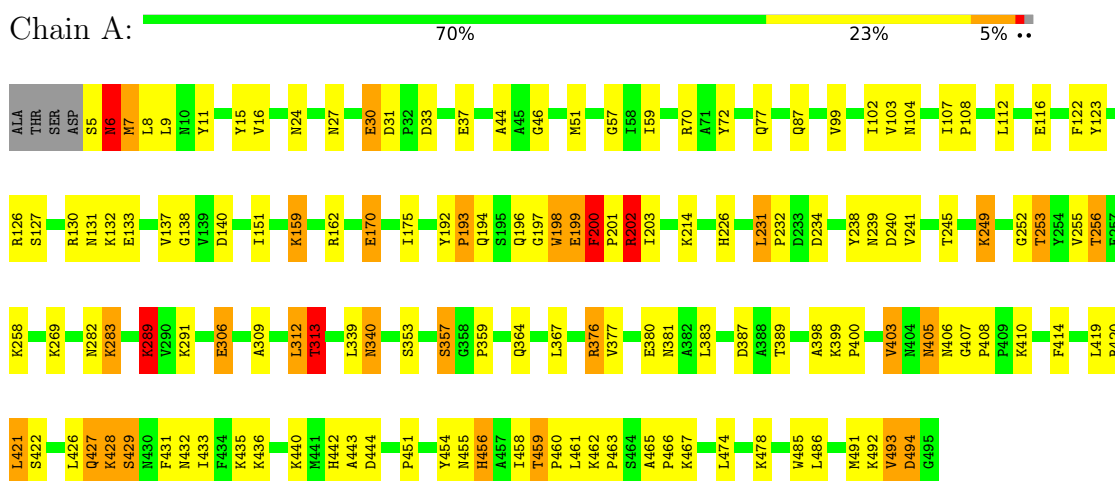
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	332	Total	O	0	0
			332	332		

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: BETA-AMYLASE



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-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 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.20 Å 86.20 Å 144.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4307	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: SO4, GLC

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	1.41	14/4032 (0.3%)	1.44	31/5479 (0.6%)

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	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	LEU	C-N	-7.77	1.22	1.33
1	A	357	SER	CA-C	-6.69	1.44	1.52
1	A	493	VAL	CA-CB	-6.29	1.45	1.54
1	A	383	LEU	CA-C	-5.93	1.46	1.52
1	A	37	GLU	CD-OE2	5.86	1.36	1.25
1	A	31	ASP	N-CA	-5.65	1.40	1.46
1	A	33	ASP	CA-C	-5.63	1.45	1.52
1	A	170	GLU	CD-OE1	5.50	1.35	1.25
1	A	306	GLU	CD-OE2	5.45	1.35	1.25
1	A	198	TRP	NE1-CE2	-5.43	1.31	1.37
1	A	104	ASN	N-CA	-5.39	1.39	1.46
1	A	162	ARG	NE-CZ	5.30	1.38	1.33
1	A	116	GLU	CD-OE2	5.29	1.35	1.25
1	A	376	ARG	NE-CZ	5.14	1.38	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	THR	N-CA-CB	12.81	132.13	110.49
1	A	200	PHE	CB-CA-C	7.79	125.51	110.17
1	A	312	LEU	O-C-N	-7.49	113.60	122.81
1	A	30	GLU	N-CA-C	7.18	118.80	110.97
1	A	193	PRO	CB-CA-C	-7.05	105.95	111.87
1	A	312	LEU	N-CA-C	-7.00	100.83	110.35
1	A	6	ASN	N-CA-C	6.88	120.66	110.48
1	A	6	ASN	CA-CB-CG	6.58	119.19	112.60
1	A	458	ILE	N-CA-CB	6.30	118.55	110.99
1	A	33	ASP	CA-CB-CG	-6.12	106.48	112.60
1	A	410	LYS	N-CA-CB	6.07	119.69	110.28
1	A	193	PRO	N-CA-CB	6.04	106.30	102.92
1	A	459	THR	N-CA-CB	-5.98	102.90	109.72
1	A	408	PRO	N-CA-CB	5.98	106.33	103.22
1	A	232	PRO	N-CA-CB	5.84	108.44	103.19
1	A	70	ARG	N-CA-C	5.59	117.06	111.07
1	A	6	ASN	CB-CA-C	5.46	119.50	109.46
1	A	138	GLY	CA-C-N	-5.39	115.57	122.26
1	A	138	GLY	C-N-CA	-5.39	115.57	122.26
1	A	432	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	289	LYS	CB-CA-C	-5.37	103.35	112.00
1	A	456	HIS	CB-CA-C	-5.33	102.29	111.45
1	A	202	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	420	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	30	GLU	CA-C-N	-5.20	117.23	122.74
1	A	30	GLU	C-N-CA	-5.20	117.23	122.74
1	A	253	THR	CB-CA-C	5.17	119.47	110.68
1	A	116	GLU	CA-C-N	-5.06	114.21	122.26
1	A	116	GLU	C-N-CA	-5.06	114.21	122.26
1	A	226	HIS	CA-C-N	5.04	124.82	119.28
1	A	226	HIS	C-N-CA	5.04	124.82	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	TYR	Sidechain

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	3925	0	3824	152	0
2	B	45	0	40	3	0
3	A	5	0	0	0	0
4	A	332	0	0	19	1
All	All	4307	0	3864	155	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 20.

All (155) 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:202:ARG:HG3	1:A:239:ASN:CA	1.40	1.47
1:A:202:ARG:CG	1:A:239:ASN:HA	1.55	1.35
1:A:201:PRO:O	1:A:202:ARG:CD	1.83	1.27
1:A:200:PHE:CG	1:A:201:PRO:HD3	1.71	1.26
1:A:201:PRO:O	1:A:202:ARG:HD3	1.31	1.20
1:A:421:LEU:C	1:A:421:LEU:HD22	1.72	1.12
1:A:202:ARG:HG3	1:A:239:ASN:C	1.75	1.11
1:A:202:ARG:CG	1:A:239:ASN:CA	2.18	1.09
1:A:202:ARG:HG2	1:A:239:ASN:HD22	1.20	1.06
1:A:99:VAL:HG12	4:A:868:HOH:O	1.56	1.05
1:A:202:ARG:HG2	1:A:239:ASN:ND2	1.72	1.04
1:A:200:PHE:CD2	1:A:201:PRO:HD3	1.92	1.04
1:A:198:TRP:CH2	1:A:200:PHE:HA	1.93	1.02
1:A:202:ARG:NE	1:A:239:ASN:O	1.96	0.97
1:A:203:ILE:HG23	1:A:240:ASP:O	1.64	0.97
1:A:202:ARG:CG	1:A:239:ASN:HD22	1.77	0.96
1:A:202:ARG:HG3	1:A:239:ASN:HA	0.99	0.96
1:A:202:ARG:HG2	1:A:239:ASN:CB	1.97	0.94
1:A:202:ARG:CG	1:A:239:ASN:CB	2.44	0.94
1:A:7:MET:HE1	1:A:403:VAL:HG13	1.50	0.93
1:A:367:LEU:HD22	1:A:377:VAL:HG11	1.53	0.90
1:A:421:LEU:C	1:A:421:LEU:CD2	2.42	0.89
1:A:405:ASN:HD22	1:A:405:ASN:H	1.18	0.89
1:A:199:GLU:H	1:A:239:ASN:HD21	1.15	0.89
1:A:201:PRO:O	1:A:202:ARG:HD2	1.73	0.89
1:A:7:MET:HE1	1:A:403:VAL:CG1	2.04	0.88
1:A:200:PHE:CG	1:A:201:PRO:CD	2.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:CB	1:A:239:ASN:HA	2.04	0.87
4:A:868:HOH:O	2:B:2:GLC:H62	1.77	0.84
1:A:289:LYS:HZ1	1:A:460:PRO:CD	1.91	0.84
1:A:5:SER:HB3	1:A:9:LEU:CD1	2.07	0.83
1:A:202:ARG:HG3	1:A:239:ASN:CB	2.08	0.82
1:A:200:PHE:CD1	1:A:201:PRO:HD3	2.16	0.81
1:A:202:ARG:CB	1:A:239:ASN:HD22	1.93	0.81
1:A:459:THR:HG22	1:A:460:PRO:HD2	1.61	0.80
1:A:289:LYS:HZ1	1:A:460:PRO:N	1.78	0.80
1:A:381:ASN:HD21	1:A:419:LEU:HB3	1.46	0.79
1:A:6:ASN:HD21	1:A:8:LEU:HB2	1.47	0.79
1:A:202:ARG:HG2	1:A:239:ASN:CG	2.06	0.79
1:A:421:LEU:HD22	1:A:421:LEU:O	1.86	0.75
1:A:6:ASN:ND2	1:A:8:LEU:HB2	2.01	0.75
1:A:357:SER:HB3	1:A:359:PRO:HD3	1.69	0.75
1:A:245:THR:O	1:A:249:LYS:HG3	1.86	0.73
1:A:202:ARG:HB3	1:A:238:TYR:O	1.89	0.72
1:A:313:THR:N	4:A:566:HOH:O	2.20	0.72
1:A:405:ASN:H	1:A:405:ASN:ND2	1.87	0.72
1:A:202:ARG:CG	1:A:239:ASN:HB3	2.18	0.71
1:A:7:MET:HE3	1:A:405:ASN:HA	1.74	0.70
1:A:459:THR:CG2	1:A:460:PRO:HD2	2.23	0.68
1:A:201:PRO:C	1:A:202:ARG:HD2	2.19	0.67
1:A:282:ASN:ND2	4:A:697:HOH:O	2.28	0.66
1:A:367:LEU:HD22	1:A:377:VAL:CG1	2.24	0.66
1:A:202:ARG:HB3	1:A:239:ASN:HA	1.77	0.66
1:A:159:LYS:HE3	4:A:556:HOH:O	1.94	0.66
1:A:403:VAL:HG21	1:A:491:MET:HE3	1.78	0.66
1:A:131:ASN:HD22	1:A:131:ASN:C	2.04	0.65
1:A:462:LYS:HB3	1:A:463:PRO:HD2	1.77	0.65
1:A:202:ARG:HG2	1:A:239:ASN:HB3	1.75	0.65
1:A:289:LYS:HZ1	1:A:460:PRO:HD3	1.61	0.63
1:A:398:ALA:HB2	4:A:658:HOH:O	1.99	0.62
2:B:3:GLC:H61	2:B:4:GLC:H5	1.81	0.62
1:A:199:GLU:O	1:A:200:PHE:C	2.43	0.62
1:A:387:ASP:OD2	1:A:389:THR:HB	1.99	0.62
1:A:376:ARG:NH2	4:A:514:HOH:O	2.32	0.62
1:A:131:ASN:HD22	1:A:132:LYS:N	1.98	0.61
1:A:5:SER:HB3	1:A:9:LEU:HD12	1.82	0.60
1:A:269:LYS:HE2	4:A:808:HOH:O	2.00	0.60
1:A:253:THR:O	1:A:256:THR:HB	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HG3	1:A:239:ASN:O	2.03	0.59
1:A:197:GLY:O	1:A:198:TRP:C	2.45	0.59
1:A:199:GLU:H	1:A:239:ASN:ND2	1.93	0.59
1:A:427:GLN:HG2	1:A:428:LYS:N	2.17	0.59
1:A:256:THR:HG22	1:A:258:LYS:H	1.69	0.57
1:A:249:LYS:C	1:A:249:LYS:HD3	2.28	0.57
1:A:201:PRO:C	1:A:202:ARG:CD	2.72	0.57
1:A:381:ASN:ND2	1:A:419:LEU:HB3	2.17	0.56
1:A:459:THR:HG22	1:A:460:PRO:CD	2.32	0.55
1:A:289:LYS:HZ2	1:A:289:LYS:HB3	1.71	0.55
1:A:131:ASN:ND2	1:A:133:GLU:H	2.05	0.55
1:A:198:TRP:CZ2	1:A:200:PHE:O	2.60	0.54
1:A:122:PHE:HB3	1:A:131:ASN:O	2.06	0.54
1:A:7:MET:HE1	1:A:403:VAL:HG11	1.86	0.54
1:A:309:ALA:O	1:A:312:LEU:O	2.25	0.54
1:A:192:TYR:HB2	1:A:198:TRP:CD2	2.43	0.54
1:A:421:LEU:HD22	1:A:422:SER:N	2.22	0.54
1:A:57:GLY:HA2	1:A:108:PRO:HD3	1.91	0.53
1:A:193:PRO:HG2	1:A:196:GLN:HB2	1.88	0.53
2:B:2:GLC:HO4	2:B:3:GLC:C1	2.12	0.53
1:A:339:LEU:HD23	1:A:339:LEU:C	2.33	0.53
1:A:202:ARG:HB2	1:A:239:ASN:HD22	1.72	0.52
1:A:123:TYR:OH	1:A:137:VAL:HG23	2.09	0.51
1:A:289:LYS:HZ2	1:A:289:LYS:CB	2.23	0.51
1:A:289:LYS:CB	1:A:289:LYS:NZ	2.73	0.51
1:A:399:LYS:NZ	4:A:782:HOH:O	2.20	0.51
1:A:405:ASN:HD22	1:A:405:ASN:N	1.97	0.50
1:A:340:ASN:HD22	1:A:340:ASN:C	2.20	0.50
1:A:306:GLU:HG2	4:A:731:HOH:O	2.11	0.50
1:A:201:PRO:HG3	4:A:506:HOH:O	2.11	0.50
1:A:381:ASN:HD21	1:A:419:LEU:CB	2.19	0.50
1:A:364:GLN:HG2	1:A:485:TRP:CE2	2.46	0.49
1:A:421:LEU:O	1:A:421:LEU:HD13	2.11	0.49
1:A:289:LYS:NZ	1:A:460:PRO:N	2.57	0.49
1:A:381:ASN:ND2	1:A:419:LEU:CB	2.75	0.49
1:A:202:ARG:CG	1:A:239:ASN:ND2	2.49	0.48
1:A:126:ARG:HH11	1:A:126:ARG:HG3	1.78	0.48
1:A:24:ASN:HD22	1:A:30:GLU:CD	2.21	0.47
1:A:414:PHE:O	1:A:456:HIS:HE1	1.97	0.47
1:A:465:ALA:HB1	1:A:466:PRO:HD2	1.96	0.47
1:A:5:SER:HB3	1:A:9:LEU:HD11	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:CE1	1:A:175:ILE:HD11	2.49	0.47
1:A:431:PHE:O	1:A:435:LYS:HG3	2.15	0.47
1:A:140:ASP:HB3	1:A:151:ILE:CD1	2.45	0.47
1:A:399:LYS:CE	4:A:782:HOH:O	2.63	0.47
1:A:44:ALA:HB3	4:A:594:HOH:O	2.15	0.47
1:A:443:ALA:O	1:A:444:ASP:HB2	2.14	0.46
1:A:200:PHE:CD2	1:A:201:PRO:CD	2.81	0.46
1:A:291:LYS:HD2	1:A:376:ARG:NH1	2.31	0.46
1:A:27:ASN:HB2	4:A:702:HOH:O	2.16	0.46
1:A:340:ASN:HD21	1:A:380:GLU:HG3	1.81	0.46
1:A:289:LYS:HZ1	1:A:459:THR:C	2.24	0.45
1:A:252:GLY:O	1:A:255:VAL:HG22	2.14	0.45
1:A:241:VAL:HG22	4:A:609:HOH:O	2.16	0.45
1:A:107:ILE:HB	1:A:108:PRO:HD2	1.97	0.45
1:A:192:TYR:HB2	1:A:198:TRP:CE2	2.52	0.45
1:A:131:ASN:C	1:A:131:ASN:ND2	2.73	0.44
1:A:494:ASP:OD1	1:A:494:ASP:N	2.50	0.44
1:A:5:SER:HB2	1:A:407:GLY:HA2	1.99	0.44
1:A:427:GLN:OE1	1:A:429:SER:N	2.51	0.44
1:A:429:SER:O	1:A:433:ILE:HG12	2.17	0.44
1:A:122:PHE:CD1	1:A:132:LYS:HA	2.52	0.44
1:A:256:THR:CG2	4:A:723:HOH:O	2.66	0.44
1:A:200:PHE:CD1	1:A:201:PRO:CD	2.93	0.44
1:A:231:LEU:HD22	4:A:692:HOH:O	2.18	0.44
1:A:51:MET:HB2	1:A:87:GLN:HE21	1.83	0.44
1:A:399:LYS:HE3	1:A:403:VAL:HG23	2.00	0.43
1:A:283:LYS:HB3	1:A:283:LYS:HE3	1.33	0.43
1:A:340:ASN:C	1:A:340:ASN:ND2	2.75	0.43
1:A:59:ILE:HD11	1:A:72:TYR:CD2	2.54	0.43
1:A:198:TRP:CZ3	1:A:200:PHE:HA	2.45	0.42
1:A:16:VAL:CG1	1:A:421:LEU:HB2	2.49	0.42
1:A:159:LYS:HD3	4:A:653:HOH:O	2.19	0.42
1:A:202:ARG:NH2	1:A:241:VAL:HG13	2.35	0.42
1:A:381:ASN:OD1	1:A:419:LEU:N	2.52	0.42
1:A:400:PRO:HB3	1:A:485:TRP:CD2	2.55	0.42
1:A:234:ASP:OD1	1:A:234:ASP:N	2.53	0.42
1:A:462:LYS:HB3	1:A:463:PRO:CD	2.46	0.41
1:A:198:TRP:CH2	1:A:200:PHE:CA	2.84	0.41
1:A:194:GLN:HE21	1:A:194:GLN:HB2	1.56	0.41
1:A:440:LYS:HA	1:A:440:LYS:HD3	1.82	0.41
1:A:256:THR:HG23	4:A:723:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:PRO:HA	1:A:454:TYR:CE2	2.56	0.41
1:A:465:ALA:HB1	1:A:466:PRO:CD	2.50	0.40
1:A:16:VAL:HG11	1:A:421:LEU:HB2	2.02	0.40
1:A:46:GLY:O	1:A:442:HIS:HE1	2.04	0.40
1:A:312:LEU:HD23	1:A:312:LEU:N	2.36	0.40

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)
4:A:647:HOH:O	4:A:829:HOH:O[2_665]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	422/425 (99%)	382 (90%)	40 (10%)	8 3

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	7	MET
1	A	77	GLN
1	A	102	ILE
1	A	103	VAL
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	127	SER
1	A	130	ARG
1	A	159	LYS
1	A	170	GLU
1	A	199	GLU
1	A	200	PHE
1	A	202	ARG
1	A	214	LYS
1	A	231	LEU
1	A	249	LYS
1	A	256	THR
1	A	283	LYS
1	A	289	LYS
1	A	313	THR
1	A	340	ASN
1	A	353	SER
1	A	403	VAL
1	A	405	ASN
1	A	406	ASN
1	A	421	LEU
1	A	426	LEU
1	A	427	GLN
1	A	428	LYS
1	A	429	SER
1	A	436	LYS
1	A	455	ASN
1	A	461	LEU
1	A	467	LYS
1	A	474	LEU
1	A	478	LYS
1	A	486	LEU
1	A	492	LYS
1	A	493	VAL
1	A	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	27	ASN
1	A	80	GLN
1	A	87	GLN

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	131	ASN
1	A	141	ASN
1	A	164	ASN
1	A	194	GLN
1	A	239	ASN
1	A	268	ASN
1	A	272	ASN
1	A	276	GLN
1	A	340	ASN
1	A	405	ASN
1	A	406	ASN
1	A	432	ASN
1	A	455	ASN

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 ⓘ

4 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	GLC	B	1	2	12,12,12	1.04	1 (8%)	17,17,17	1.63	4 (23%)
2	GLC	B	2	2	11,11,12	0.96	1 (9%)	15,15,17	1.44	2 (13%)
2	GLC	B	3	2	11,11,12	0.86	1 (9%)	15,15,17	1.54	4 (26%)
2	GLC	B	4	2	11,11,12	1.03	1 (9%)	15,15,17	1.40	3 (20%)

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	B	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1
2	GLC	B	4	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	B	1	GLC	C1-C2	-2.50	1.46	1.52
2	B	4	GLC	O5-C1	2.41	1.47	1.43
2	B	3	GLC	O2-C2	-2.08	1.39	1.43
2	B	2	GLC	C4-C3	2.05	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	GLC	C1-O5-C5	3.31	116.62	112.19
2	B	1	GLC	C1-C2-C3	-3.16	103.91	110.36
2	B	1	GLC	C1-O5-C5	-3.12	107.62	113.65
2	B	3	GLC	O5-C1-C2	-2.98	103.69	110.79
2	B	1	GLC	O5-C1-C2	-2.89	105.22	110.30
2	B	1	GLC	O1-C1-O5	2.63	118.22	110.41
2	B	2	GLC	O3-C3-C2	-2.50	104.96	110.05
2	B	3	GLC	C1-C2-C3	-2.46	106.07	109.64
2	B	2	GLC	O4-C4-C3	2.45	116.15	110.38
2	B	4	GLC	O2-C2-C1	2.39	114.70	109.22
2	B	3	GLC	C3-C4-C5	-2.31	106.03	110.23
2	B	3	GLC	C1-O5-C5	-2.15	109.31	112.19
2	B	4	GLC	O6-C6-C5	2.11	118.53	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	GLC	C1

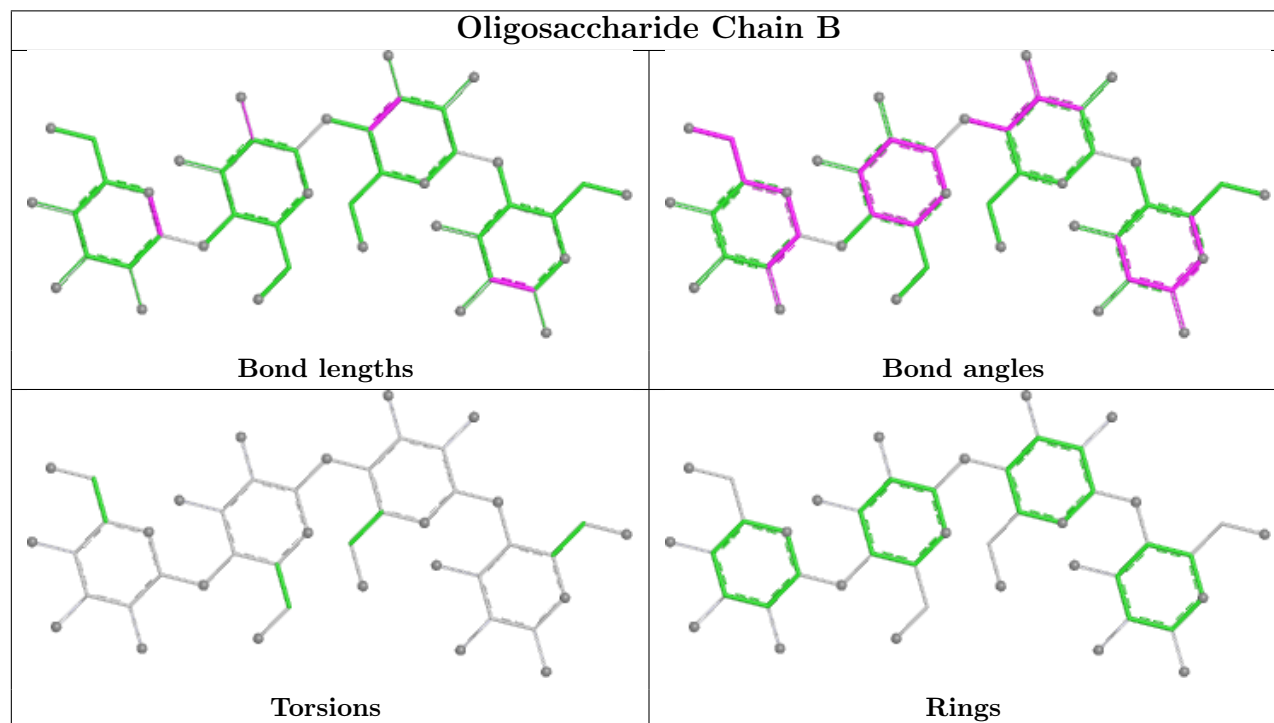
There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	GLC	2	0
2	B	2	GLC	2	0
2	B	4	GLC	1	0

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 [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	SO4	A	860	-	4,4,4	0.35	0	6,6,6	0.44	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 [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 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.