Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:49 PM EDT

PDB ID	:	1BTC
Title	:	THREE-DIMENSIONAL STRUCTURE OF SOYBEAN BETA-AMYLASE DETERMINED AT 3.0 ANGSTROMS RESOLUTION: PRELIMINARY CHAIN TRACING OF THE COMPLEX WITH ALPHA-CYCLODEXTRIN
Authors	:	Mikami, B.; Hehre, E.J.; Sato, M.; Katsube, Y.; Hirose, M.; Morita, Y.; Sacchettini, 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 (i) 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 (i)) were used in the production of this report:

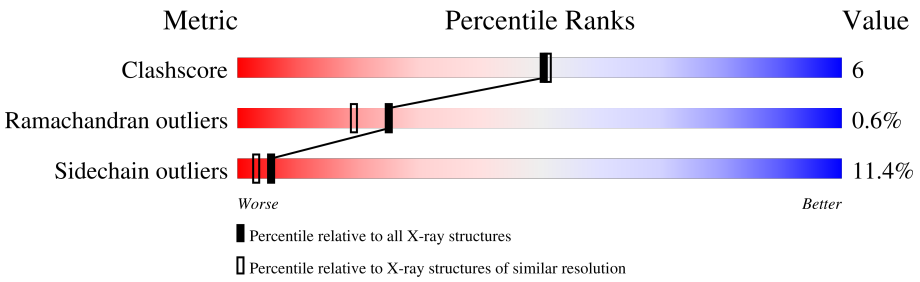
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	76% 18% 5% •
2	B	6	100%

2 Entry composition (i)

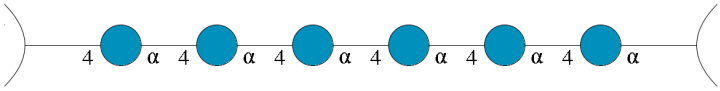
There are 5 unique types of molecules in this entry. The entry contains 4334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

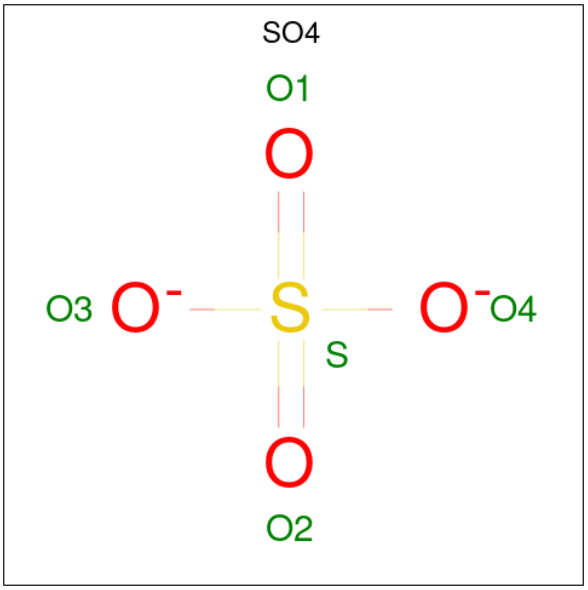
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	3929	2520	662	730	17	0	0	0

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



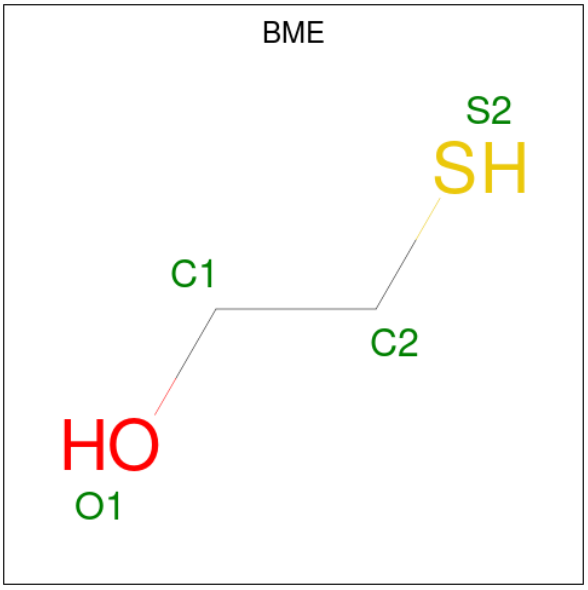
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	6	66	36	30	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 5 is water.

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

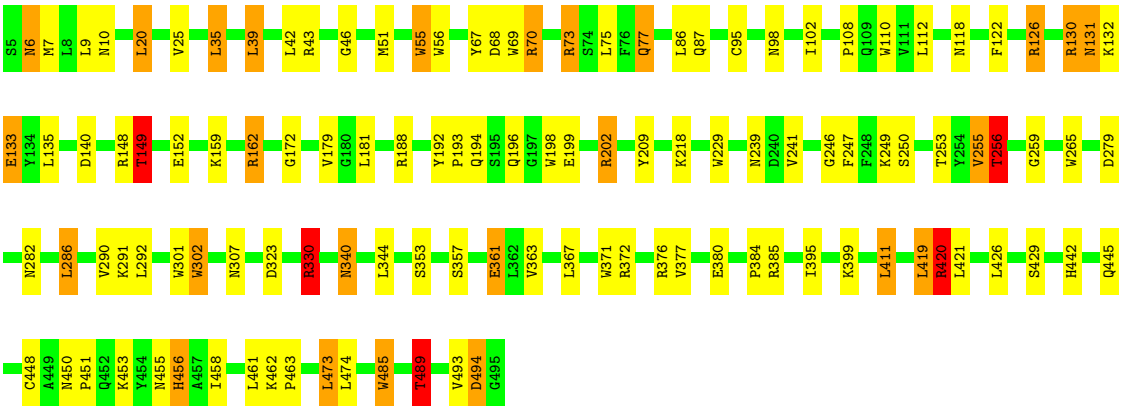
3 Residue-property plots (i)

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

Chain A: 76% 18% 5%



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

Chain B: 100%

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, SO4, BME

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	0.87	0/4036	1.58	79/5482 (1.4%)

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	70	ARG	NE-CZ-NH2	-14.57	113.01	120.30
1	A	73	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	A	70	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	A	330	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	A	371	TRP	CD1-CG-CD2	9.30	113.74	106.30
1	A	385	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	86	LEU	CA-CB-CG	8.79	135.52	115.30
1	A	419	LEU	CA-C-N	-8.67	98.12	117.20
1	A	73	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	265	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	A	330	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	202	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	229	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	485	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	A	148	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	485	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	371	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	110	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	55	TRP	CD1-CG-CD2	7.63	112.41	106.30
1	A	385	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	485	TRP	CB-CG-CD1	-7.60	117.11	127.00
1	A	301	TRP	CD1-CG-CD2	7.45	112.26	106.30
1	A	198	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	55	TRP	CE2-CD2-CG	-7.36	101.41	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	A	301	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	110	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	419	LEU	O-C-N	6.94	133.81	122.70
1	A	56	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	265	TRP	CE2-CD2-CG	-6.91	101.78	107.30
1	A	302	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	229	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	A	69	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	A	363	VAL	CG1-CB-CG2	-6.58	100.37	110.90
1	A	198	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	A	493	VAL	CA-CB-CG2	-6.55	101.07	110.90
1	A	69	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	A	420	ARG	CA-C-N	-6.48	102.94	117.20
1	A	485	TRP	CG-CD2-CE3	6.46	139.71	133.90
1	A	458	ILE	CA-C-N	-6.35	103.24	117.20
1	A	265	TRP	CG-CD1-NE1	-6.22	103.88	110.10
1	A	371	TRP	CG-CD1-NE1	-6.14	103.96	110.10
1	A	420	ARG	N-CA-C	6.14	127.57	111.00
1	A	301	TRP	CG-CD2-CE3	6.13	139.41	133.90
1	A	301	TRP	CB-CG-CD1	-6.08	119.09	127.00
1	A	55	TRP	CG-CD2-CE3	6.04	139.34	133.90
1	A	302	TRP	CD1-CG-CD2	6.02	111.11	106.30
1	A	420	ARG	CA-CB-CG	-5.97	100.28	113.40
1	A	372	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	67	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	A	130	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	56	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	A	357	SER	N-CA-CB	-5.70	101.95	110.50
1	A	302	TRP	CB-CG-CD1	-5.66	119.64	127.00
1	A	255	VAL	CA-CB-CG2	-5.63	102.45	110.90
1	A	209	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	A	188	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	361	GLU	CA-CB-CG	5.61	125.74	113.40
1	A	411	LEU	CA-CB-CG	5.57	128.12	115.30
1	A	489	THR	CB-CA-C	-5.57	96.55	111.60
1	A	256	THR	N-CA-CB	-5.56	99.74	110.30
1	A	126	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	55	TRP	CB-CG-CD1	-5.50	119.86	127.00
1	A	162	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	302	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	133	GLU	CB-CA-C	-5.34	99.73	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	A	110	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	419	LEU	C-N-CA	5.26	134.85	121.70
1	A	218	LYS	CA-CB-CG	-5.25	101.84	113.40
1	A	149	THR	N-CA-CB	-5.24	100.34	110.30
1	A	202	ARG	N-CA-CB	-5.22	101.20	110.60
1	A	489	THR	N-CA-CB	5.20	120.18	110.30
1	A	188	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	344	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	198	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	A	323	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	301	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	A	192	TYR	CB-CG-CD2	-5.02	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

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	3929	0	3823	45	0
2	B	66	0	54	0	0
3	A	5	0	0	0	0
4	A	16	0	20	0	0
5	A	318	0	0	10	0
All	All	4334	0	3897	45	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 (45) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	25 19

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%)	374 (89%)	48 (11%)	5 3

All (48) 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	35	LEU
1	A	39	LEU
1	A	42	LEU
1	A	43	ARG
1	A	73	ARG
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	131	ASN
1	A	135	LEU
1	A	149	THR
1	A	162	ARG
1	A	179	VAL
1	A	181	LEU
1	A	194	GLN
1	A	250	SER
1	A	255	VAL
1	A	256	THR
1	A	279	ASP
1	A	286	LEU
1	A	290	VAL
1	A	292	LEU
1	A	307	ASN
1	A	330	ARG
1	A	340	ASN
1	A	353	SER
1	A	361	GLU
1	A	411	LEU
1	A	421	LEU
1	A	426	LEU
1	A	429	SER
1	A	445	GLN
1	A	455	ASN
1	A	456	HIS
1	A	461	LEU
1	A	462	LYS

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Mol	Chain	Res	Type
1	A	473	LEU
1	A	474	LEU
1	A	485	TRP
1	A	489	THR
1	A	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	87	GLN
1	A	98	ASN
1	A	118	ASN
1	A	131	ASN
1	A	196	GLN
1	A	207	GLN
1	A	239	ASN
1	A	268	ASN
1	A	276	GLN
1	A	307	ASN
1	A	340	ASN
1	A	364	GLN
1	A	401	GLN
1	A	445	GLN
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	0.64	0	15,15,17	1.35	1 (6%)
2	GLC	B	2	2	11,11,12	0.58	0	15,15,17	1.24	3 (20%)
2	GLC	B	3	2	11,11,12	0.72	0	15,15,17	1.37	2 (13%)
2	GLC	B	4	2	11,11,12	0.73	0	15,15,17	1.42	3 (20%)
2	GLC	B	5	2	11,11,12	0.50	0	15,15,17	1.07	2 (13%)
2	GLC	B	6	2	11,11,12	0.72	0	15,15,17	1.33	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 (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	GLC	O4-C4-C3	-3.57	102.10	110.35
2	B	1	GLC	C1-O5-C5	3.19	116.52	112.19
2	B	4	GLC	O4-C4-C3	-3.15	103.07	110.35
2	B	6	GLC	O4-C4-C3	-2.97	103.47	110.35
2	B	3	GLC	C1-O5-C5	2.96	116.21	112.19
2	B	4	GLC	C1-O5-C5	2.94	116.18	112.19
2	B	2	GLC	C1-O5-C5	2.54	115.63	112.19
2	B	6	GLC	C1-O5-C5	2.49	115.57	112.19
2	B	2	GLC	O4-C4-C3	-2.43	104.72	110.35
2	B	2	GLC	C2-C3-C4	-2.24	107.01	110.89
2	B	5	GLC	C1-O5-C5	2.22	115.20	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4	GLC	O5-C1-C2	2.18	114.14	110.77
2	B	5	GLC	O4-C4-C3	-2.14	105.40	110.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

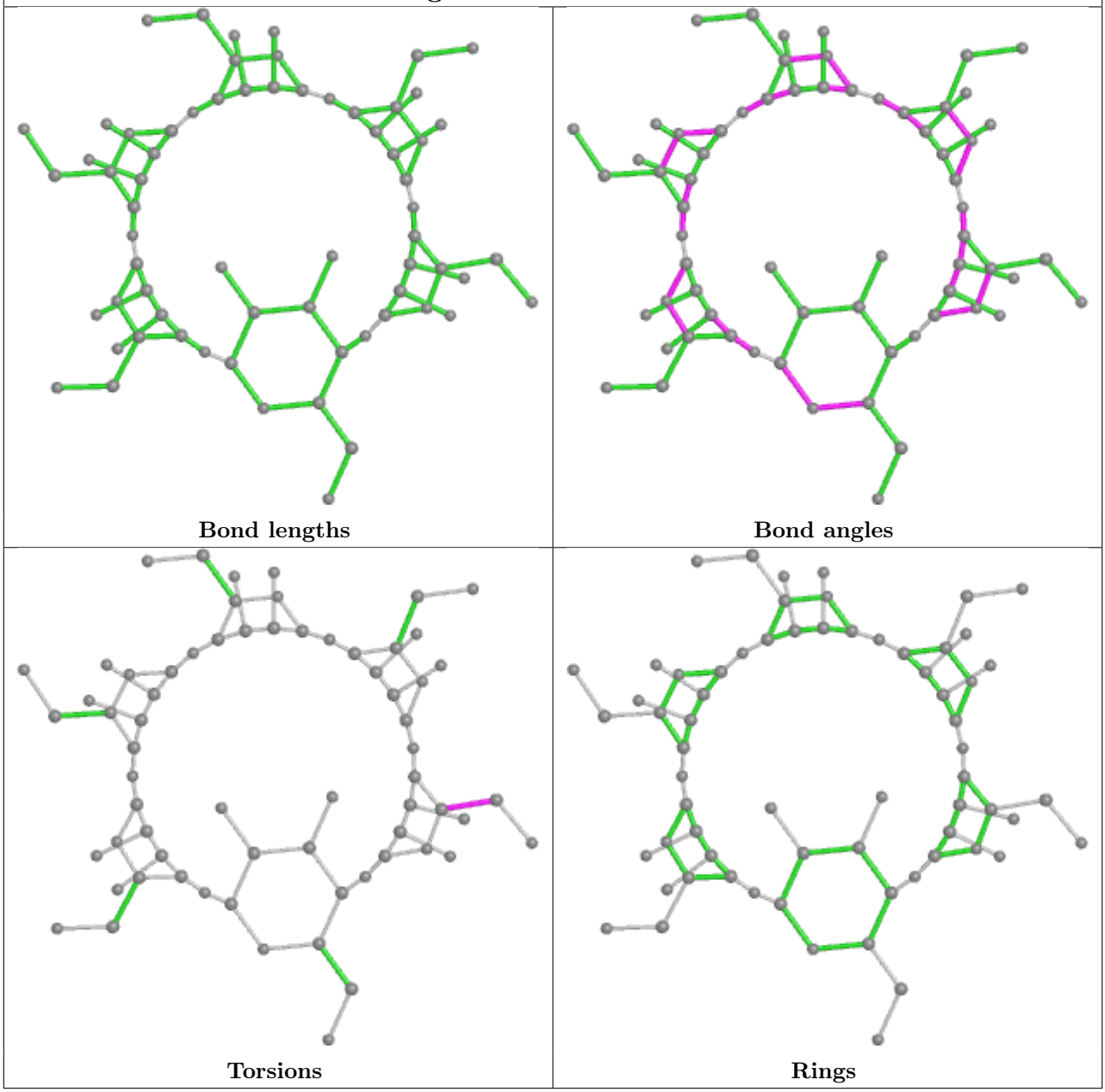
Mol	Chain	Res	Type	Atoms
2	B	2	GLC	O5-C5-C6-O6

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.

Oligosaccharide Chain B



5.6 Ligand geometry (i)

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	505	1	3,3,3	0.31	0	1,2,2	0.51	0
4	BME	A	502	1	3,3,3	0.77	0	1,2,2	0.43	0
4	BME	A	504	1	3,3,3	0.42	0	1,2,2	0.60	0
3	SO4	A	1	-	4,4,4	0.42	0	6,6,6	0.50	0
4	BME	A	503	1	3,3,3	0.24	0	1,2,2	0.50	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	505	1	-	1/1/1/1	-
4	BME	A	502	1	-	0/1/1/1	-
4	BME	A	504	1	-	0/1/1/1	-
4	BME	A	503	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.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.