Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 01:12 PM EST

PDB ID	:	1B9Z
Title	:	BACILLUS CEREUS BETA-AMYLASE COMPLEXED WITH MALTOSE
Authors	:	Mikami, B.; Adachi, M.; Kage, T.; Sarikaya, E.; Nanmori, T.; Shinke, R.; Utsumi, S.
Deposited on	:	1999-03-06
Resolution	:	2.10 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:

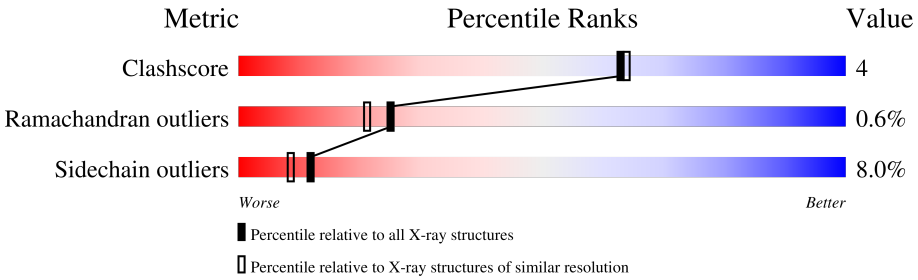
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	516	79% 17% .
2	B	2	100%
2	C	2	50% 50%
2	D	2	100%
2	E	2	50% 50%

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	GLC	D	1	X	-	-	-
2	GLC	E	1	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4496 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.

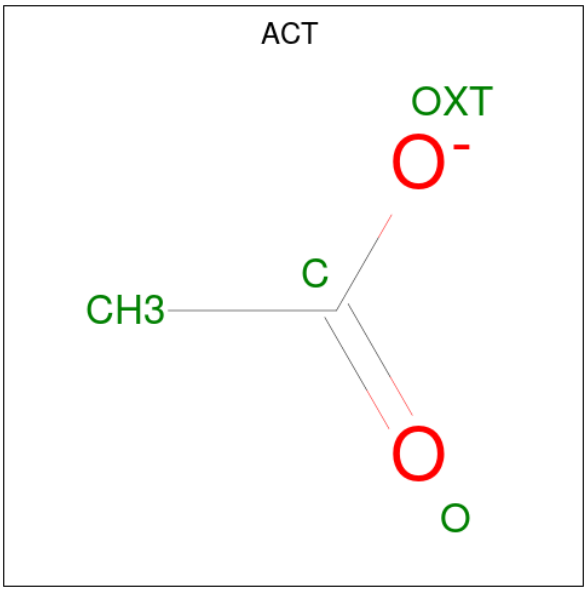
- Molecule 1 is a protein called PROTEIN (BETA-AMYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			

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

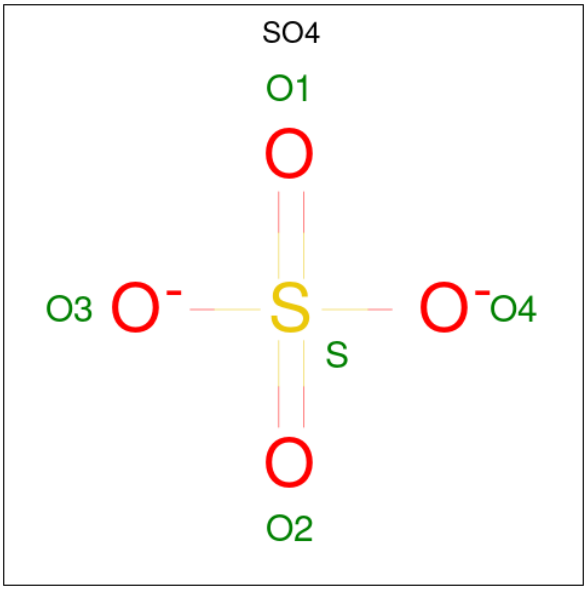
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	275	Total O 275 275	0	0

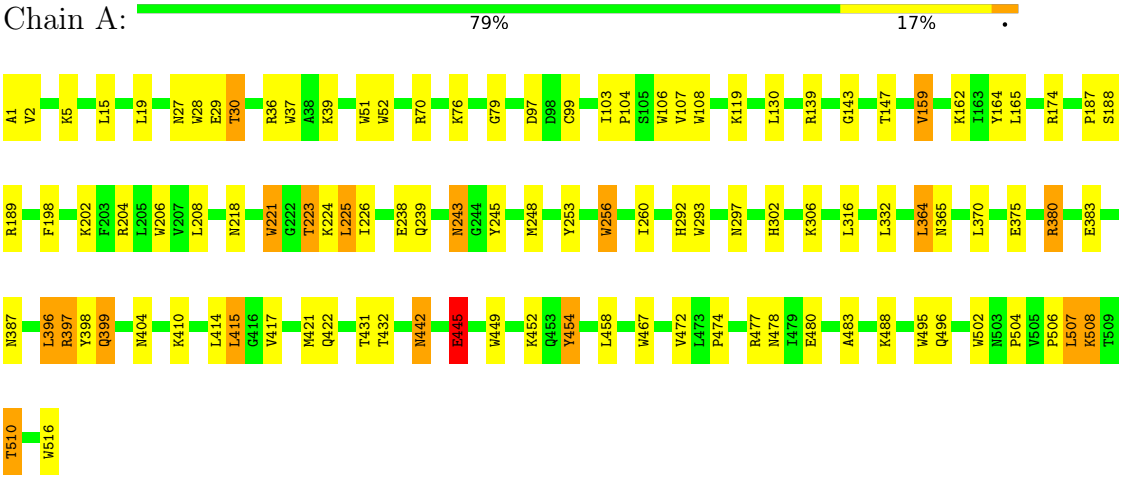
3 Residue-property plots (i)

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.

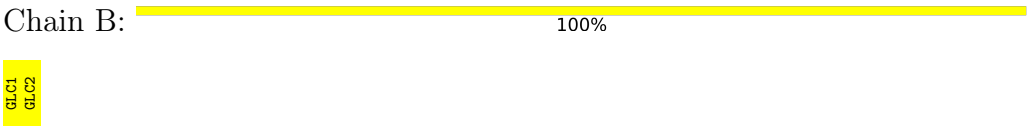
• Molecule 1: PROTEIN (BETA-AMYLASE)

Chain A:



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

Chain B:

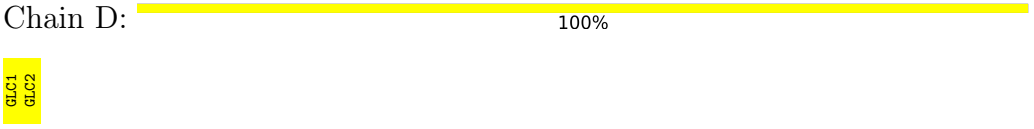


• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

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

Chain D:



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

Chain E:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.16Å 93.74Å 66.66Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	11.00 – 2.10	Depositor
% Data completeness (in resolution range)	82.3 (11.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.170 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4496	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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, ACT, CA, 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	0.86	0/4234	1.60	85/5751 (1.5%)

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	397	ARG	NE-CZ-NH2	-21.59	109.50	120.30
1	A	397	ARG	NE-CZ-NH1	16.40	128.50	120.30
1	A	70	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	454	TYR	CB-CG-CD2	-9.56	115.27	121.00
1	A	477	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	28	TRP	CD1-CG-CD2	8.59	113.17	106.30
1	A	396	LEU	CA-CB-CG	8.37	134.54	115.30
1	A	108	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	449	TRP	CD1-CG-CD2	8.27	112.91	106.30
1	A	36	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	106	TRP	CD1-CG-CD2	8.11	112.78	106.30
1	A	189	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	293	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	70	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	516	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	A	495	TRP	CD1-CG-CD2	7.86	112.58	106.30
1	A	174	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	28	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	449	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	A	37	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	108	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	A	106	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	A	206	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	A	293	TRP	CE2-CD2-CG	-7.63	101.20	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	A	37	TRP	CD1-CG-CD2	7.52	112.32	106.30
1	A	51	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	A	495	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	516	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	221	TRP	CE2-CD2-CG	-7.08	101.63	107.30
1	A	206	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	52	TRP	CE2-CD2-CG	-7.02	101.69	107.30
1	A	51	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	397	ARG	CG-CD-NE	-6.97	97.15	111.80
1	A	139	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	454	TYR	N-CA-C	6.56	128.70	111.00
1	A	52	TRP	CD1-CG-CD2	6.54	111.53	106.30
1	A	445	GLU	CA-CB-CG	6.53	127.76	113.40
1	A	477	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	502	TRP	CD1-CG-CD2	6.44	111.45	106.30
1	A	502	TRP	CE2-CD2-CG	-6.37	102.21	107.30
1	A	467	TRP	CD1-CG-CD2	6.30	111.34	106.30
1	A	364	LEU	CB-CG-CD1	-6.26	100.35	111.00
1	A	206	TRP	CB-CG-CD1	-6.22	118.92	127.00
1	A	223	THR	N-CA-CB	-6.18	98.55	110.30
1	A	467	TRP	CE2-CD2-CG	-6.16	102.38	107.30
1	A	256	TRP	CD1-CG-CD2	6.14	111.22	106.30
1	A	256	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	A	380	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	332	LEU	N-CA-C	5.95	127.05	111.00
1	A	106	TRP	CB-CG-CD1	-5.87	119.37	127.00
1	A	507	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	188	SER	N-CA-CB	-5.78	101.83	110.50
1	A	189	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	502	TRP	N-CA-C	-5.73	95.53	111.00
1	A	37	TRP	CB-CG-CD1	-5.67	119.62	127.00
1	A	454	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	245	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	106	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	A	502	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	A	417	VAL	N-CA-CB	-5.56	99.27	111.50
1	A	221	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	164	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	28	TRP	CB-CG-CD1	-5.47	119.89	127.00
1	A	293	TRP	CG-CD2-CE3	5.44	138.79	133.90
1	A	28	TRP	CG-CD1-NE1	-5.42	104.68	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	221	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	A	206	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	A	108	TRP	CB-CG-CD1	-5.38	120.01	127.00
1	A	293	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	A	99	CYS	CA-CB-SG	-5.32	104.42	114.00
1	A	449	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	119	LYS	CB-CG-CD	-5.22	98.02	111.60
1	A	204	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	364	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	108	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	A	495	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	A	28	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	A	495	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	A	449	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	A	495	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	A	206	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	A	159	VAL	CA-CB-CG2	-5.02	103.37	110.90
1	A	415	LEU	CA-CB-CG	5.01	126.82	115.30

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	4119	0	3984	36	0
2	B	23	0	21	0	0
2	C	23	0	21	1	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
3	A	4	0	3	0	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	275	0	0	4	0
All	All	4496	0	4071	36	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 4.

All (36) 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:1:ALA:HA	1:A:387:ASN:HD22	1.48	0.78
1:A:422:GLN:HE22	1:A:510:THR:H	1.38	0.72
1:A:198:PHE:O	1:A:202:LYS:HG2	1.91	0.69
1:A:383:GLU:HG2	6:A:751:HOH:O	1.95	0.67
1:A:365:ASN:HB3	6:A:779:HOH:O	2.00	0.61
1:A:422:GLN:NE2	1:A:510:THR:H	2.00	0.59
1:A:218:ASN:OD1	1:A:223:THR:HG23	2.02	0.59
1:A:27:ASN:HD22	1:A:29:GLU:H	1.51	0.58
1:A:162:LYS:HD3	6:A:768:HOH:O	2.03	0.57
1:A:442:ASN:ND2	1:A:480:GLU:H	2.05	0.55
1:A:483:ALA:H	1:A:496:GLN:HE21	1.54	0.55
1:A:218:ASN:HA	1:A:223:THR:CG2	2.41	0.51
1:A:445:GLU:HG3	1:A:474:PRO:HD3	1.94	0.49
1:A:483:ALA:H	1:A:496:GLN:NE2	2.11	0.49
1:A:218:ASN:HA	1:A:223:THR:HG22	1.95	0.48
1:A:397:ARG:HG2	1:A:399:GLN:HE22	1.79	0.47
1:A:143:GLY:O	1:A:147:THR:HG23	2.15	0.47
1:A:375:GLU:HB2	1:A:410:LYS:HD3	1.96	0.47
1:A:478:ASN:HB3	6:A:881:HOH:O	2.15	0.46
1:A:27:ASN:ND2	1:A:29:GLU:HB3	2.30	0.46
1:A:223:THR:OG1	1:A:225:LEU:HD13	2.16	0.45
1:A:39:LYS:NZ	1:A:79:GLY:O	2.49	0.45
1:A:421:MET:CE	1:A:472:VAL:HG22	2.46	0.45
1:A:104:PRO:O	1:A:107:VAL:HG12	2.18	0.44
1:A:506:PRO:HB2	1:A:508:LYS:HD2	2.00	0.44
1:A:221:TRP:HB2	1:A:223:THR:HG22	2.01	0.43
1:A:27:ASN:ND2	1:A:30:THR:H	2.16	0.43
1:A:292:HIS:HE1	2:C:1:GLC:O3	2.01	0.43
1:A:256:TRP:CZ2	1:A:260:ILE:HD11	2.53	0.43
1:A:19:LEU:CD1	1:A:97:ASP:HA	2.49	0.42
1:A:380:ARG:HH11	1:A:380:ARG:HD2	1.69	0.42
1:A:103:ILE:HD13	1:A:103:ILE:HG21	1.84	0.41
1:A:2:VAL:O	1:A:5:LYS:HG2	2.20	0.41
1:A:302:HIS:HB2	1:A:306:LYS:HE3	2.02	0.41
1:A:27:ASN:HD22	1:A:29:GLU:N	2.16	0.40
1:A:1:ALA:HB3	1:A:5:LYS:O	2.21	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	514/516 (100%)	493 (96%)	18 (4%)	3 (1%)	25 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	TYR
1	A	243	ASN
1	A	454	TYR

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	440/440 (100%)	405 (92%)	35 (8%)	12 8

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	30	THR
1	A	76	LYS
1	A	130	LEU
1	A	159	VAL
1	A	165	LEU
1	A	187	PRO
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	224	LYS
1	A	225	LEU
1	A	226	ILE
1	A	238	GLU
1	A	239	GLN
1	A	243	ASN
1	A	248	MET
1	A	297	ASN
1	A	316	LEU
1	A	364	LEU
1	A	370	LEU
1	A	396	LEU
1	A	399	GLN
1	A	404	ASN
1	A	414	LEU
1	A	415	LEU
1	A	431	THR
1	A	432	THR
1	A	442	ASN
1	A	445	GLU
1	A	452	LYS
1	A	458	LEU
1	A	488	LYS
1	A	504	PRO
1	A	507	LEU
1	A	508	LYS
1	A	510	THR

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	27	ASN
1	A	33	ASN
1	A	41	ASN
1	A	73	GLN
1	A	274	ASN
1	A	292	HIS
1	A	297	ASN
1	A	351	GLN
1	A	387	ASN
1	A	399	GLN
1	A	404	ASN

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Mol	Chain	Res	Type
1	A	422	GLN
1	A	442	ASN
1	A	463	HIS
1	A	470	ASN
1	A	496	GLN
1	A	512	HIS

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

8 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	0.85	1 (8%)	17,17,17	0.88	1 (5%)
2	GLC	B	2	2	11,11,12	0.98	0	15,15,17	1.09	1 (6%)
2	GLC	C	1	2	12,12,12	0.78	0	17,17,17	1.16	2 (11%)
2	GLC	C	2	2	11,11,12	1.07	2 (18%)	15,15,17	2.04	6 (40%)
2	GLC	D	1	2	12,12,12	0.68	0	17,17,17	1.19	1 (5%)
2	GLC	D	2	2	11,11,12	0.66	0	15,15,17	0.95	1 (6%)
2	GLC	E	1	2	12,12,12	0.68	0	17,17,17	1.19	1 (5%)
2	GLC	E	2	2	11,11,12	0.96	0	15,15,17	0.84	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
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	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	1/1/5/5	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	O4-C4	-2.33	1.37	1.43
2	C	2	GLC	C1-C2	2.11	1.57	1.52
2	B	1	GLC	C4-C5	2.09	1.57	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	O5-C1-C2	3.85	116.71	110.77
2	B	2	GLC	C1-O5-C5	3.74	117.27	112.19
2	C	2	GLC	C2-C3-C4	-3.19	105.38	110.89
2	E	1	GLC	O4-C4-C3	-3.14	103.09	110.35
2	C	2	GLC	O5-C5-C4	-3.03	103.47	110.83
2	D	1	GLC	C1-C2-C3	-2.97	104.15	110.31
2	C	2	GLC	O5-C5-C6	2.91	111.77	107.20
2	C	1	GLC	O5-C5-C4	-2.40	105.33	109.69
2	C	2	GLC	C6-C5-C4	2.29	118.38	113.00
2	C	2	GLC	O3-C3-C2	2.29	114.37	109.99
2	C	1	GLC	C6-C5-C4	2.27	118.33	113.00
2	D	2	GLC	C1-O5-C5	2.20	115.18	112.19
2	B	1	GLC	C6-C5-C4	2.03	117.75	113.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	GLC	C1
2	D	1	GLC	C1
2	E	1	GLC	C1

All (4) torsion outliers are listed below:

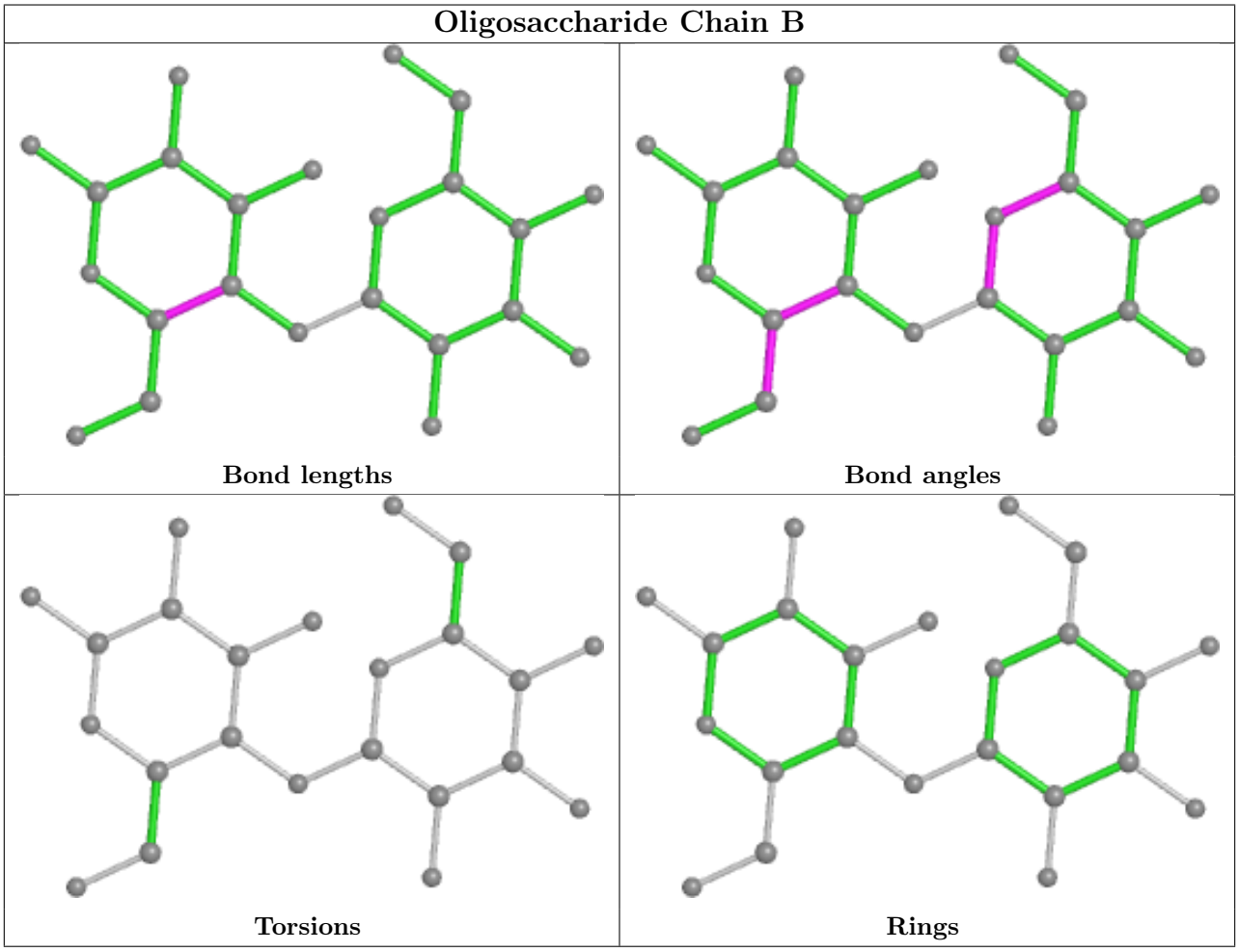
Mol	Chain	Res	Type	Atoms
2	C	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6

There are no ring outliers.

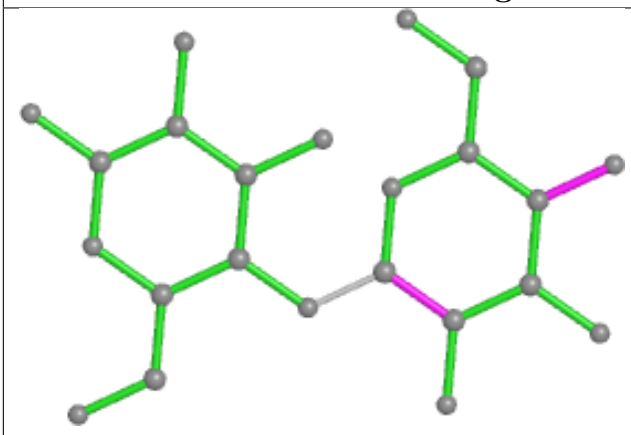
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	0

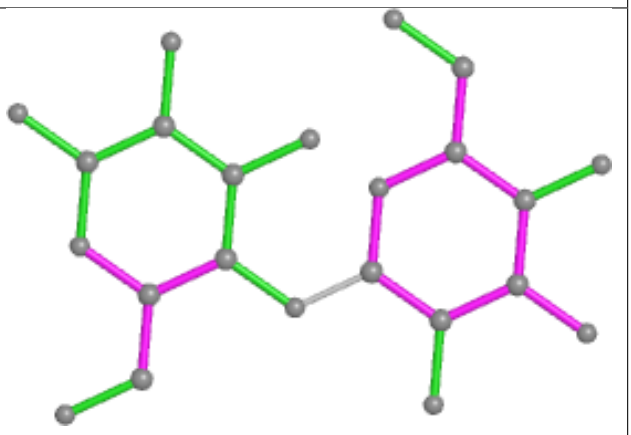
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



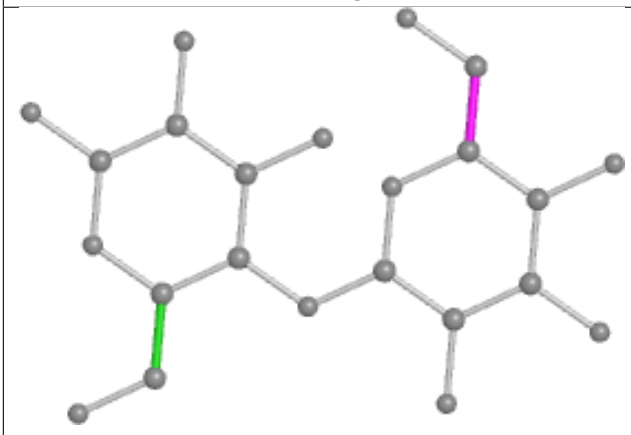
Oligosaccharide Chain C



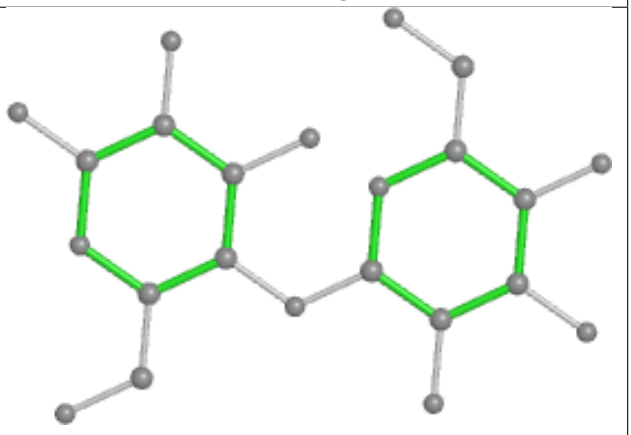
Bond lengths



Bond angles

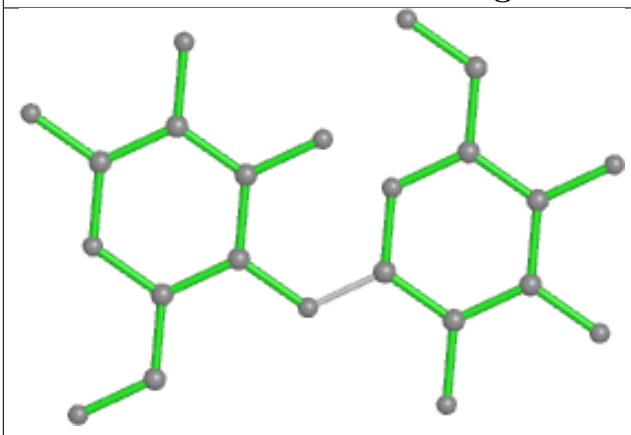


Torsions

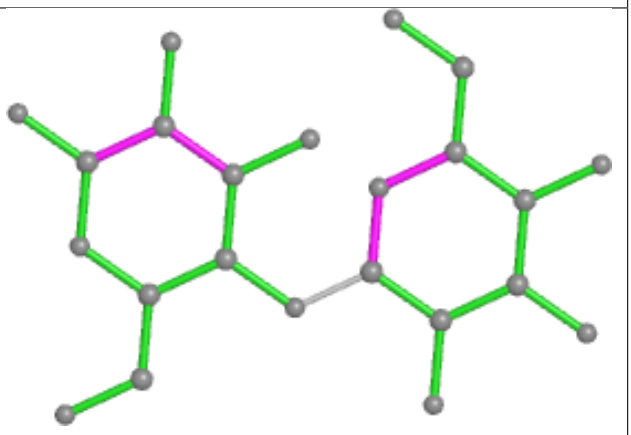


Rings

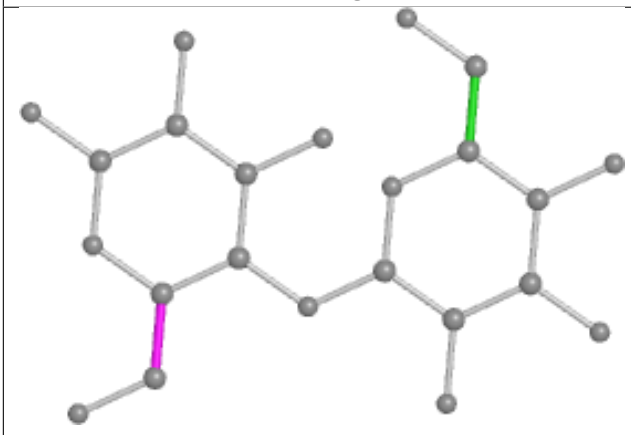
Oligosaccharide Chain D



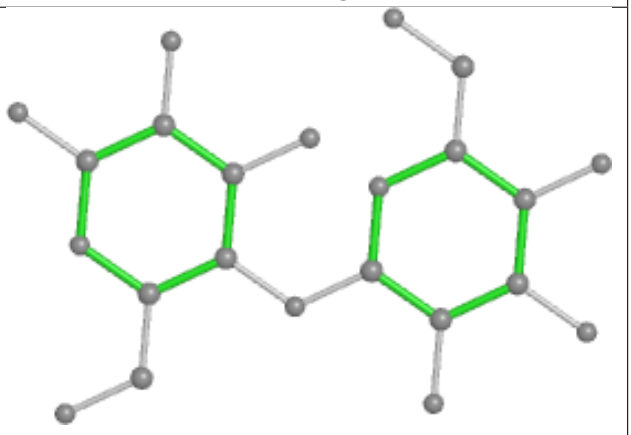
Bond lengths



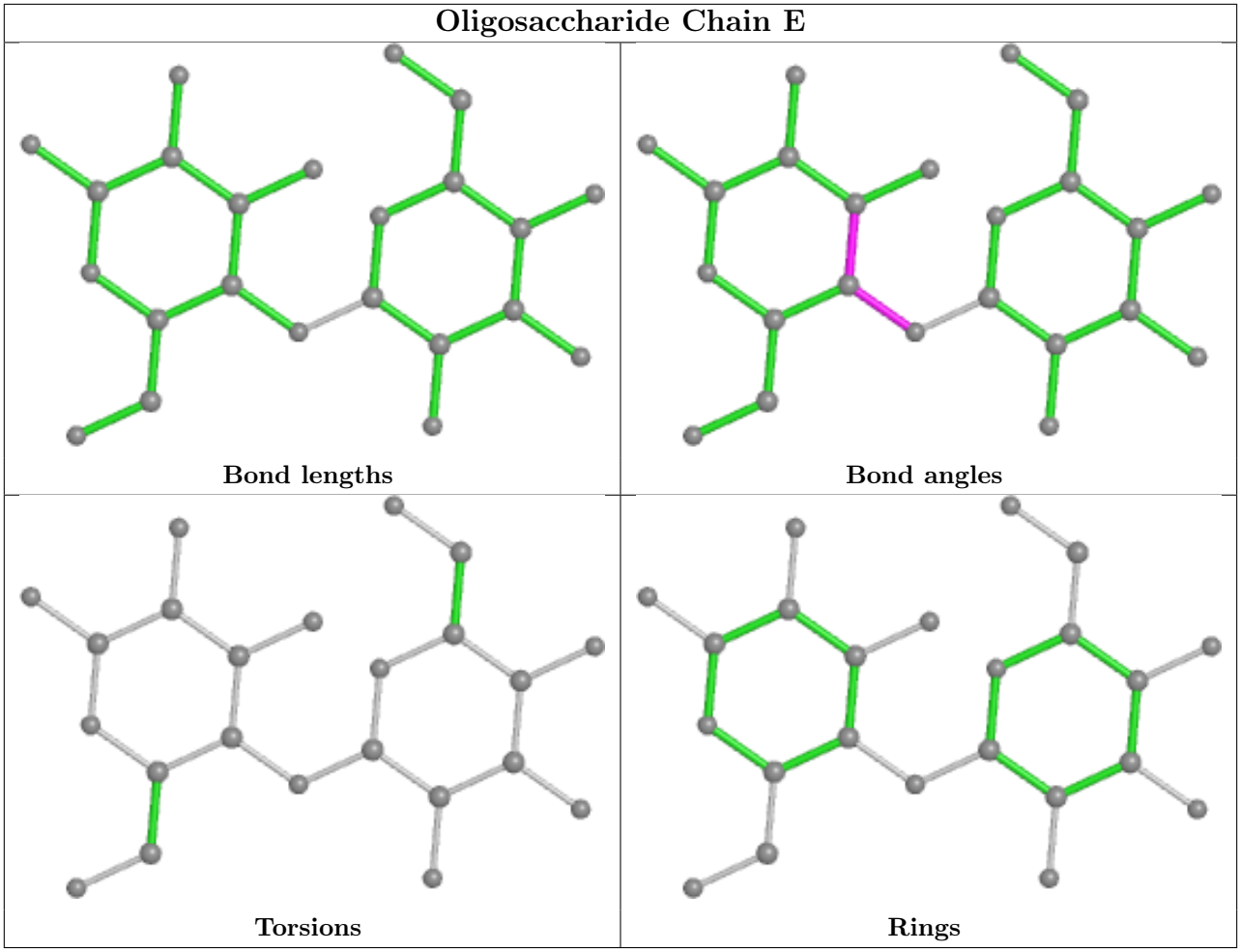
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	ACT	A	920	-	3,3,3	1.03	0	3,3,3	0.77	0
4	SO4	A	921	-	4,4,4	0.32	0	6,6,6	0.51	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.