



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:15 AM UTC

PDB ID : 1BTC / pdb_00001btc
Title : THREE-DIMENSIONAL STRUCTURE OF SOYBEAN BETA-AMYLASE
DETERMINED AT 3.0 ANGSTROMS RESOLUTION: PRELIMINARY
CHAIN TRACING OF THE COMPLEX WITH ALPHA-CYCLODEXTRIN
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chettini, J.C.
Deposited on : 1993-02-18
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

<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

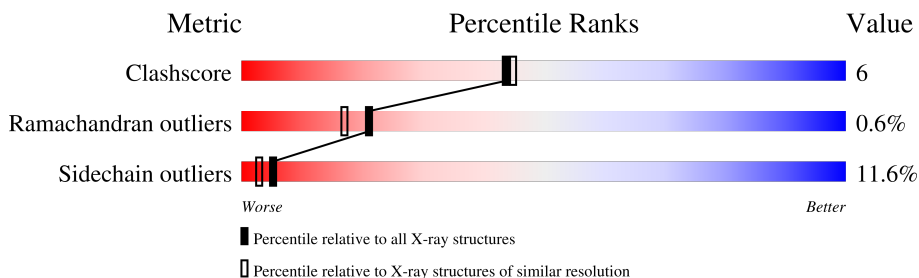
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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	491	 70% 22% 7% •
2	B	6	 100%

2 Entry composition [i](#)

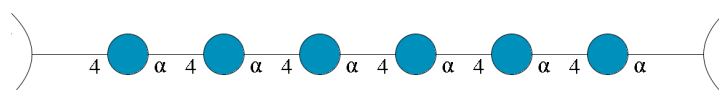
There are 5 unique types of molecules in this entry. The entry contains 4334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

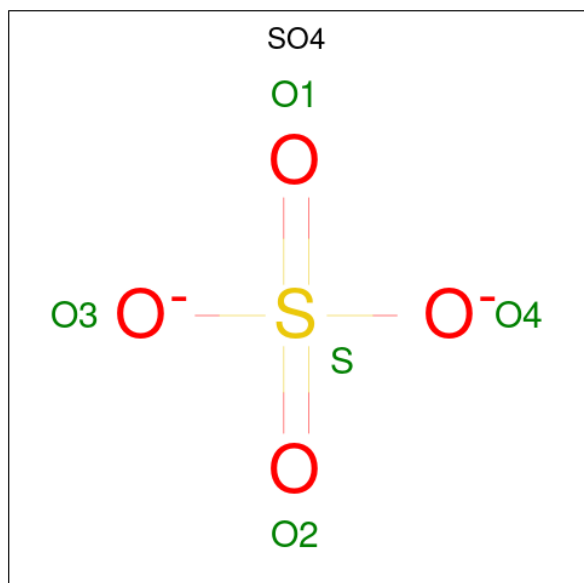
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	3929	2520	662	730	17	0	0	0

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



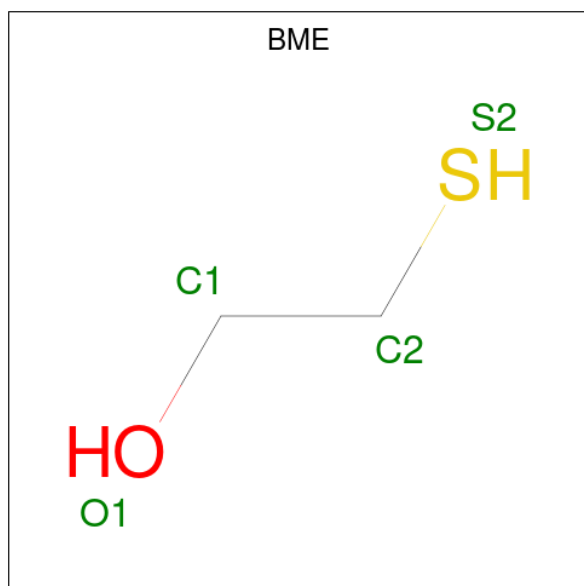
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	6	66	36	30	0	0	0

- 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 BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is water.

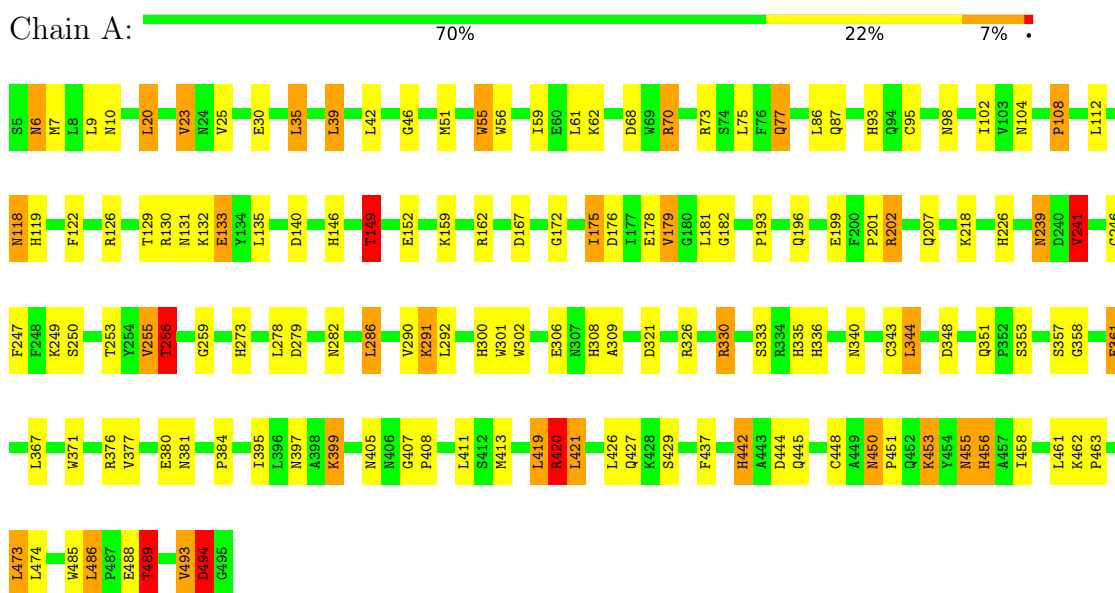
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	318	Total	O	0	0
			318	318		

3 Residue-property plots

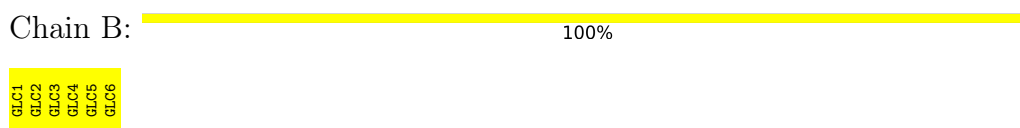
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Cyclohexakis-(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	86.10Å 86.10Å 144.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4334	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: SO4, BME, 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	1.09	20/4036 (0.5%)	1.78	93/5482 (1.7%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	HIS	CD2-NE2	-7.89	1.29	1.37
1	A	308	HIS	CD2-NE2	-7.48	1.29	1.37
1	A	179	VAL	CA-CB	7.12	1.62	1.54
1	A	335	HIS	CD2-NE2	-7.05	1.30	1.37
1	A	300	HIS	CD2-NE2	-6.87	1.30	1.37
1	A	93	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	119	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	146	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	273	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	442	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	335	HIS	CG-ND1	-5.97	1.31	1.38
1	A	23	VAL	CA-CB	5.76	1.61	1.54
1	A	308	HIS	CG-ND1	-5.64	1.32	1.38
1	A	119	HIS	CG-ND1	-5.49	1.32	1.38
1	A	226	HIS	CD2-NE2	-5.32	1.31	1.37
1	A	273	HIS	CG-ND1	-5.31	1.32	1.38
1	A	336	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	300	HIS	CG-ND1	-5.19	1.32	1.38
1	A	108	PRO	CA-CB	-5.12	1.46	1.53
1	A	456	HIS	CG-ND1	-5.10	1.32	1.38

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	GLU	N-CA-C	10.06	123.51	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	LEU	O-C-N	8.45	133.81	122.82
1	A	309	ALA	N-CA-C	8.08	120.81	111.11
1	A	456	HIS	CB-CG-CD2	-8.00	120.80	131.20
1	A	489	THR	CB-CA-C	-7.93	96.55	109.72
1	A	420	ARG	N-CA-C	7.87	127.57	110.80
1	A	405	ASN	CA-CB-CG	7.65	120.25	112.60
1	A	256	THR	N-CA-CB	-7.36	99.74	110.26
1	A	59	ILE	N-CA-C	7.33	118.12	110.72
1	A	241	VAL	N-CA-CB	-7.06	101.33	111.21
1	A	419	LEU	CA-C-N	6.97	134.85	121.54
1	A	419	LEU	C-N-CA	6.97	134.85	121.54
1	A	420	ARG	CA-CB-CG	-6.91	100.28	114.10
1	A	70	ARG	NE-CZ-NH2	-6.87	113.01	119.20
1	A	489	THR	N-CA-CB	6.86	120.18	109.83
1	A	458	ILE	CA-C-O	6.86	127.75	120.48
1	A	437	PHE	CA-CB-CG	6.76	120.56	113.80
1	A	133	GLU	CB-CG-CD	-6.70	101.20	112.60
1	A	176	ASP	CA-CB-CG	6.61	119.20	112.60
1	A	149	THR	N-CA-CB	-6.55	100.34	110.29
1	A	485	TRP	CB-CG-CD1	-6.52	117.11	126.90
1	A	419	LEU	CA-C-O	6.28	127.69	120.60
1	A	450	ASN	CA-C-N	6.27	126.18	119.28
1	A	450	ASN	C-N-CA	6.27	126.18	119.28
1	A	308	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	A	486	LEU	N-CA-C	-6.23	101.48	110.08
1	A	421	LEU	N-CA-C	-6.22	99.88	109.76
1	A	175	ILE	N-CA-CB	-6.14	101.68	110.52
1	A	218	LYS	CA-CB-CG	-6.13	101.84	114.10
1	A	351	GLN	N-CA-C	6.09	117.48	109.93
1	A	146	HIS	CA-CB-CG	-6.08	107.72	113.80
1	A	256	THR	CA-CB-OG1	-6.07	100.50	109.60
1	A	61	LEU	N-CA-C	6.02	117.51	111.07
1	A	70	ARG	CA-C-O	-6.02	114.68	121.00
1	A	399	LYS	CA-C-N	5.97	125.84	119.28
1	A	399	LYS	C-N-CA	5.97	125.84	119.28
1	A	62	LYS	N-CA-C	5.87	119.54	112.38
1	A	361	GLU	CA-CB-CG	5.82	125.74	114.10
1	A	485	TRP	CG-CD2-CE3	5.81	139.71	133.90
1	A	420	ARG	CA-C-O	5.80	128.81	120.51
1	A	146	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	A	182	GLY	CA-C-N	5.78	126.07	119.83
1	A	182	GLY	C-N-CA	5.78	126.07	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	119	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	306	GLU	N-CA-C	5.71	118.28	111.71
1	A	408	PRO	CA-C-O	-5.70	116.23	120.73
1	A	407	GLY	CA-C-N	5.66	123.74	119.66
1	A	407	GLY	C-N-CA	5.66	123.74	119.66
1	A	202	ARG	N-CA-CB	-5.65	101.20	110.41
1	A	444	ASP	N-CA-C	5.62	121.37	113.56
1	A	129	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	301	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	86	LEU	CA-CB-CG	5.49	135.52	116.30
1	A	104	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	493	VAL	CA-CB-CG2	-5.49	101.07	110.40
1	A	494	ASP	O-C-N	5.46	129.86	122.59
1	A	73	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	167	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	207	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	A	55	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	A	437	PHE	N-CA-C	-5.42	105.37	111.28
1	A	118	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	226	HIS	CA-C-N	5.38	125.05	119.56
1	A	226	HIS	C-N-CA	5.38	125.05	119.56
1	A	488	GLU	N-CA-CB	-5.37	101.86	110.77
1	A	397	ASN	OD1-CG-ND2	-5.28	117.33	122.60
1	A	129	THR	CA-C-O	5.24	126.46	120.54
1	A	93	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	A	458	ILE	O-C-N	5.21	128.65	123.18
1	A	301	TRP	CB-CG-CD1	-5.20	119.09	126.90
1	A	335	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	381	ASN	N-CA-C	-5.16	102.84	110.48
1	A	239	ASN	N-CA-C	5.15	118.70	112.93
1	A	56	TRP	CG-CD2-CE3	5.14	139.04	133.90
1	A	86	LEU	N-CA-CB	-5.13	101.94	111.13
1	A	348	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	255	VAL	N-CA-CB	-5.13	100.89	111.76
1	A	453	LYS	CB-CG-CD	-5.13	99.51	111.30
1	A	485	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	371	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	202	ARG	CB-CA-C	5.11	118.25	109.51
1	A	357	SER	N-CA-CB	-5.11	101.95	110.23
1	A	201	PRO	CA-C-N	-5.10	113.36	122.07
1	A	201	PRO	C-N-CA	-5.10	113.36	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	O-C-N	-5.08	115.47	121.32
1	A	133	GLU	CB-CA-C	-5.06	99.73	110.31
1	A	333	SER	CA-C-O	-5.04	114.41	120.10
1	A	358	GLY	CA-C-N	5.03	124.47	119.24
1	A	358	GLY	C-N-CA	5.03	124.47	119.24
1	A	256	THR	CA-CB-CG2	5.02	119.03	110.50
1	A	455	ASN	N-CA-C	5.01	118.50	111.74
1	A	178	GLU	O-C-N	-5.01	116.86	123.02

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	3929	0	3823	48	0
2	B	66	0	54	0	0
3	A	5	0	0	0	0
4	A	16	0	20	1	0
5	A	318	0	0	10	0
All	All	4334	0	3897	48	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 6.

All (48) 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:367:LEU:HD22	1:A:377:VAL:HG11	1.61	0.81
1:A:202:ARG:HB3	1:A:239:ASN:HA	1.62	0.78
1:A:395:ILE:HG22	1:A:489:THR:HG21	1.70	0.71
1:A:149:THR:HG22	1:A:152:GLU:H	1.56	0.70
1:A:149:THR:HG21	5:A:692:HOH:O	1.92	0.69
1:A:68:ASP:OD1	1:A:70:ARG:HD3	1.99	0.63
1:A:140:ASP:O	1:A:149:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:CYS:SG	4:A:504:BME:O1	2.54	0.61
1:A:172:GLY:HA2	5:A:662:HOH:O	2.01	0.60
1:A:199:GLU:H	1:A:239:ASN:HD21	1.49	0.59
1:A:131:ASN:HD21	1:A:133:GLU:HG3	1.70	0.57
1:A:193:PRO:HG2	1:A:196:GLN:HB2	1.87	0.57
1:A:202:ARG:CB	1:A:239:ASN:HA	2.31	0.57
1:A:35:LEU:HD22	1:A:39:LEU:HD13	1.88	0.55
1:A:367:LEU:HD22	1:A:377:VAL:CG1	2.35	0.55
1:A:253:THR:O	1:A:256:THR:HB	2.10	0.52
1:A:51:MET:HE3	1:A:87:GLN:NE2	2.26	0.51
1:A:20:LEU:HD23	1:A:102:ILE:HD11	1.93	0.51
1:A:25:VAL:HG23	5:A:672:HOH:O	2.11	0.51
1:A:291:LYS:HE2	1:A:376:ARG:NH1	2.26	0.51
1:A:286:LEU:HD21	1:A:463:PRO:HD3	1.93	0.50
1:A:7:MET:O	1:A:10:ASN:HB2	2.13	0.49
1:A:126:ARG:NH1	5:A:713:HOH:O	2.46	0.49
1:A:241:VAL:HG22	1:A:302:TRP:CH2	2.48	0.48
1:A:256:THR:HG22	1:A:259:GLY:H	1.77	0.48
1:A:291:LYS:HE2	1:A:376:ARG:HH12	1.78	0.48
1:A:122:PHE:HB3	1:A:131:ASN:O	2.14	0.48
1:A:20:LEU:HD13	1:A:420:ARG:NH1	2.29	0.47
1:A:55:TRP:CH2	1:A:95:CYS:HB2	2.50	0.46
1:A:330:ARG:HG2	1:A:473:LEU:HD12	1.98	0.46
1:A:340:ASN:HD21	1:A:380:GLU:HG3	1.80	0.45
1:A:456:HIS:HD2	5:A:596:HOH:O	1.99	0.45
1:A:489:THR:HG23	5:A:529:HOH:O	2.17	0.44
1:A:448:CYS:SG	1:A:453:LYS:HD2	2.57	0.44
1:A:159:LYS:HE2	5:A:553:HOH:O	2.18	0.43
1:A:384:PRO:HD3	1:A:419:LEU:HD22	2.01	0.43
1:A:131:ASN:ND2	1:A:133:GLU:HG3	2.32	0.43
1:A:122:PHE:CD1	1:A:132:LYS:HA	2.54	0.42
1:A:247:PHE:CD1	1:A:253:THR:HB	2.54	0.42
1:A:399:LYS:HE2	5:A:528:HOH:O	2.18	0.42
1:A:77:GLN:HG3	5:A:723:HOH:O	2.20	0.42
1:A:51:MET:HB2	1:A:87:GLN:HE21	1.84	0.42
1:A:246:GLY:HA2	1:A:249:LYS:HE3	2.02	0.42
1:A:344:LEU:HD11	1:A:413:MET:HE1	2.03	0.41
1:A:456:HIS:HE1	5:A:521:HOH:O	2.02	0.41
1:A:46:GLY:O	1:A:442:HIS:HE1	2.04	0.41
1:A:282:ASN:OD1	1:A:463:PRO:HA	2.21	0.40
1:A:450:ASN:HA	1:A:451:PRO:HD3	1.94	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	489/491 (100%)	470 (96%)	16 (3%)	3 (1%)	21 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	ARG
1	A	6	ASN
1	A	494	ASP

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	422/422 (100%)	373 (88%)	49 (12%)	5 3

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	LEU
1	A	20	LEU
1	A	23	VAL
1	A	35	LEU

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Mol	Chain	Res	Type
1	A	39	LEU
1	A	42	LEU
1	A	75	LEU
1	A	77	GLN
1	A	98	ASN
1	A	108	PRO
1	A	112	LEU
1	A	118	ASN
1	A	130	ARG
1	A	135	LEU
1	A	149	THR
1	A	162	ARG
1	A	175	ILE
1	A	179	VAL
1	A	181	LEU
1	A	241	VAL
1	A	250	SER
1	A	255	VAL
1	A	256	THR
1	A	278	LEU
1	A	279	ASP
1	A	286	LEU
1	A	290	VAL
1	A	291	LYS
1	A	292	LEU
1	A	330	ARG
1	A	344	LEU
1	A	353	SER
1	A	361	GLU
1	A	411	LEU
1	A	421	LEU
1	A	426	LEU
1	A	427	GLN
1	A	429	SER
1	A	445	GLN
1	A	455	ASN
1	A	461	LEU
1	A	462	LYS
1	A	473	LEU
1	A	474	LEU
1	A	486	LEU
1	A	489	THR

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Mol	Chain	Res	Type
1	A	493	VAL
1	A	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	87	GLN
1	A	98	ASN
1	A	104	ASN
1	A	118	ASN
1	A	131	ASN
1	A	194	GLN
1	A	239	ASN
1	A	268	ASN
1	A	276	GLN
1	A	340	ASN
1	A	351	GLN
1	A	364	GLN
1	A	393	GLN
1	A	445	GLN
1	A	450	ASN
1	A	456	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](#)

6 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	11,11,12	0.62	0	15,15,17	1.28	1 (6%)
2	GLC	B	2	2	11,11,12	0.57	0	15,15,17	1.22	3 (20%)
2	GLC	B	3	2	11,11,12	0.71	0	15,15,17	1.36	2 (13%)
2	GLC	B	4	2	11,11,12	0.71	0	15,15,17	1.34	2 (13%)
2	GLC	B	5	2	11,11,12	0.49	0	15,15,17	1.03	2 (13%)
2	GLC	B	6	2	11,11,12	0.70	0	15,15,17	1.28	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	GLC	B	1	2	-	0/2/19/22	0/1/1/1
2	GLC	B	2	2	-	1/2/19/22	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
2	GLC	B	5	2	-	0/2/19/22	0/1/1/1
2	GLC	B	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	GLC	O4-C4-C3	-3.51	102.10	110.38
2	B	1	GLC	C1-O5-C5	3.23	116.52	112.19
2	B	4	GLC	O4-C4-C3	-3.10	103.07	110.38
2	B	3	GLC	C1-O5-C5	3.00	116.21	112.19
2	B	4	GLC	C1-O5-C5	2.98	116.18	112.19
2	B	6	GLC	O4-C4-C3	-2.93	103.47	110.38
2	B	2	GLC	C1-O5-C5	2.57	115.63	112.19
2	B	6	GLC	C1-O5-C5	2.52	115.57	112.19
2	B	2	GLC	O4-C4-C3	-2.40	104.72	110.38
2	B	5	GLC	C1-O5-C5	2.25	115.20	112.19
2	B	2	GLC	C2-C3-C4	-2.19	107.01	110.86
2	B	5	GLC	O4-C4-C3	-2.11	105.40	110.38

There are no chirality outliers.

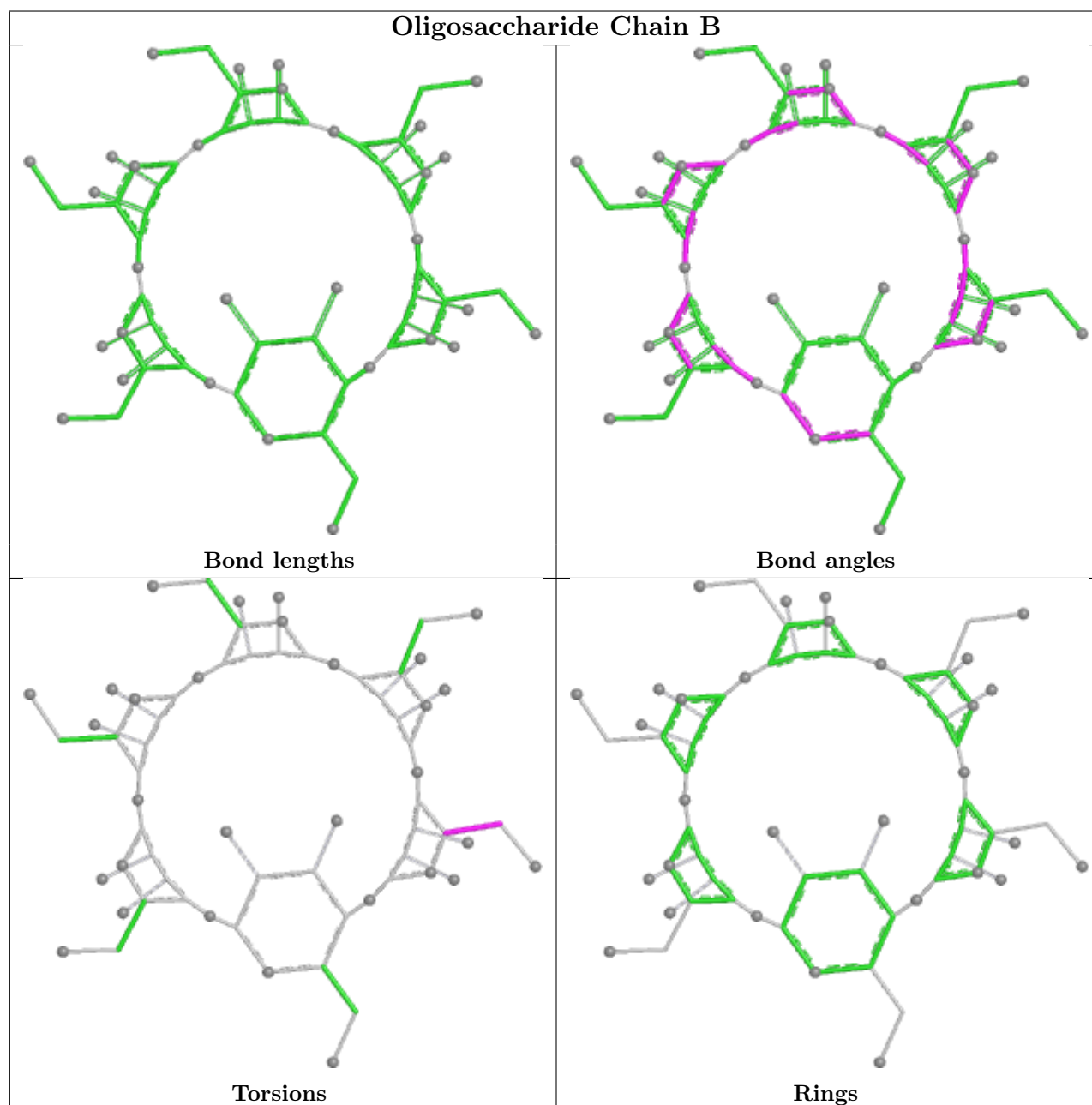
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

5 ligands 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	$\# Z > 2$
4	BME	A	502	1	3,3,3	0.76	0	2,2,2	0.72	0
4	BME	A	503	1	3,3,3	0.18	0	2,2,2	0.51	0
3	SO4	A	1	-	4,4,4	0.40	0	6,6,6	0.52	0
4	BME	A	504	1	3,3,3	0.30	0	2,2,2	0.56	0
4	BME	A	505	1	3,3,3	0.31	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	BME	A	502	1	-	0/1/1/1	-
4	BME	A	503	1	-	0/1/1/1	-
4	BME	A	505	1	-	1/1/1/1	-
4	BME	A	504	1	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	BME	1	0

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.