



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:25 AM EDT

PDB ID : 2FHC / pdb_00002fhc
Title : Crystal Structure Analysis of Klebsiella pneumoniae pullulanase complexed with maltotriose
Authors : Mikami, B.; Iwamoto, H.; Katsuya, Y.; Yoon, H.-J.; Demirkan-Sarikaya, E.; Malle, D.
Deposited on : 2005-12-23
Resolution : 1.85 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

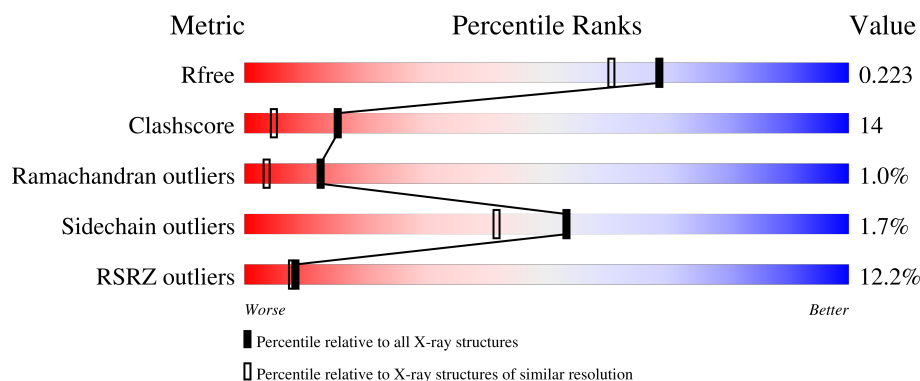
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 $\leq 5\%$. 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	1083	
2	B	3	
2	C	3	
3	D	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9357 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 Alpha-dextrin endo-1,6-alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	20	0
			8142	5088	1388	1639	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	conflict	UNP W9BQ28

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	3	Total	C	O	0	0	0
			34	18	16			
2	C	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

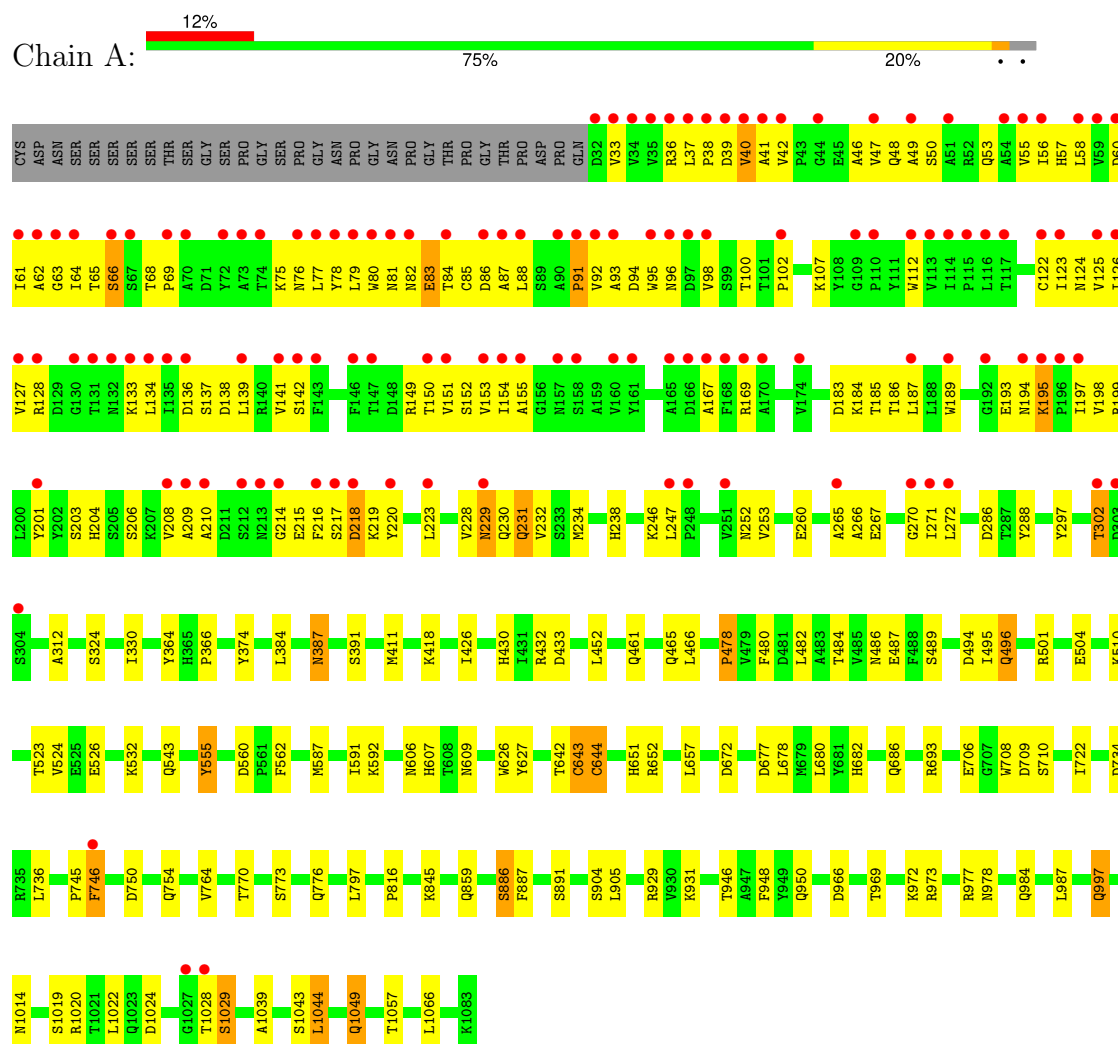
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1119	Total 1119	O 1119	0	0

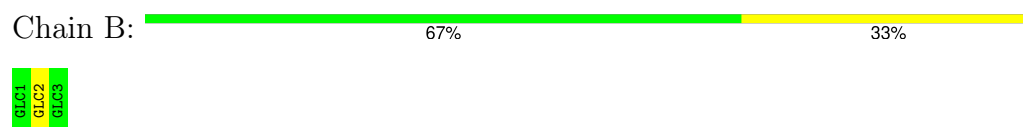
3 Residue-property plots

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 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: Alpha-dextrin endo-1,6-alpha-glucosidase



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



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

Chain C:  33% 67%

GLC1
GLC2
GLC3

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.54Å 60.66Å 135.39Å 90.00° 113.59° 90.00°	Depositor
Resolution (Å)	14.99 – 1.85 14.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.9 (14.99-1.85) 91.8 (14.99-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.214 0.187 , 0.223	Depositor DCC
R_{free} test set	8791 reflections (9.32%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9357	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GLC, CA

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	0.36	0/8387	0.90	26/11418 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	644	CYS	N-CA-CB	-9.53	102.72	111.59
1	A	555	TYR	N-CA-C	7.82	121.99	109.24
1	A	484	THR	N-CA-C	7.71	122.07	113.21
1	A	652	ARG	N-CA-C	7.26	119.83	111.11
1	A	426	ILE	N-CA-C	7.18	119.79	108.87
1	A	931	LYS	N-CA-C	6.93	119.43	111.11
1	A	845	LYS	N-CA-C	6.79	121.86	113.50
1	A	891	SER	N-CA-C	6.61	120.33	112.93
1	A	480	PHE	N-CA-C	-6.13	100.86	110.36
1	A	644	CYS	N-CA-C	6.10	117.30	108.34
1	A	288	TYR	N-CA-C	5.93	121.18	113.88
1	A	312	ALA	CA-C-N	5.70	125.37	119.56
1	A	312	ALA	C-N-CA	5.70	125.37	119.56
1	A	1044	LEU	N-CA-C	-5.69	106.19	113.01
1	A	905	LEU	N-CA-C	5.62	119.43	112.58
1	A	189	TRP	CA-C-N	5.58	124.78	118.97
1	A	189	TRP	C-N-CA	5.58	124.78	118.97
1	A	904	SER	N-CA-C	-5.53	106.53	113.28
1	A	1019	SER	N-CA-C	-5.40	101.66	110.20
1	A	489	SER	N-CA-C	5.36	117.81	111.33
1	A	297	TYR	N-CA-C	5.28	117.88	109.81
1	A	562	PHE	N-CA-C	-5.19	106.03	112.93
1	A	532	LYS	N-CA-C	5.17	116.60	111.07
1	A	770	THR	N-CA-C	5.10	117.29	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	764	VAL	N-CA-C	5.04	117.39	111.09
1	A	302	THR	N-CA-C	-5.03	101.81	109.65

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	8142	0	7841	219	0
2	B	34	0	30	0	0
2	C	34	0	30	2	0
3	D	23	0	21	0	0
4	A	5	0	0	0	0
5	A	1119	0	0	13	0
All	All	9357	0	7922	219	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 14.

All (219) 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:81:ASN:HB2	1:A:86:ASP:HA	1.44	0.98
1:A:978:ASN:HD21	1:A:984:GLN:H	1.16	0.92
1:A:40:VAL:HG13	1:A:41:ALA:H	1.38	0.89
1:A:81:ASN:HD22	1:A:88:LEU:HB2	1.38	0.89
1:A:83:GLU:HG3	1:A:84:THR:H	1.39	0.88
1:A:680:LEU:HD11	5:A:1543:HOH:O	1.78	0.84
1:A:127:VAL:HG21	1:A:153:VAL:HG21	1.59	0.82
1:A:972[A]:LYS:HE2	1:A:973:ARG:HE	1.47	0.80
1:A:606:ASN:HD21	1:A:607:HIS:HD2	1.31	0.79
1:A:452[A]:LEU:HD12	1:A:587:MET:HG3	1.64	0.78
1:A:229:ASN:HD21	1:A:232:VAL:CG2	1.99	0.76
1:A:229:ASN:HD21	1:A:232:VAL:HG23	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:HD2	1:A:185:THR:H	1.50	0.75
1:A:972[A]:LYS:HG3	1:A:973:ARG:HG3	1.69	0.75
1:A:79:LEU:HB3	1:A:88:LEU:HD13	1.70	0.74
1:A:722:ILE:HD12	5:A:2376:HOH:O	1.87	0.74
1:A:82:ASN:ND2	1:A:83:GLU:HG2	2.02	0.73
1:A:37:LEU:HD13	1:A:169:ARG:HB3	1.73	0.71
1:A:76:ASN:ND2	1:A:128:ARG:HH21	1.90	0.69
1:A:219:LYS:H	1:A:219:LYS:HD3	1.58	0.69
1:A:560:ASP:HB3	1:A:609:ASN:ND2	2.09	0.68
1:A:680:LEU:HG	1:A:710:SER:HB3	1.76	0.67
1:A:523:THR:OG1	1:A:526:GLU:HG3	1.93	0.67
1:A:606:ASN:ND2	1:A:607:HIS:HD2	1.90	0.67
1:A:184:LYS:HD2	1:A:185:THR:N	2.10	0.66
1:A:501:ARG:O	1:A:504:GLU:HG2	1.96	0.66
1:A:50:SER:H	1:A:53:GLN:NE2	1.94	0.66
1:A:82:ASN:HD22	1:A:83:GLU:HG2	1.60	0.66
1:A:627:TYR:O	1:A:651:HIS:HD2	1.79	0.66
1:A:40:VAL:HG13	1:A:41:ALA:N	2.10	0.65
1:A:972[A]:LYS:HE2	1:A:973:ARG:NE	2.11	0.65
1:A:76:ASN:HD21	1:A:128:ARG:HH21	1.45	0.65
1:A:1049:GLN:HG3	1:A:1057:THR:HB	1.78	0.65
1:A:680:LEU:HD13	1:A:708:TRP:HB2	1.80	0.64
1:A:61:ILE:O	1:A:64:ILE:HG12	1.98	0.63
1:A:1028:THR:O	1:A:1029:SER:HB3	1.99	0.63
1:A:680:LEU:HD23	1:A:680:LEU:H	1.65	0.62
1:A:560:ASP:HB3	1:A:609:ASN:HD22	1.64	0.62
1:A:40:VAL:HG22	1:A:41:ALA:N	2.15	0.62
1:A:184:LYS:HD3	1:A:185:THR:HG23	1.80	0.61
1:A:324:SER:HB3	1:A:330[A]:ILE:HD11	1.81	0.61
1:A:75:LYS:O	1:A:102:PRO:HD3	2.00	0.61
1:A:78:TYR:HB3	1:A:126:ILE:HB	1.83	0.60
1:A:123:ILE:HD11	1:A:141:VAL:HB	1.83	0.60
1:A:193:GLU:O	1:A:194:ASN:HB2	2.00	0.60
1:A:81:ASN:CB	1:A:86:ASP:HA	2.28	0.59
1:A:411[A]:MET:HE3	5:A:2250:HOH:O	2.02	0.59
1:A:987:LEU:HD21	1:A:1022:LEU:HD21	1.84	0.59
1:A:465:GLN:HG3	1:A:950:GLN:HE22	1.67	0.58
1:A:452[A]:LEU:HD12	1:A:587:MET:CG	2.32	0.58
1:A:87:ALA:HB3	1:A:123:ILE:HG23	1.84	0.58
1:A:55:VAL:HG23	1:A:150:THR:HG23	1.85	0.58
1:A:969:THR:HA	1:A:972[A]:LYS:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HD12	1:A:123:ILE:O	2.04	0.57
1:A:197:ILE:HD12	1:A:270:GLY:HA2	1.86	0.57
1:A:706:GLU:OE2	2:C:1:GLC:H1	2.05	0.57
1:A:80:TRP:CZ3	1:A:126:ILE:HG13	2.40	0.57
1:A:79:LEU:O	1:A:92:VAL:HG22	2.04	0.57
1:A:680:LEU:HD23	1:A:680:LEU:N	2.19	0.57
1:A:50:SER:H	1:A:53:GLN:HE21	1.52	0.56
1:A:682:HIS:HD2	1:A:686:GLN:NE2	2.03	0.56
1:A:80:TRP:HZ3	1:A:126:ILE:HG13	1.69	0.56
1:A:411[B]:MET:HE2	1:A:672:ASP:OD1	2.05	0.56
1:A:246:LYS:HD3	1:A:247:LEU:N	2.21	0.56
1:A:95:TRP:HH2	1:A:133:LYS:HG2	1.71	0.55
1:A:139:LEU:HD12	1:A:139:LEU:H	1.70	0.55
1:A:1039:ALA:HB3	1:A:1043:SER:HB2	1.88	0.55
1:A:85:CYS:HB3	1:A:122:CYS:O	2.07	0.55
1:A:195:LYS:HE3	1:A:195:LYS:N	2.21	0.55
1:A:682:HIS:HD2	1:A:686:GLN:HE22	1.54	0.55
1:A:107:LYS:H	1:A:107:LYS:HD2	1.71	0.55
1:A:272:LEU:HD23	1:A:272:LEU:C	2.31	0.55
1:A:816:PRO:HG2	5:A:1995:HOH:O	2.07	0.55
1:A:229:ASN:HD21	1:A:232:VAL:CB	2.20	0.54
1:A:929:ARG:HD2	5:A:1588:HOH:O	2.07	0.54
1:A:76:ASN:HD21	1:A:128:ARG:NH2	2.06	0.54
1:A:229:ASN:HD22	1:A:229:ASN:N	2.06	0.53
1:A:642:THR:O	1:A:643:CYS:HB3	2.08	0.53
1:A:678:LEU:C	1:A:680:LEU:HD23	2.33	0.53
1:A:496:GLN:H	1:A:496:GLN:NE2	2.06	0.53
1:A:977:ARG:NH1	1:A:1024:ASP:HB3	2.24	0.53
1:A:495:ILE:HA	1:A:524:VAL:HB	1.91	0.53
1:A:81:ASN:HB2	1:A:86:ASP:CA	2.30	0.53
1:A:98:VAL:O	1:A:98:VAL:HG22	2.09	0.52
1:A:81:ASN:HD21	1:A:91:PRO:HD3	1.74	0.52
1:A:418:LYS:HD2	1:A:966[A]:ASP:OD1	2.09	0.52
1:A:55:VAL:CG2	1:A:150:THR:HG23	2.40	0.52
1:A:65:THR:HG23	1:A:66:SER:H	1.74	0.52
1:A:680:LEU:H	1:A:680:LEU:CD2	2.22	0.52
1:A:122:CYS:HB3	1:A:142:SER:HA	1.92	0.52
1:A:977:ARG:HH11	1:A:1024:ASP:HB3	1.75	0.52
1:A:387:ASN:ND2	1:A:487:GLU:H	2.08	0.52
1:A:969:THR:HG23	1:A:972[A]:LYS:NZ	2.25	0.52
1:A:36:ARG:HB3	1:A:215:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:HG23	1:A:66:SER:N	2.25	0.51
1:A:85:CYS:HB3	1:A:122:CYS:C	2.35	0.51
1:A:208:VAL:HG22	1:A:260:GLU:OE2	2.11	0.51
1:A:56:ILE:HD11	1:A:153:VAL:HG13	1.92	0.51
1:A:452[A]:LEU:HD13	1:A:591:ILE:HD11	1.93	0.50
1:A:56:ILE:HD13	1:A:151:VAL:HG23	1.93	0.50
1:A:946:THR:O	1:A:950:GLN:HG3	2.11	0.50
1:A:60:ASP:OD2	1:A:62:ALA:HB3	2.12	0.50
1:A:49:ALA:HB1	1:A:53:GLN:O	2.12	0.50
1:A:229:ASN:ND2	1:A:232:VAL:HB	2.27	0.50
1:A:745:PRO:HG2	1:A:746:PHE:CE1	2.46	0.50
1:A:38:PRO:HG3	1:A:271:ILE:HD11	1.93	0.49
1:A:33:VAL:HG21	1:A:197:ILE:CD1	2.42	0.49
1:A:682:HIS:CD2	1:A:686:GLN:HE22	2.31	0.49
1:A:466:LEU:HD23	1:A:950:GLN:HE21	1.76	0.49
1:A:324:SER:HB3	1:A:330[B]:ILE:HD11	1.95	0.49
1:A:198:VAL:HG12	1:A:223:LEU:HD12	1.95	0.49
1:A:55:VAL:HA	1:A:112:TRP:O	2.12	0.49
1:A:87:ALA:HB3	1:A:123:ILE:CG2	2.43	0.48
1:A:128:ARG:HA	1:A:134:LEU:H	1.77	0.48
1:A:1049:GLN:CG	1:A:1057:THR:HB	2.43	0.48
1:A:80:TRP:CZ2	1:A:124:ASN:HB3	2.48	0.48
1:A:465:GLN:HG3	1:A:950:GLN:NE2	2.28	0.48
1:A:134:LEU:HD22	1:A:155:ALA:HA	1.95	0.48
1:A:38:PRO:HA	1:A:271:ILE:HD11	1.95	0.48
1:A:154:ILE:HD11	1:A:167:ALA:HB1	1.94	0.48
1:A:267:GLU:HB2	1:A:271:ILE:HG22	1.95	0.48
1:A:680:LEU:HD12	1:A:709:ASP:C	2.38	0.48
1:A:39:ASP:HA	1:A:42:VAL:HG21	1.95	0.48
1:A:184:LYS:HG3	1:A:286:ASP:OD2	2.13	0.48
1:A:465:GLN:CG	1:A:950:GLN:HE22	2.27	0.48
1:A:643:CYS:SG	1:A:644:CYS:N	2.87	0.48
1:A:58:LEU:CD2	1:A:75:LYS:HD3	2.44	0.47
1:A:77:LEU:CD2	1:A:127:VAL:HA	2.44	0.47
1:A:125:VAL:HG12	1:A:126:ILE:N	2.29	0.47
1:A:139:LEU:HD12	1:A:139:LEU:N	2.30	0.47
1:A:80:TRP:O	1:A:124:ASN:HB2	2.15	0.47
1:A:123:ILE:HD12	1:A:123:ILE:C	2.40	0.47
1:A:230:GLN:O	1:A:234:MET:HG2	2.15	0.47
1:A:461[B]:GLN:NE2	5:A:1950:HOH:O	2.47	0.47
1:A:606:ASN:ND2	1:A:607:HIS:CD2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:HB3	1:A:57:HIS:CE1	2.50	0.47
1:A:139:LEU:H	1:A:139:LEU:CD1	2.28	0.46
1:A:642:THR:O	1:A:643:CYS:CB	2.63	0.46
1:A:246:LYS:HD3	1:A:247:LEU:O	2.15	0.46
1:A:302:THR:HG23	5:A:1944:HOH:O	2.15	0.46
1:A:693[B]:ARG:NH2	5:A:1547:HOH:O	2.49	0.46
1:A:154:ILE:HG22	1:A:155:ALA:N	2.31	0.46
1:A:231:GLN:N	1:A:231:GLN:OE1	2.49	0.46
1:A:430:HIS:HD2	1:A:433:ASP:H	1.62	0.46
1:A:79:LEU:CD2	1:A:125:VAL:HG22	2.45	0.46
1:A:187:LEU:HD13	1:A:187:LEU:C	2.41	0.46
1:A:197:ILE:HB	1:A:266:ALA:HB3	1.98	0.46
1:A:123:ILE:HD13	1:A:125:VAL:HG23	1.97	0.46
1:A:199:ARG:HD3	1:A:220:TYR:CE2	2.51	0.46
1:A:154:ILE:HD11	1:A:167:ALA:O	2.15	0.46
1:A:38:PRO:CA	1:A:271:ILE:HD11	2.46	0.45
1:A:219:LYS:HD3	1:A:219:LYS:N	2.28	0.45
1:A:592:LYS:HE2	1:A:672:ASP:OD2	2.16	0.45
1:A:1028:THR:O	1:A:1029:SER:CB	2.64	0.45
1:A:680:LEU:HD12	1:A:710:SER:N	2.32	0.45
1:A:98:VAL:HG12	5:A:2386:HOH:O	2.15	0.45
1:A:195:LYS:HE3	1:A:195:LYS:CA	2.47	0.45
1:A:56:ILE:CG2	1:A:112:TRP:HB2	2.47	0.45
1:A:123:ILE:CD1	1:A:141:VAL:HB	2.46	0.45
1:A:229:ASN:HD21	1:A:232:VAL:HB	1.81	0.45
1:A:430:HIS:CD2	1:A:432:ARG:H	2.35	0.45
1:A:94:ASP:OD2	1:A:96:ASN:HB2	2.18	0.44
1:A:68:THR:OG1	1:A:69:PRO:HD2	2.18	0.44
1:A:229:ASN:N	1:A:229:ASN:ND2	2.66	0.44
1:A:1014:ASN:HD21	1:A:1020:ARG:HH11	1.65	0.44
1:A:61:ILE:C	1:A:63:GLY:H	2.26	0.44
1:A:657:LEU:C	1:A:657:LEU:HD23	2.42	0.44
1:A:736:LEU:C	1:A:736:LEU:HD23	2.43	0.44
1:A:886:SER:O	1:A:887:PHE:HB2	2.17	0.44
1:A:217:SER:O	1:A:218:ASP:C	2.61	0.44
1:A:33:VAL:HG21	1:A:197:ILE:HD13	1.99	0.43
1:A:81:ASN:HD22	1:A:88:LEU:CB	2.19	0.43
1:A:210:ALA:HA	1:A:215:GLU:O	2.17	0.43
1:A:366:PRO:HB2	1:A:626:TRP:CE2	2.52	0.43
1:A:750:ASP:HB3	1:A:754:GLN:HE21	1.83	0.43
1:A:107:LYS:HD2	1:A:107:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:HIS:HE1	5:A:1154:HOH:O	2.00	0.43
1:A:677:ASP:OD1	2:C:1:GLC:H1	2.19	0.43
1:A:56:ILE:HG21	1:A:77:LEU:CD1	2.49	0.43
1:A:100:THR:O	1:A:100:THR:HG22	2.17	0.43
1:A:77:LEU:HD23	1:A:127:VAL:HA	2.00	0.43
1:A:773:SER:OG	1:A:776:GLN:HG3	2.19	0.43
1:A:57:HIS:HB2	1:A:152:SER:OG	2.18	0.43
1:A:228:VAL:O	1:A:228:VAL:HG13	2.18	0.42
1:A:510:LYS:HE2	5:A:1189:HOH:O	2.19	0.42
1:A:238:HIS:H	1:A:238:HIS:CD2	2.37	0.42
1:A:40:VAL:CG1	1:A:41:ALA:N	2.78	0.42
1:A:430:HIS:HB3	1:A:433:ASP:HB2	2.00	0.42
1:A:260:GLU:HB2	1:A:364:TYR:CE1	2.55	0.42
1:A:486:ASN:HB2	5:A:1693:HOH:O	2.19	0.42
1:A:47:VAL:HG22	1:A:48:GLN:N	2.35	0.42
1:A:722:ILE:HG13	5:A:1665:HOH:O	2.20	0.42
1:A:36:ARG:HB2	1:A:214:GLY:O	2.20	0.42
1:A:39:ASP:HA	1:A:42:VAL:CG2	2.50	0.42
1:A:252:ASN:C	1:A:252:ASN:HD22	2.28	0.42
1:A:216:PHE:CZ	1:A:272:LEU:HD13	2.55	0.41
1:A:494:ASP:HB3	1:A:496:GLN:HE22	1.84	0.41
1:A:797:LEU:HD12	1:A:797:LEU:C	2.45	0.41
1:A:948:PHE:CD1	1:A:1044:LEU:HG	2.55	0.41
1:A:56:ILE:HG21	1:A:77:LEU:HD11	2.03	0.41
1:A:83:GLU:HG3	1:A:84:THR:N	2.19	0.41
1:A:734:ASP:OD1	1:A:734:ASP:N	2.53	0.41
1:A:199:ARG:HB2	1:A:201:TYR:HE1	1.85	0.41
1:A:203:SER:OG	1:A:206:SER:HB2	2.19	0.41
1:A:128:ARG:HA	1:A:134:LEU:HB2	2.03	0.41
1:A:194:ASN:O	1:A:195:LYS:C	2.63	0.41
1:A:555:TYR:CD1	1:A:555:TYR:C	2.98	0.41
1:A:126:ILE:HD11	1:A:138:ASP:OD1	2.21	0.41
1:A:197:ILE:O	1:A:265:ALA:HA	2.21	0.41
1:A:136:ASP:O	1:A:137:SER:HB2	2.20	0.40
1:A:680:LEU:CG	1:A:710:SER:HB3	2.49	0.40
1:A:746:PHE:CD1	1:A:746:PHE:N	2.88	0.40
1:A:149:ARG:HG3	1:A:149:ARG:HH11	1.87	0.40
1:A:183:ASP:OD2	1:A:186:THR:N	2.54	0.40
1:A:682:HIS:CD2	1:A:686:GLN:NE2	2.87	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	1070/1083 (99%)	1008 (94%)	52 (5%)	10 (1%)	14 4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	66	SER
1	A	83	GLU
1	A	218	ASP
1	A	93	ALA
1	A	478	PRO
1	A	643	CYS
1	A	1029	SER
1	A	209	ALA
1	A	91	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	886/891 (99%)	869 (98%)	17 (2%)	50 38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LYS

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	231	GLN
1	A	374	TYR
1	A	387	ASN
1	A	391[A]	SER
1	A	391[B]	SER
1	A	478	PRO
1	A	482	LEU
1	A	496	GLN
1	A	543	GLN
1	A	746	PHE
1	A	859	GLN
1	A	886	SER
1	A	997[A]	GLN
1	A	997[B]	GLN
1	A	1049	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	53	GLN
1	A	76	ASN
1	A	81	ASN
1	A	204	HIS
1	A	213	ASN
1	A	229	ASN
1	A	230	GLN
1	A	238	HIS
1	A	252	ASN
1	A	279	GLN
1	A	316	GLN
1	A	317	GLN
1	A	367	GLN
1	A	387	ASN
1	A	392	GLN
1	A	397	ASN
1	A	413	HIS
1	A	430	HIS
1	A	439	GLN
1	A	455	GLN
1	A	458	ASN

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Mol	Chain	Res	Type
1	A	465	GLN
1	A	496	GLN
1	A	533	GLN
1	A	534	ASN
1	A	541	GLN
1	A	543	GLN
1	A	551	GLN
1	A	563	HIS
1	A	606	ASN
1	A	607	HIS
1	A	609	ASN
1	A	629	GLN
1	A	651	HIS
1	A	682	HIS
1	A	686	GLN
1	A	712	GLN
1	A	754	GLN
1	A	835	ASN
1	A	859	GLN
1	A	899	ASN
1	A	906	GLN
1	A	911	ASN
1	A	950	GLN
1	A	978	ASN
1	A	984	GLN
1	A	1014	ASN
1	A	1023	GLN
1	A	1037	GLN
1	A	1049	GLN
1	A	1074	GLN

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	0.46	0	17,17,17	0.40	0
2	GLC	B	2	2	11,11,12	0.46	0	15,15,17	0.68	1 (6%)
2	GLC	B	3	2	11,11,12	0.49	0	15,15,17	0.53	0
2	GLC	C	1	2	12,12,12	0.50	0	17,17,17	0.66	0
2	GLC	C	2	2	11,11,12	0.57	0	15,15,17	0.64	1 (6%)
2	GLC	C	3	2	11,11,12	0.47	0	15,15,17	0.51	0
3	GLC	D	1	3	12,12,12	0.42	0	17,17,17	0.31	0
3	GLC	D	2	3	11,11,12	0.48	0	15,15,17	0.62	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	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	2/2/19/22	0/1/1/1
2	GLC	B	3	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	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	2/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GLC	C1-O5-C5	2.28	115.24	112.19
2	C	2	GLC	C1-O5-C5	2.09	114.99	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

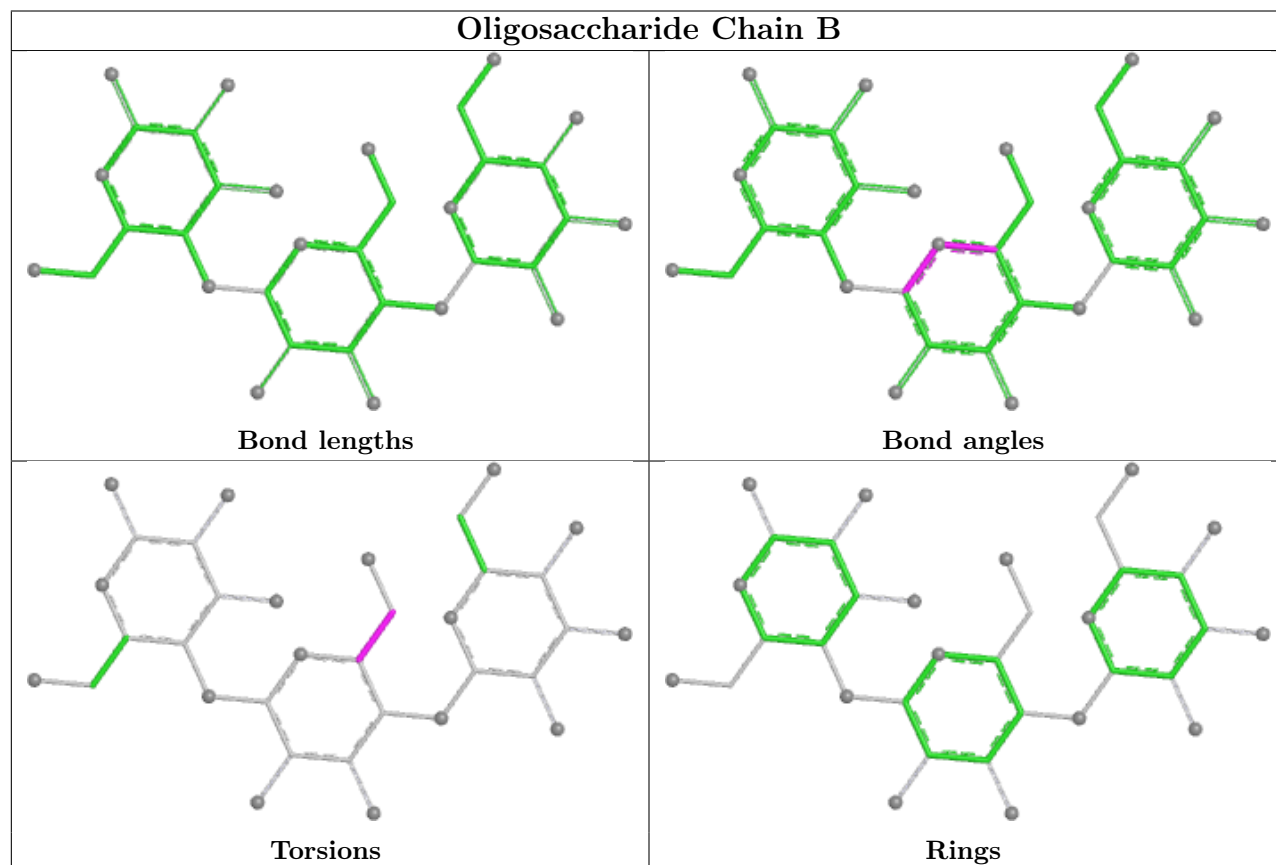
Mol	Chain	Res	Type	Atoms
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
2	B	2	GLC	O5-C5-C6-O6
3	D	1	GLC	O5-C5-C6-O6
2	B	2	GLC	C4-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6

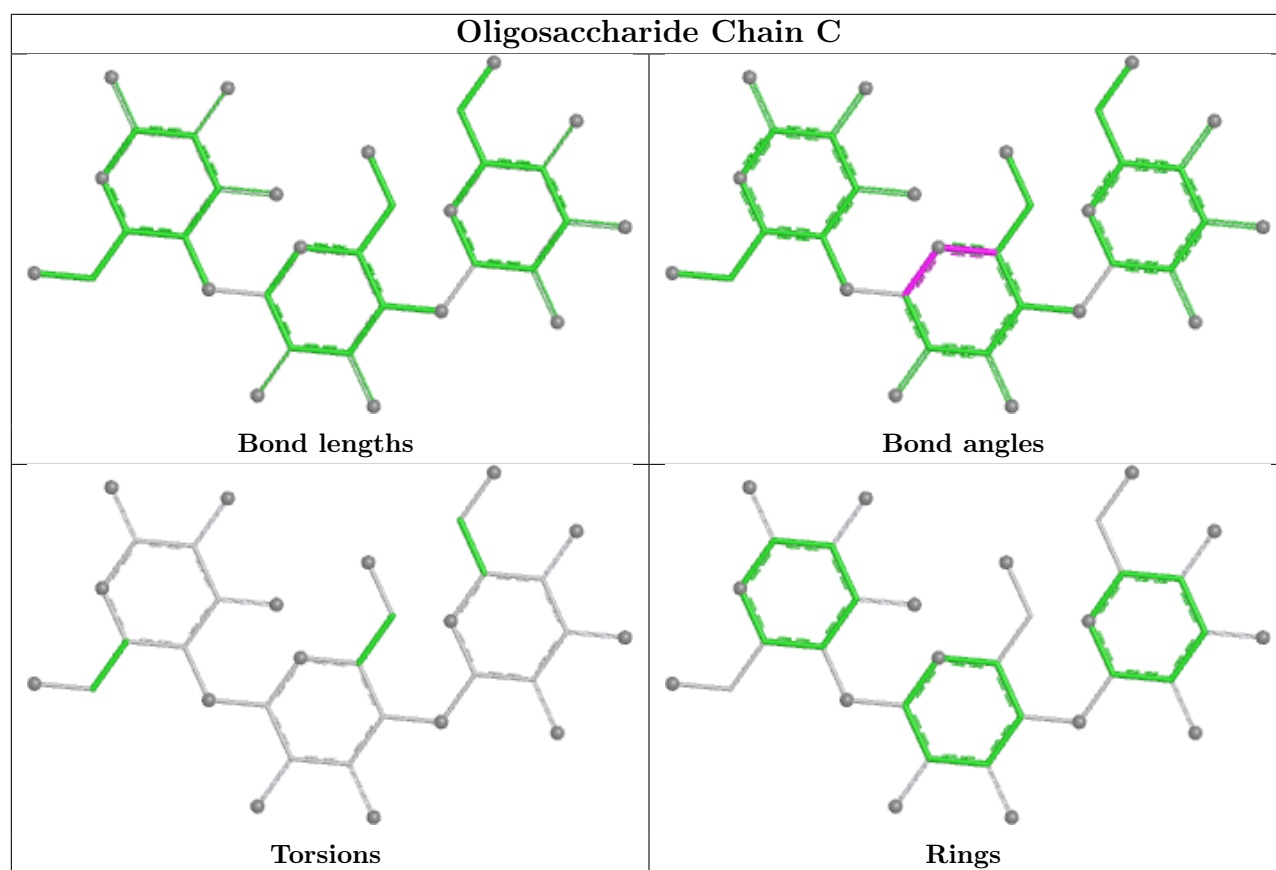
There are no ring outliers.

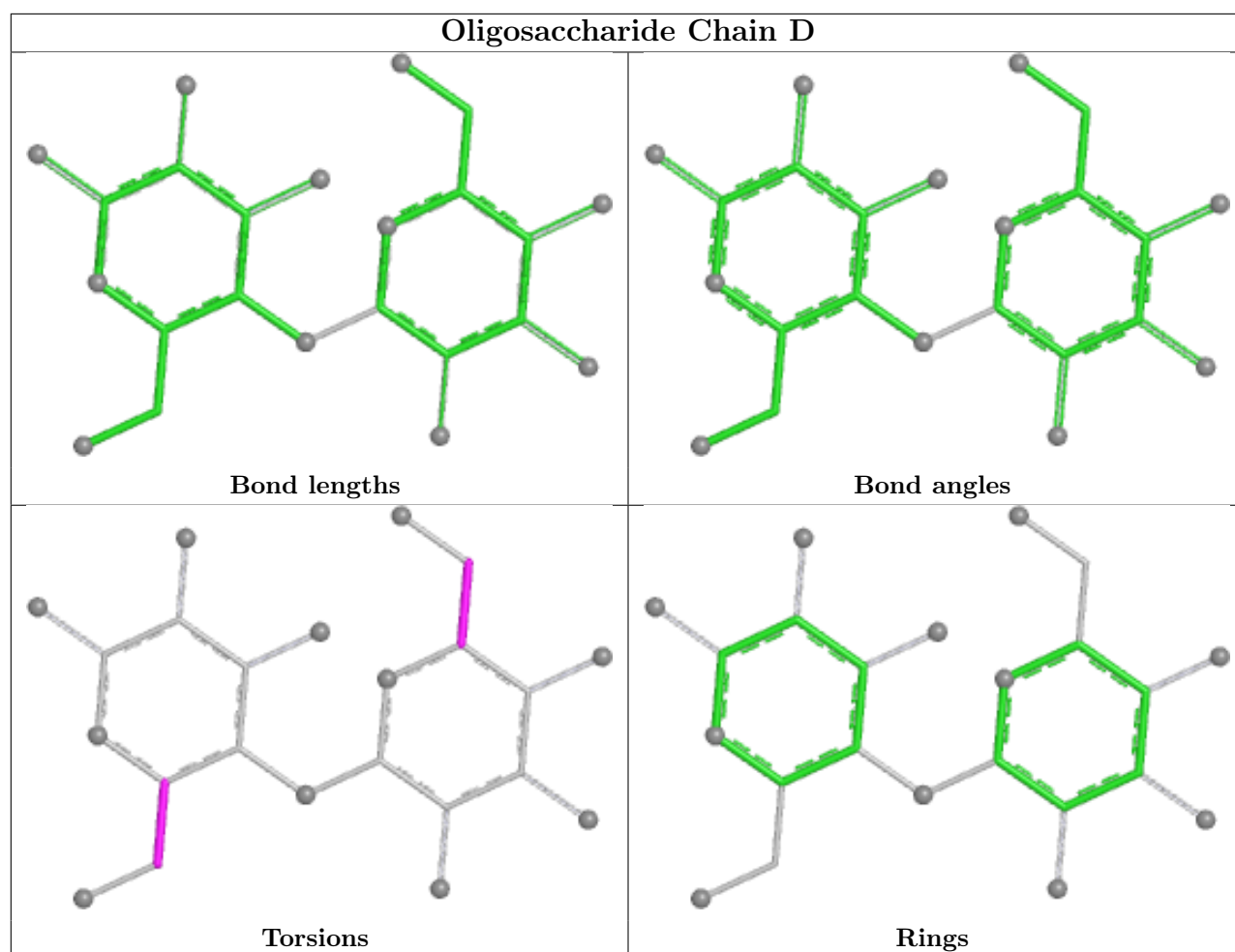
1 monomer is involved in 2 short contacts:

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

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







5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 ⓘ

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, 95th 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	1052/1083 (97%)	0.29	128 (12%) 8 8	10, 20, 66, 77	144 (13%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	VAL	5.2
1	A	135	ILE	4.9
1	A	95	TRP	4.8
1	A	61	ILE	4.7
1	A	64	ILE	4.6
1	A	80	TRP	4.6
1	A	134	LEU	4.3
1	A	303	ASP	4.2
1	A	150	THR	4.2
1	A	79	LEU	4.2
1	A	98	VAL	4.2
1	A	69	PRO	4.1
1	A	122	CYS	4.1
1	A	746	PHE	4.1
1	A	272	LEU	4.1
1	A	82	ASN	4.1
1	A	76	ASN	4.0
1	A	155	ALA	4.0
1	A	54	ALA	3.9
1	A	141	VAL	3.9
1	A	40	VAL	3.8
1	A	42	VAL	3.8
1	A	126	ILE	3.7
1	A	208	VAL	3.7
1	A	161	TYR	3.7
1	A	58	LEU	3.6
1	A	128	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	3.6
1	A	34	VAL	3.6
1	A	35	VAL	3.6
1	A	62	ALA	3.5
1	A	194	ASN	3.5
1	A	127	VAL	3.5
1	A	78	TYR	3.4
1	A	59	VAL	3.4
1	A	67	SER	3.4
1	A	142	SER	3.4
1	A	154	ILE	3.4
1	A	271	ILE	3.4
1	A	116	LEU	3.4
1	A	90	ALA	3.3
1	A	216	PHE	3.3
1	A	165	ALA	3.3
1	A	39	ASP	3.2
1	A	70	ALA	3.2
1	A	87	ALA	3.2
1	A	88	LEU	3.2
1	A	167	ALA	3.1
1	A	270	GLY	3.1
1	A	157	ASN	3.1
1	A	73	ALA	3.1
1	A	143	PHE	3.0
1	A	38	PRO	3.0
1	A	146	PHE	3.0
1	A	168	PHE	3.0
1	A	63	GLY	3.0
1	A	33	VAL	2.9
1	A	147	THR	2.9
1	A	49	ALA	2.9
1	A	1028	THR	2.8
1	A	72	TYR	2.8
1	A	209	ALA	2.8
1	A	56	ILE	2.8
1	A	197	ILE	2.8
1	A	130	GLY	2.8
1	A	213	ASN	2.8
1	A	91	PRO	2.8
1	A	115	PRO	2.8
1	A	169	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	74	THR	2.8
1	A	77	LEU	2.8
1	A	174	VAL	2.8
1	A	196	PRO	2.7
1	A	81	ASN	2.7
1	A	166	ASP	2.7
1	A	47	VAL	2.7
1	A	55	VAL	2.7
1	A	1027	GLY	2.7
1	A	218	ASP	2.7
1	A	123	ILE	2.6
1	A	151	VAL	2.6
1	A	131	THR	2.6
1	A	214	GLY	2.6
1	A	170	ALA	2.6
1	A	217	SER	2.6
1	A	229	ASN	2.5
1	A	84	THR	2.5
1	A	60	ASP	2.5
1	A	192	GLY	2.5
1	A	96	ASN	2.5
1	A	302	THR	2.5
1	A	212	SER	2.4
1	A	93	ALA	2.4
1	A	265	ALA	2.4
1	A	97	ASP	2.4
1	A	125	VAL	2.4
1	A	153	VAL	2.4
1	A	66	SER	2.4
1	A	195	LYS	2.4
1	A	220	TYR	2.4
1	A	251	VAL	2.4
1	A	187	LEU	2.3
1	A	36	ARG	2.3
1	A	41	ALA	2.3
1	A	132	ASN	2.3
1	A	44	GLY	2.3
1	A	160	VAL	2.3
1	A	117	THR	2.3
1	A	113	VAL	2.2
1	A	247	LEU	2.2
1	A	133	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	32	ASP	2.2
1	A	210	ALA	2.2
1	A	114	ILE	2.2
1	A	112	TRP	2.2
1	A	201	TYR	2.1
1	A	189	TRP	2.1
1	A	223	LEU	2.1
1	A	248	PRO	2.1
1	A	51	ALA	2.1
1	A	158	SER	2.1
1	A	110	PRO	2.1
1	A	139	LEU	2.1
1	A	86	ASP	2.1
1	A	136	ASP	2.1
1	A	304	SER	2.0
1	A	109	GLY	2.0
1	A	102	PRO	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 ⓘ

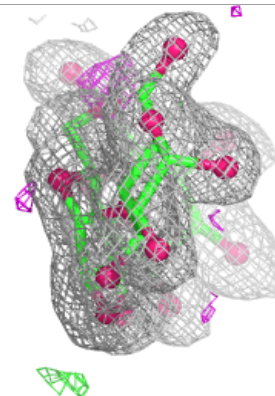
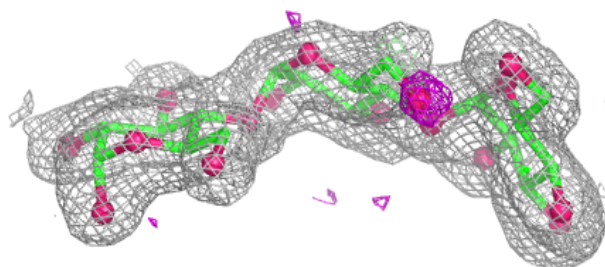
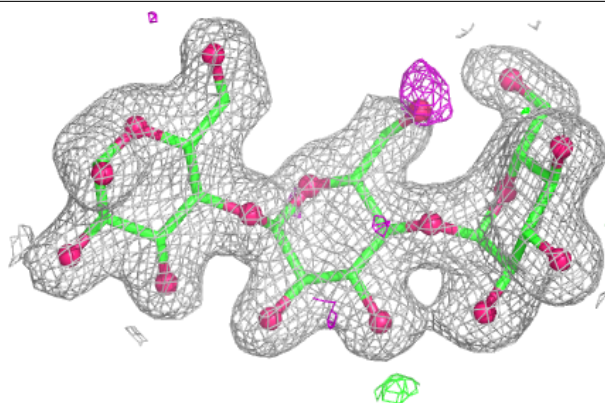
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GLC	D	1	12/12	0.57	0.13	88,88,88,88	0
3	GLC	D	2	11/12	0.58	0.13	87,88,88,88	0
2	GLC	C	1	12/12	0.91	0.08	17,21,23,27	0
2	GLC	B	3	11/12	0.92	0.07	21,23,26,27	0
2	GLC	B	2	11/12	0.92	0.07	21,22,27,36	0
2	GLC	C	3	11/12	0.93	0.07	21,24,28,31	0
2	GLC	B	1	12/12	0.94	0.06	18,19,21,25	0
2	GLC	C	2	11/12	0.95	0.06	13,17,18,18	0

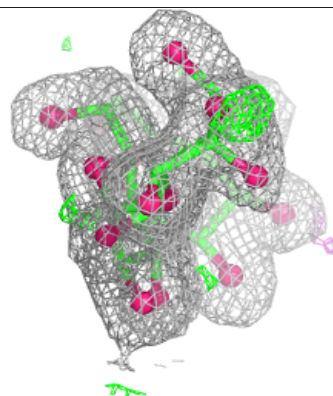
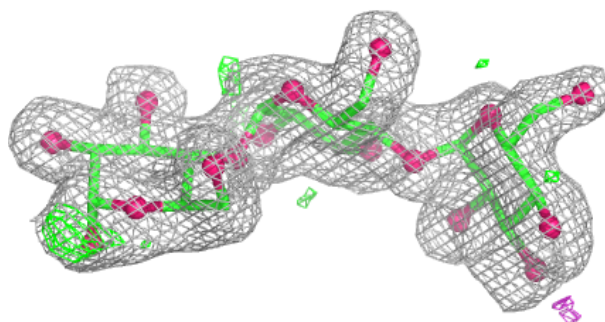
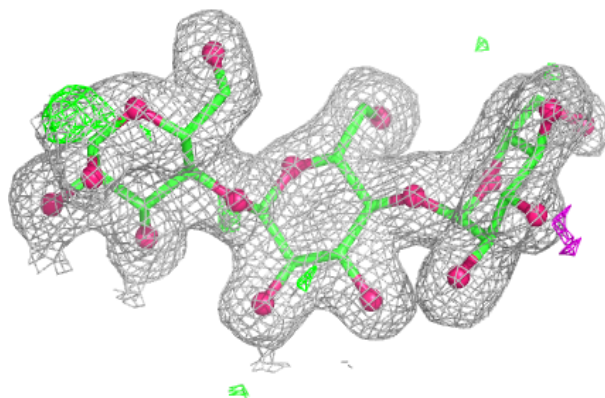
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

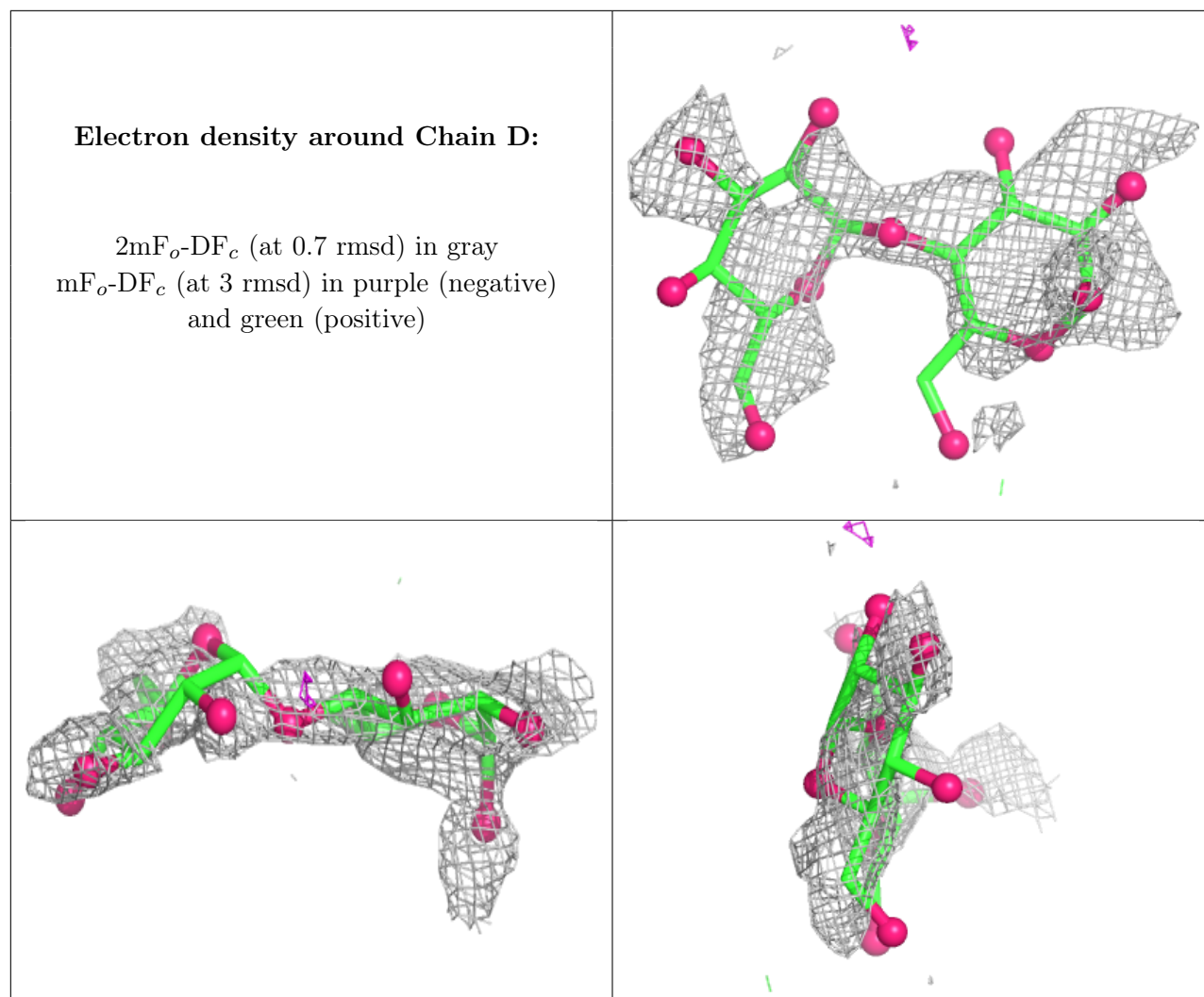
Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain C:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	CA	A	2405	1/1	0.93	0.09	59,59,59,59	0
4	CA	A	2402	1/1	0.95	0.09	34,34,34,34	0
4	CA	A	2403	1/1	0.98	0.07	36,36,36,36	0
4	CA	A	2404	1/1	0.99	0.01	16,16,16,16	0
4	CA	A	2401	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.