Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 12:59 PM EDT

PDB ID	:	1JDD
Title	:	MUTANT (E219Q) MALTOTETRAOSE-FORMING EXO-AMYLASE COCRYSTALLIZED WITH MALTOTETRAOSE (CRYSTAL TYPE 2)
Authors	:	Yoshioka, Y.; Hasegawa, K.; Matsuura, Y.; Katsube, Y.; Kubota, M.
Deposited on	:	1997-06-16
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

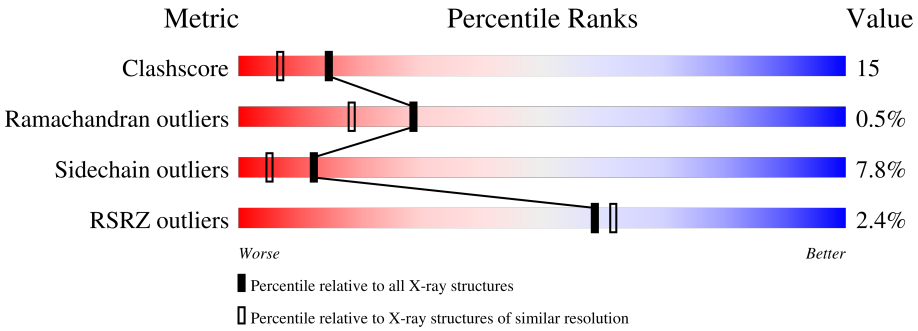
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	2% 68% 22% 7%
2	B	4	75% 25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3496 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 1,4-ALPHA MALTOTETRAHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3297	2070	597	620	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLN	GLU	engineered mutation	UNP P13507
A	334	ASP	SER	conflict	UNP P13507

- 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
2	B	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

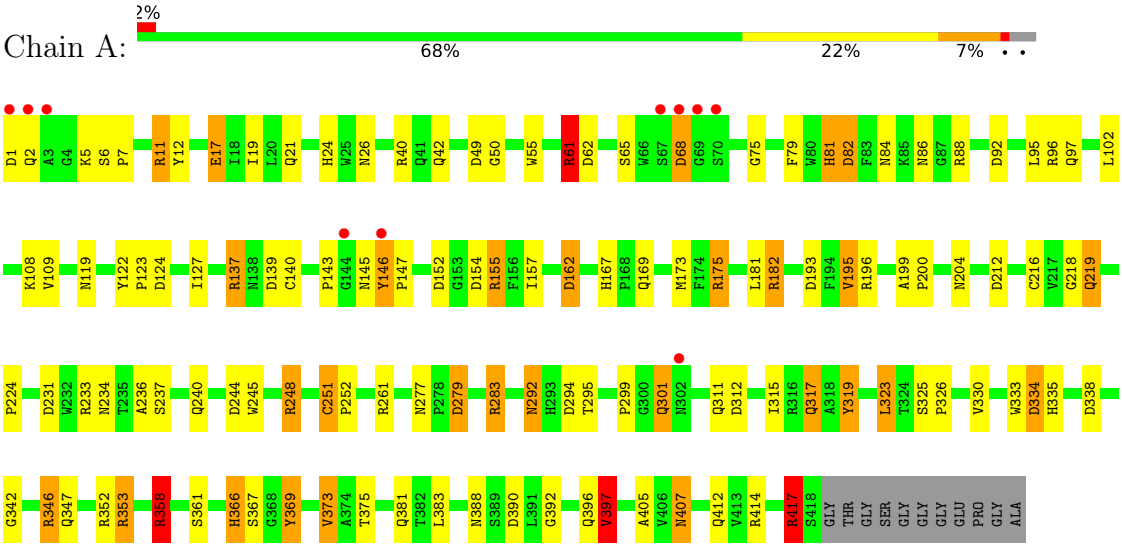
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

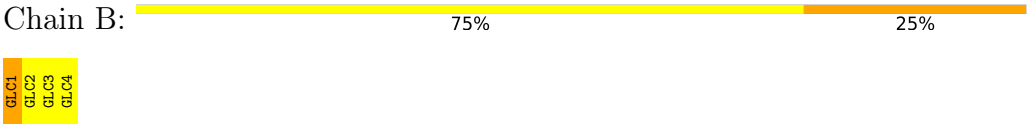
• Molecule 1: 1,4-ALPHA MALTOTETRAHYDROLASE

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.60Å 170.70Å 46.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 26.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 83.9 (26.10-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 1.91Å)	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.191 , (Not available) 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3496	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.91	2/3402 (0.1%)	1.89	65/4631 (1.4%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ASP	CA-CB	6.79	1.68	1.53
1	A	17	GLU	CD-OE2	-5.02	1.20	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	ARG	CD-NE-CZ	40.12	179.78	123.60
1	A	346	ARG	CD-NE-CZ	28.56	163.59	123.60
1	A	346	ARG	NE-CZ-NH1	24.01	132.31	120.30
1	A	175	ARG	NE-CZ-NH1	17.44	129.02	120.30
1	A	82	ASP	CB-CG-OD1	-17.16	102.85	118.30
1	A	61	ARG	NE-CZ-NH1	16.93	128.77	120.30
1	A	137	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	A	61	ARG	NE-CZ-NH2	-14.22	113.19	120.30
1	A	414	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	358	ARG	NE-CZ-NH1	-10.39	115.10	120.30
1	A	358	ARG	NE-CZ-NH2	10.15	125.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	A	248	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	175	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	175	ARG	CD-NE-CZ	9.44	136.81	123.60
1	A	417	ARG	CD-NE-CZ	-9.25	110.64	123.60
1	A	233	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	A	233	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	346	ARG	NH1-CZ-NH2	-8.70	109.83	119.40
1	A	11	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	A	96	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	347	GLN	CA-CB-CG	8.50	132.09	113.40
1	A	231	ASP	CB-CG-OD1	8.46	125.91	118.30
1	A	82	ASP	CB-CA-C	-8.23	93.95	110.40
1	A	137	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	283	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	A	414	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	61	ARG	CD-NE-CZ	7.54	134.16	123.60
1	A	139	ASP	CB-CG-OD2	7.46	125.02	118.30
1	A	82	ASP	CB-CG-OD2	7.45	125.01	118.30
1	A	279	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	139	ASP	CB-CG-OD1	-7.18	111.83	118.30
1	A	319	TYR	CB-CG-CD1	-7.11	116.73	121.00
1	A	390	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	152	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	353	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	A	68	ASP	N-CA-CB	6.85	122.92	110.60
1	A	352	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	182	ARG	CD-NE-CZ	-6.68	114.25	123.60
1	A	244	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	A	82	ASP	CA-CB-CG	-6.41	99.30	113.40
1	A	397	VAL	N-CA-CB	-6.22	97.82	111.50
1	A	373	VAL	CA-CB-CG1	6.13	120.09	110.90
1	A	417	ARG	CB-CA-C	-6.11	98.17	110.40
1	A	140	CYS	CA-CB-SG	5.92	124.67	114.00
1	A	414	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	146	TYR	CB-CG-CD2	5.69	124.41	121.00
1	A	261	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	397	VAL	CG1-CB-CG2	5.57	119.80	110.90
1	A	334	ASP	CA-CB-CG	-5.51	101.28	113.40
1	A	369	TYR	CA-CB-CG	-5.42	103.09	113.40
1	A	155	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	353	ARG	NE-CZ-NH2	5.32	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	366	HIS	C-N-CA	5.28	134.90	121.70
1	A	88	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	251	CYS	CA-CB-SG	5.25	123.44	114.00
1	A	17	GLU	CG-CD-OE2	5.24	128.79	118.30
1	A	212	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	124	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	347	GLN	N-CA-CB	5.21	119.97	110.60
1	A	81	HIS	C-N-CA	5.12	134.51	121.70
1	A	417	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	152	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	88	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	196	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	ARG	Sidechain

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	3297	0	3015	97	0
2	B	45	0	38	1	0
3	A	2	0	0	0	0
4	A	152	0	0	7	0
All	All	3496	0	3053	97	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 15.

All (97) 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:299:PRO:HD3	1:A:334:ASP:OD2	1.55	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:CYS:HB3	4:A:623:HOH:O	1.59	1.00
1:A:237:SER:H	1:A:240:GLN:HE21	1.10	1.00
1:A:405:ALA:HB2	1:A:417:ARG:HD3	1.48	0.96
1:A:193:ASP:OD1	2:B:1:GLC:H1	1.65	0.95
1:A:167:HIS:HD2	1:A:169:GLN:H	1.14	0.92
1:A:277:ASN:HD22	1:A:279:ASP:H	1.21	0.88
1:A:317:GLN:H	1:A:317:GLN:HE21	1.20	0.85
1:A:61:ARG:HD2	1:A:84:ASN:HB3	1.62	0.82
1:A:237:SER:H	1:A:240:GLN:NE2	1.77	0.81
1:A:61:ARG:CD	1:A:84:ASN:HB3	2.13	0.79
1:A:216:CYS:O	1:A:252:PRO:HD2	1.84	0.78
1:A:145:ASN:ND2	1:A:155:ARG:H	1.82	0.78
1:A:11:ARG:HH22	1:A:204:ASN:ND2	1.83	0.77
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.19	0.73
1:A:11:ARG:HH12	1:A:204:ASN:HD22	1.33	0.73
1:A:145:ASN:HD21	1:A:154:ASP:HB3	1.56	0.71
1:A:195:VAL:HG13	1:A:245:TRP:NE1	2.06	0.71
1:A:167:HIS:CD2	1:A:169:GLN:H	2.05	0.70
1:A:299:PRO:CD	1:A:334:ASP:OD2	2.37	0.69
1:A:146:TYR:CD1	1:A:147:PRO:HD2	2.27	0.69
1:A:82:ASP:HB3	1:A:84:ASN:H	1.58	0.69
1:A:277:ASN:ND2	1:A:279:ASP:H	1.90	0.69
1:A:145:ASN:HD21	1:A:155:ARG:H	1.39	0.69
1:A:127:ILE:HG21	1:A:173:MET:HE1	1.76	0.66
1:A:61:ARG:HD3	1:A:82:ASP:HB2	1.77	0.65
1:A:366:HIS:HB2	1:A:373:VAL:HG22	1.81	0.62
1:A:237:SER:N	1:A:240:GLN:HE21	1.90	0.60
1:A:407:ASN:C	1:A:407:ASN:HD22	2.05	0.59
1:A:405:ALA:CB	1:A:417:ARG:HD3	2.28	0.59
1:A:61:ARG:HD3	1:A:82:ASP:CB	2.33	0.58
1:A:81:HIS:HD2	4:A:509:HOH:O	1.87	0.57
1:A:86:ASN:ND2	1:A:92:ASP:H	2.04	0.56
1:A:381:GLN:OE1	1:A:417:ARG:HG2	2.08	0.54
1:A:127:ILE:CG2	1:A:173:MET:HE1	2.37	0.54
1:A:50:GLY:HA2	1:A:353:ARG:HH12	1.74	0.53
1:A:292:ASN:C	1:A:292:ASN:HD22	2.12	0.53
1:A:11:ARG:NH1	1:A:204:ASN:HD22	2.06	0.52
1:A:167:HIS:HD2	1:A:169:GLN:N	1.96	0.52
1:A:146:TYR:CE1	1:A:147:PRO:HD2	2.45	0.52
1:A:251:CYS:CB	4:A:623:HOH:O	2.34	0.51
1:A:292:ASN:ND2	1:A:295:THR:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLN:HE22	1:A:358:ARG:NH1	2.11	0.49
1:A:24:HIS:HD2	1:A:26:ASN:H	1.60	0.48
1:A:17:GLU:OE2	1:A:108:LYS:HE2	2.14	0.48
1:A:137:ARG:NH2	1:A:146:TYR:O	2.28	0.47
1:A:317:GLN:HE21	1:A:317:GLN:N	2.02	0.47
1:A:342:GLY:O	1:A:346:ARG:HB2	2.14	0.47
1:A:167:HIS:CD2	1:A:169:GLN:HB3	2.50	0.47
1:A:277:ASN:O	1:A:283:ARG:HD3	2.15	0.47
1:A:326:PRO:HG3	1:A:361:SER:O	2.14	0.47
1:A:325:SER:HB2	1:A:326:PRO:HD2	1.96	0.46
1:A:127:ILE:HD13	1:A:173:MET:HE1	1.98	0.46
1:A:301:GLN:HG2	4:A:643:HOH:O	2.15	0.46
1:A:317:GLN:H	1:A:317:GLN:NE2	2.01	0.46
1:A:195:VAL:CG1	1:A:245:TRP:CE2	2.99	0.45
1:A:195:VAL:HG11	1:A:245:TRP:CE2	2.52	0.45
1:A:40:ARG:HD3	1:A:97:GLN:HB3	1.99	0.45
1:A:319:TYR:OH	1:A:335:HIS:CD2	2.69	0.45
1:A:319:TYR:OH	1:A:335:HIS:HD2	2.00	0.45
1:A:62:ASP:O	1:A:75:GLY:HA2	2.17	0.45
1:A:334:ASP:OD1	1:A:338:ASP:OD2	2.35	0.44
1:A:388:ASN:HD22	1:A:412:GLN:HB3	1.82	0.44
1:A:24:HIS:CD2	1:A:299:PRO:HD2	2.52	0.44
1:A:292:ASN:ND2	1:A:294:ASP:H	2.15	0.44
1:A:199:ALA:HA	1:A:200:PRO:HD3	1.91	0.44
1:A:388:ASN:ND2	1:A:412:GLN:HB3	2.33	0.44
1:A:146:TYR:CG	1:A:147:PRO:HD2	2.52	0.44
1:A:236:ALA:HB1	1:A:240:GLN:NE2	2.33	0.44
1:A:200:PRO:HG2	1:A:248:ARG:CZ	2.49	0.43
1:A:219:GLN:O	1:A:219:GLN:HG3	2.17	0.43
1:A:366:HIS:HE1	1:A:375:THR:OG1	2.01	0.43
1:A:1:ASP:OD2	1:A:108:LYS:NZ	2.48	0.43
1:A:19:ILE:HB	1:A:330:VAL:HG22	2.00	0.43
1:A:224:PRO:O	1:A:234:ASN:HA	2.19	0.43
1:A:155:ARG:HA	1:A:162:ASP:OD2	2.18	0.43
1:A:122:TYR:CD1	1:A:123:PRO:HD2	2.54	0.43
1:A:407:ASN:C	1:A:407:ASN:ND2	2.72	0.42
1:A:122:TYR:HA	1:A:123:PRO:HD2	1.91	0.42
1:A:11:ARG:NH2	1:A:204:ASN:ND2	2.60	0.42
1:A:42:GLN:HG3	4:A:620:HOH:O	2.19	0.42
1:A:218:GLY:HA3	1:A:245:TRP:CH2	2.54	0.42
1:A:392:GLY:N	1:A:396:GLN:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TYR:HB2	1:A:373:VAL:HG11	2.02	0.42
1:A:6:SER:HB2	1:A:7:PRO:CD	2.49	0.42
1:A:417:ARG:HD2	4:A:552:HOH:O	2.20	0.41
1:A:42:GLN:CG	4:A:620:HOH:O	2.67	0.41
1:A:21:GLN:O	1:A:333:TRP:HB2	2.20	0.41
1:A:325:SER:HB2	1:A:326:PRO:CD	2.50	0.41
1:A:319:TYR:O	1:A:323:LEU:HB2	2.21	0.41
1:A:2:GLN:NE2	1:A:358:ARG:NH1	2.69	0.41
1:A:311:GLN:HE21	1:A:311:GLN:HB3	1.68	0.41
1:A:366:HIS:CG	1:A:397:VAL:HG22	2.56	0.40
1:A:50:GLY:HA2	1:A:353:ARG:NH1	2.37	0.40
1:A:146:TYR:CD1	1:A:147:PRO:CD	3.01	0.40
1:A:49:ASP:CG	1:A:346:ARG:HH11	2.25	0.40
1:A:312:ASP:HA	1:A:315:ILE:CD1	2.52	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	416/429 (97%)	396 (95%)	18 (4%)	2 (0%)	29 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ILE
1	A	143	PRO

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	333/337 (99%)	307 (92%)	26 (8%)	12 5

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	12	TYR
1	A	55	TRP
1	A	61	ARG
1	A	65	SER
1	A	68	ASP
1	A	79	PHE
1	A	95	LEU
1	A	102	LEU
1	A	109	VAL
1	A	119	ASN
1	A	162	ASP
1	A	175	ARG
1	A	181	LEU
1	A	182	ARG
1	A	195	VAL
1	A	219	GLN
1	A	292	ASN
1	A	301	GLN
1	A	317	GLN
1	A	323	LEU
1	A	358	ARG
1	A	367	SER
1	A	383	LEU
1	A	397	VAL
1	A	407	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	24	HIS
1	A	26	ASN
1	A	81	HIS
1	A	86	ASN
1	A	119	ASN
1	A	128	ASN
1	A	145	ASN
1	A	167	HIS
1	A	204	ASN
1	A	240	GLN
1	A	264	ASN
1	A	277	ASN
1	A	292	ASN
1	A	311	GLN
1	A	317	GLN
1	A	335	HIS
1	A	347	GLN
1	A	366	HIS
1	A	388	ASN
1	A	407	ASN

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)

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	1.27	1 (8%)	17,17,17	2.49	5 (29%)
2	GLC	B	2	2	11,11,12	0.96	0	15,15,17	1.89	3 (20%)
2	GLC	B	3	2	11,11,12	0.49	0	15,15,17	1.24	2 (13%)
2	GLC	B	4	2	11,11,12	0.59	0	15,15,17	1.55	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	-	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	-	2/2/19/22	0/1/1/1
2	GLC	B	4	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	C1-C2	-2.10	1.47	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	GLC	C1-O5-C5	7.49	127.79	113.66
2	B	2	GLC	C1-O5-C5	4.75	118.63	112.19
2	B	1	GLC	O5-C1-C2	4.07	117.54	110.28
2	B	2	GLC	O5-C1-C2	3.53	116.23	110.77
2	B	4	GLC	O3-C3-C2	3.29	116.29	109.99
2	B	4	GLC	C1-O5-C5	3.28	116.64	112.19
2	B	1	GLC	O3-C3-C2	-2.74	104.03	110.35
2	B	4	GLC	C1-C2-C3	2.64	112.91	109.67
2	B	2	GLC	O4-C4-C5	2.48	115.45	109.30
2	B	3	GLC	C1-O5-C5	2.30	115.31	112.19
2	B	1	GLC	O2-C2-C1	2.30	114.48	109.16
2	B	1	GLC	O1-C1-C2	2.27	115.43	109.03
2	B	3	GLC	O3-C3-C2	-2.07	106.02	109.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

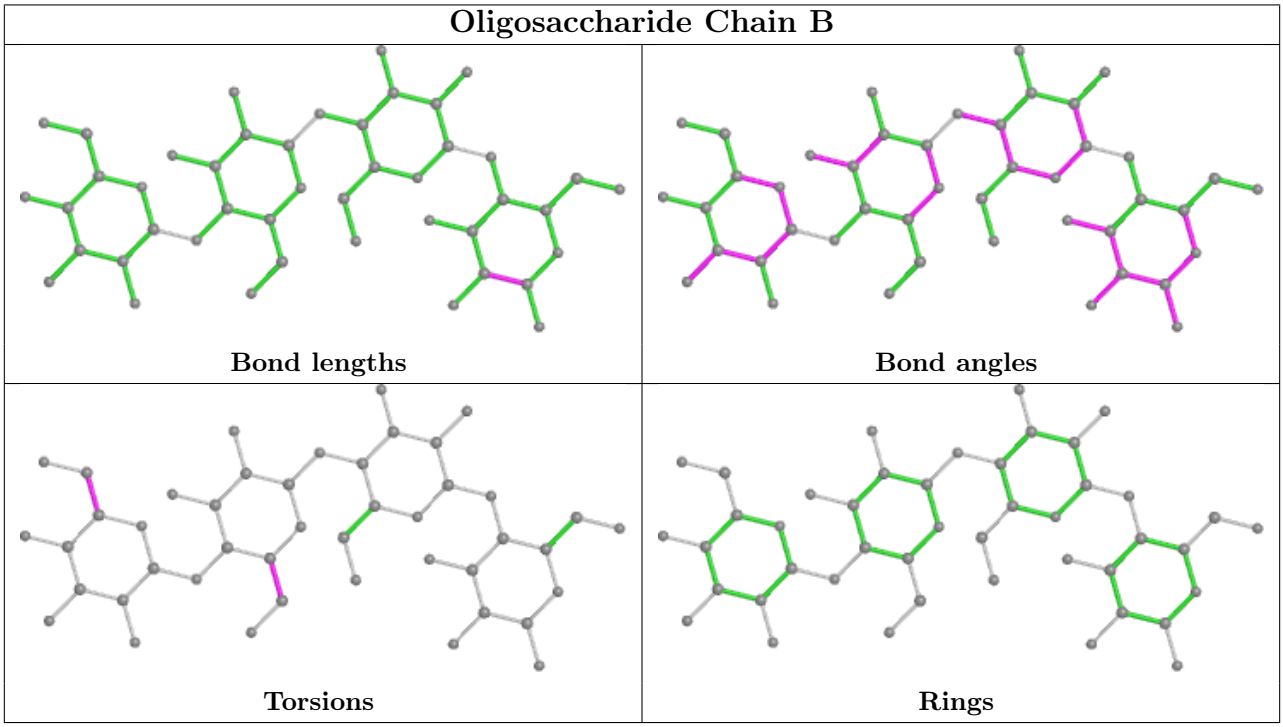
Mol	Chain	Res	Type	Atoms
2	B	3	GLC	O5-C5-C6-O6
2	B	4	GLC	O5-C5-C6-O6
2	B	4	GLC	C4-C5-C6-O6
2	B	3	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	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.



5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	418/429 (97%)	-0.34	10 (2%) 59 62	11, 19, 33, 54	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLN	6.5
1	A	3	ALA	5.3
1	A	1	ASP	4.8
1	A	146	TYR	3.4
1	A	68	ASP	2.9
1	A	70	SER	2.5
1	A	69	GLY	2.4
1	A	302	ASN	2.4
1	A	144	GLY	2.3
1	A	67	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	B	4	11/12	0.96	0.07	23,24,26,26	0
2	GLC	B	2	11/12	0.97	0.07	16,17,18,19	0

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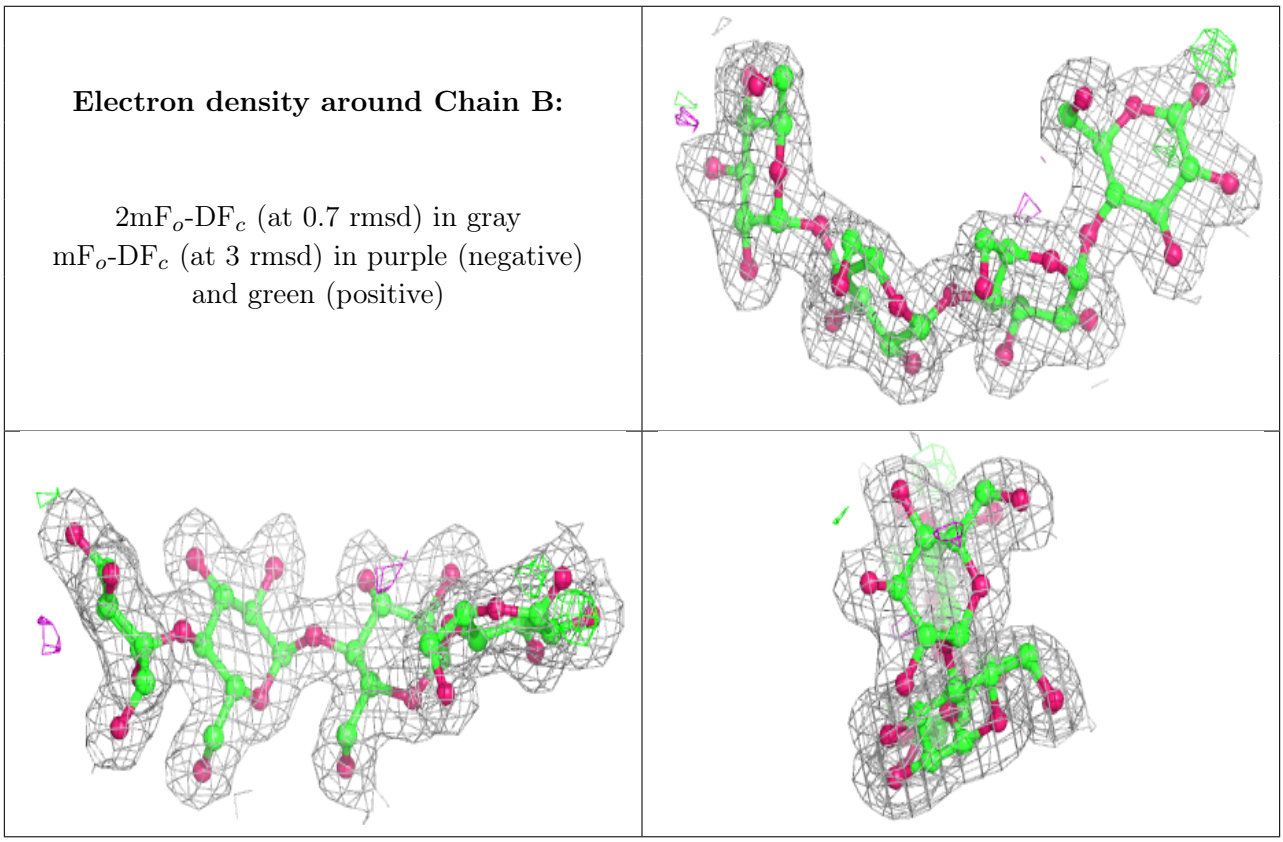
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	B	3	11/12	0.97	0.05	21,22,23,24	0
2	GLC	B	1	12/12	0.97	0.10	15,15,16,17	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	A	452	1/1	0.97	0.20	43,43,43,43	0
3	CA	A	451	1/1	0.99	0.06	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.