Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 04:07 PM EDT

PDB ID	:	5E70
Title	:	Crystal structure of Ecoli Branching Enzyme with gamma cyclodextrin
Authors	:	Feng, L.; Nosrati, M.; Geiger, J.H.
Deposited on	:	2015-10-11
Resolution	:	2.33 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:

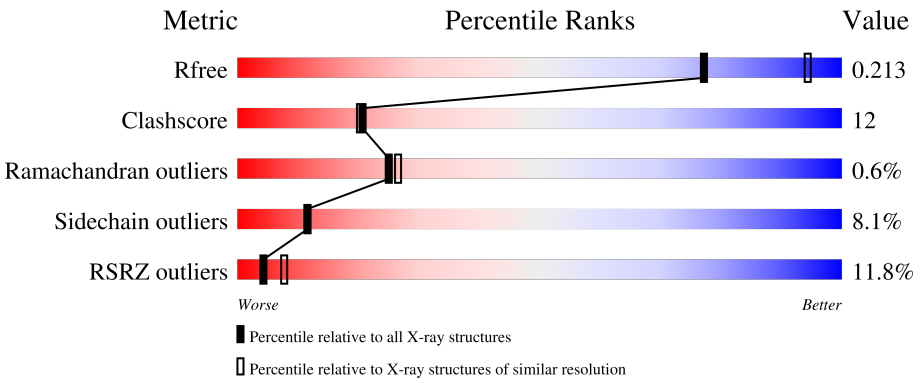
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.33 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	612	11% 72% 20% • •
1	B	612	% 77% 17% • •
1	C	612	32% 70% 21% • 6%
1	D	612	2% 73% 19% • •
2	E	8	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	8	88% 12%
2	G	8	38% 50% 12%
2	H	8	75% 25%
2	I	8	12% 75% 12%

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	E	2	-	-	X	-
2	GLC	E	8	-	-	-	X
2	GLC	G	1	-	-	-	X
2	GLC	G	2	-	-	-	X
2	GLC	G	5	-	-	-	X
2	GLC	G	6	-	-	-	X
2	GLC	G	7	-	-	-	X
2	GLC	G	8	-	-	-	X
2	GLC	I	6	-	-	-	X
2	GLC	I	7	-	-	-	X

2 Entry composition (i)

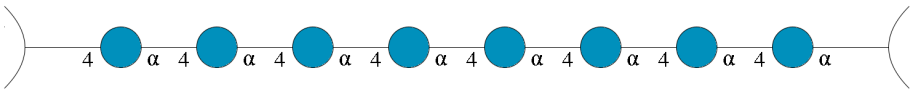
There are 4 unique types of molecules in this entry. The entry contains 21132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-glucan branching enzyme GlgB.

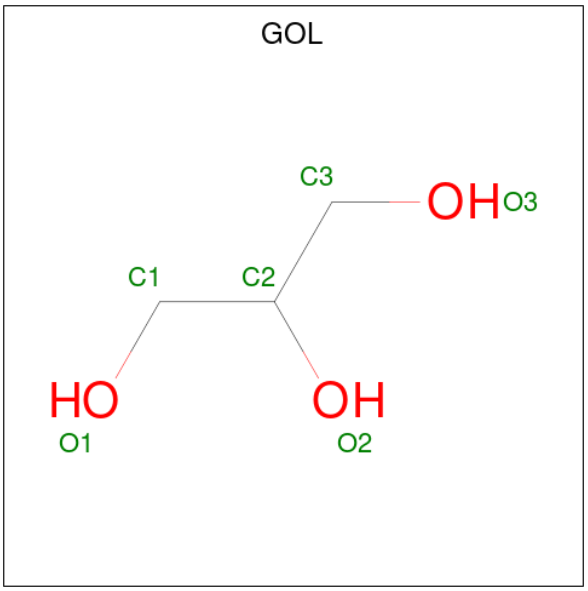
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	586	4871	3110	868	877	16	0	6	0
1	B	600	4960	3170	880	894	16	0	2	0
1	C	578	4768	3052	845	855	16	0	2	0
1	D	588	4852	3103	862	871	16	0	2	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	8	88	48	40	0	0	0
2	F	8	88	48	40	0	0	0
2	G	8	88	48	40	0	0	0
2	H	8	88	48	40	0	0	0
2	I	8	88	48	40	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0

- Molecule 4 is water.

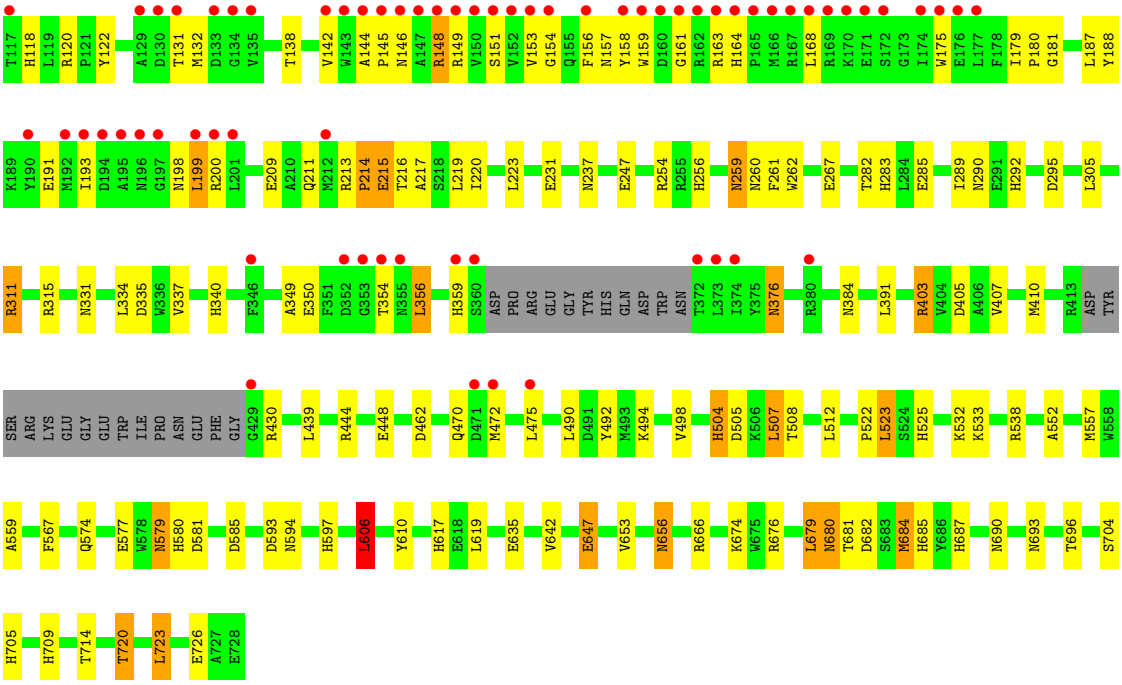
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	310	310	310	0	0
			Total	O		
4	B	480	480	480	0	0
			Total	O		
4	C	75	75	75	0	0
			Total	O		
4	D	340	340	340	0	0

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 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.

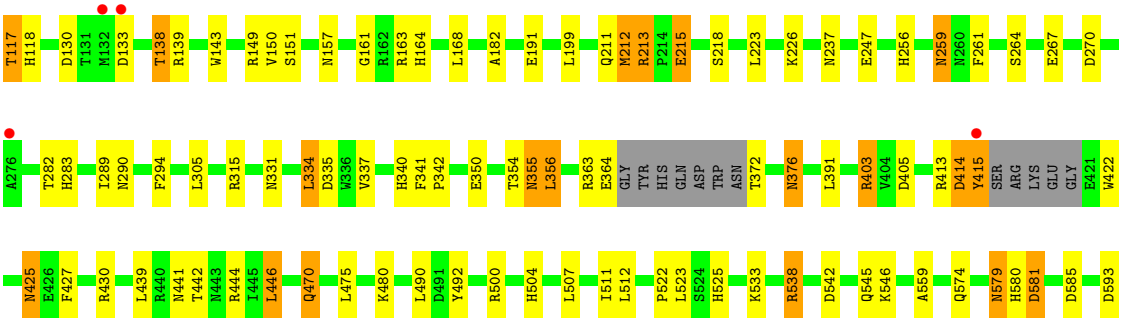
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

Chain A:



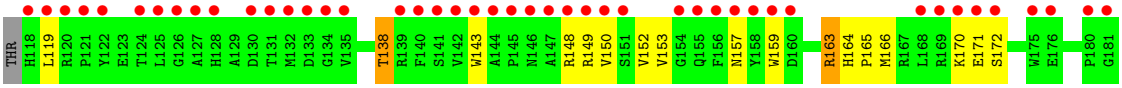
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

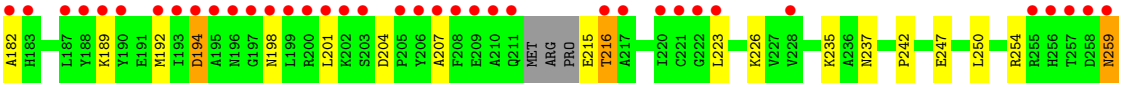
Chain B:

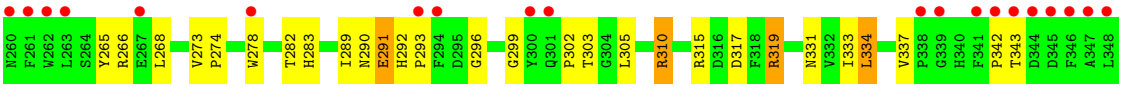


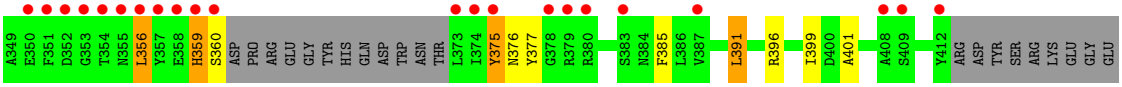
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

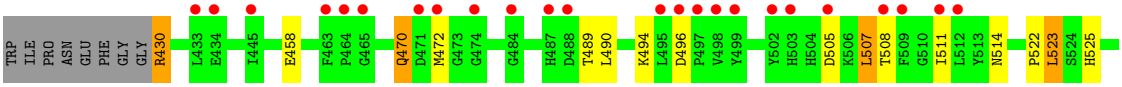
Chain C:

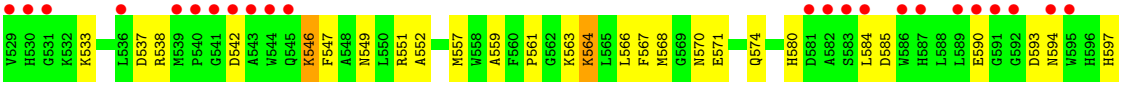


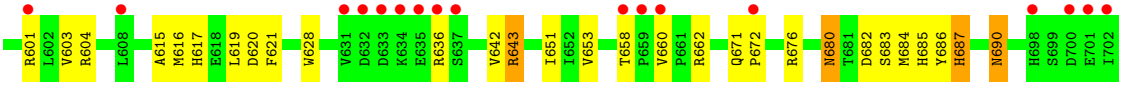


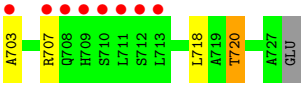






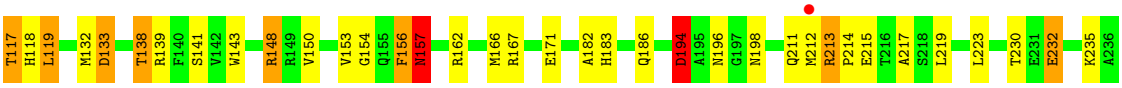


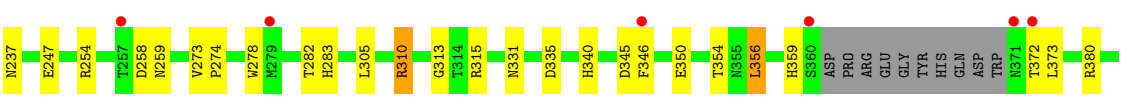


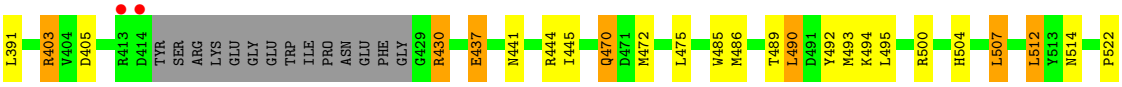


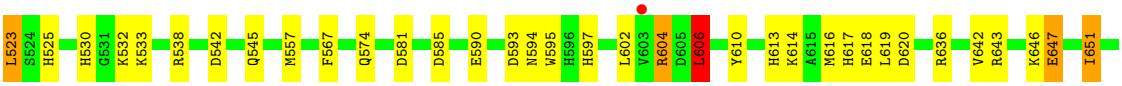
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

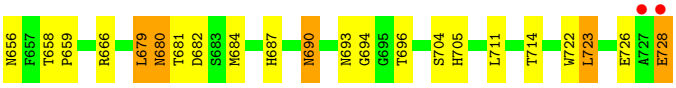
Chain D:











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

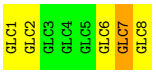
Chain E:

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

Chain F:

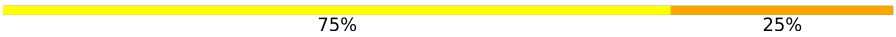
- Molecule 2: Cyclooctakis-(1-4)-(alpha-D-glucopyranose)

Chain G:



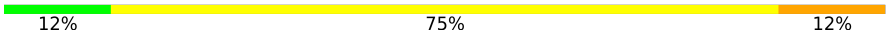
- Molecule 2: Cyclooctakis-(1-4)-(alpha-D-glucopyranose)

Chain H:



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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.10Å 103.22Å 186.69Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	50.00 – 2.33 45.60 – 2.33	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.33) 94.6 (45.60-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.170 , 0.217 0.167 , 0.213	Depositor DCC
R_{free} test set	14049 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21132	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.65	0/5028	0.68	5/6827 (0.1%)
1	B	0.77	0/5120	0.77	7/6953 (0.1%)
1	C	0.40	0/4918	0.51	0/6677
1	D	0.65	0/5006	0.73	8/6796 (0.1%)
All	All	0.64	0/20072	0.68	20/27253 (0.1%)

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	D	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	538	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	723	LEU	CA-CB-CG	7.54	132.64	115.30
1	A	723	LEU	CA-CB-CG	6.89	131.15	115.30
1	D	723	LEU	CA-CB-CG	6.65	130.59	115.30
1	D	403	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	D	636	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	606	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	403	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	D	604	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	355	ASN	CB-CA-C	-5.96	98.48	110.40
1	D	194	ASP	CB-CG-OD1	-5.93	112.97	118.30
1	A	606	LEU	CB-CG-CD1	5.90	121.03	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	606	LEU	CA-CB-CG	5.62	128.21	115.30
1	A	311	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	D	157	ASN	N-CA-CB	-5.39	100.89	110.60
1	B	622	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	604	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	606	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	403	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	604	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	156	PHE	Peptide

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	4871	0	4596	131	0
1	B	4960	0	4666	109	0
1	C	4768	0	4505	111	0
1	D	4852	0	4584	119	1
2	E	88	0	72	13	0
2	F	88	0	72	1	0
2	G	88	0	72	1	0
2	H	88	0	72	1	1
2	I	88	0	72	2	0
3	A	12	0	16	3	0
3	B	12	0	16	2	0
3	D	12	0	16	1	0
4	A	310	0	0	17	0
4	B	480	0	0	17	0
4	C	75	0	0	8	0
4	D	340	0	0	19	0
All	All	21132	0	18759	475	1

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 12.

All (475) 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:211:GLN:NE2	1:A:217:ALA:HB3	1.54	1.21
1:D:117:THR:N	1:D:118:HIS:HB2	1.56	1.21
1:D:470:GLN:H	1:D:470:GLN:NE2	1.45	1.13
1:D:470:GLN:HE21	1:D:470:GLN:N	1.48	1.12
1:D:213:ARG:H	1:D:213:ARG:HD3	1.16	1.03
1:A:666:ARG:H	3:A:802:GOL:H31	1.27	0.97
1:D:437:GLU:HG3	4:D:924:HOH:O	1.65	0.96
1:B:444:ARG:HD3	4:B:927:HOH:O	1.64	0.96
1:C:470:GLN:HE21	1:C:470:GLN:H	0.96	0.95
1:A:213:ARG:HA	1:A:214:PRO:O	1.65	0.94
1:B:470:GLN:H	1:B:470:GLN:NE2	1.66	0.92
1:C:319:ARG:NH2	1:C:396:ARG:O	2.02	0.92
1:A:157:ASN:HB3	4:A:1053:HOH:O	1.70	0.92
1:B:157:ASN:HD22	1:B:164:HIS:HD2	1.17	0.91
1:A:211:GLN:OE1	1:A:215:GLU:HB3	1.70	0.91
1:B:138:THR:HG22	1:B:182:ALA:O	1.70	0.91
1:C:470:GLN:HE21	1:C:470:GLN:N	1.70	0.90
1:B:470:GLN:HE21	1:B:470:GLN:N	1.69	0.89
1:D:278:TRP:O	1:D:604:ARG:HD2	1.73	0.89
1:B:666:ARG:O	3:B:803:GOL:H32	1.73	0.88
1:C:594:ASN:H	1:C:597:HIS:HD2	1.19	0.88
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.11	0.86
1:B:164:HIS:HE1	4:B:1282:HOH:O	1.57	0.85
1:D:138:THR:HG22	1:D:182:ALA:O	1.77	0.85
1:C:684[A]:MET:CE	1:D:684:MET:SD	2.66	0.84
1:A:211:GLN:HE21	1:A:217:ALA:HB3	1.42	0.83
1:A:512:LEU:HD21	2:E:4:GLC:H61	1.61	0.83
1:D:154:GLY:O	1:D:157:ASN:HB3	1.79	0.82
1:D:213:ARG:H	1:D:213:ARG:CD	1.92	0.82
1:C:658:THR:HG22	1:C:660:VAL:H	1.42	0.82
1:B:415:TYR:CD1	1:B:430:ARG:HD3	2.14	0.82
1:C:163:ARG:CG	1:C:163:ARG:HH11	1.91	0.81
1:A:594:ASN:H	1:A:597:HIS:HD2	1.25	0.81
1:D:117:THR:CA	1:D:118:HIS:HB2	2.10	0.81
1:B:157:ASN:HD22	1:B:164:HIS:CD2	1.99	0.80
1:C:684[A]:MET:HE1	1:D:684:MET:SD	2.21	0.80
1:C:430:ARG:HE	1:C:430:ARG:HA	1.46	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ARG:HD3	1:D:213:ARG:N	1.96	0.79
1:A:574:GLN:NE2	1:A:585:ASP:H	1.81	0.79
1:A:676[B]:ARG:HG3	1:A:676[B]:ARG:HH11	1.48	0.78
4:C:961:HOH:O	1:D:590:GLU:HG2	1.84	0.78
1:A:157:ASN:CB	4:A:1053:HOH:O	2.30	0.77
1:C:470:GLN:H	1:C:470:GLN:NE2	1.80	0.77
1:A:262:TRP:CH2	1:A:311:ARG:HG2	2.19	0.77
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.82	0.77
1:C:334:LEU:HD23	1:C:399:ILE:HG21	1.65	0.76
2:E:6:GLC:H61	2:E:7:GLC:H5	1.67	0.76
1:B:247:GLU:OE1	1:B:525:HIS:HD2	1.69	0.76
1:B:594:ASN:H	1:B:597:HIS:HD2	1.33	0.76
1:A:533:LYS:O	1:A:538:ARG:NH2	2.19	0.75
1:D:156:PHE:HD1	1:D:186:GLN:OE1	1.68	0.75
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.68	0.75
1:A:676[B]:ARG:HH11	1:A:676[B]:ARG:CG	1.99	0.75
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.68	0.74
1:B:211:GLN:HG2	1:B:212:MET:SD	2.28	0.74
1:A:148:ARG:O	1:A:149:ARG:HB3	1.88	0.74
1:A:676[B]:ARG:HG3	1:A:676[B]:ARG:NH1	1.98	0.74
1:D:684:MET:H	1:D:690:ASN:ND2	1.86	0.74
1:C:163:ARG:HH11	1:C:163:ARG:HG2	1.52	0.73
1:C:594:ASN:H	1:C:597:HIS:CD2	2.06	0.73
1:B:658:THR:HG22	1:B:660:VAL:H	1.54	0.73
1:A:709:HIS:HD2	4:A:1059:HOH:O	1.71	0.73
1:A:282:THR:OG1	1:A:283:HIS:HD2	1.71	0.73
1:A:666:ARG:H	3:A:802:GOL:C3	2.02	0.72
1:C:170:LYS:HA	1:C:170:LYS:HE2	1.71	0.72
1:C:542:ASP:O	1:C:546:LYS:HG3	1.89	0.72
1:C:686:TYR:O	1:C:687:HIS:HB2	1.89	0.72
1:C:302:PRO:O	1:C:342:PRO:HB3	1.89	0.72
1:D:504:HIS:HD2	4:D:982:HOH:O	1.72	0.71
1:B:470:GLN:H	1:B:470:GLN:HE21	0.83	0.71
1:A:693:ASN:HD21	1:A:714:THR:H	1.39	0.71
1:B:415:TYR:CD1	1:B:415:TYR:C	2.64	0.70
1:D:117:THR:HA	1:D:119:LEU:H	1.56	0.70
1:D:693:ASN:HD21	1:D:714:THR:H	1.38	0.70
1:D:138:THR:CG2	1:D:182:ALA:O	2.39	0.70
1:A:153:VAL:HA	4:A:1053:HOH:O	1.92	0.70
1:A:120:ARG:NH1	4:A:902:HOH:O	2.24	0.70
1:A:161:GLY:HA3	1:A:191:GLU:OE2	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.27	0.70
1:B:415:TYR:C	1:B:415:TYR:HD1	1.95	0.69
1:B:425:ASN:HD22	1:B:427:PHE:H	1.41	0.69
1:A:211:GLN:NE2	1:A:217:ALA:CB	2.45	0.69
1:C:601[B]:ARG:HG2	1:C:601[B]:ARG:HH11	1.57	0.69
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.76	0.69
1:B:289:ILE:HG13	1:B:334:LEU:HD11	1.75	0.69
1:B:413:ARG:O	1:B:414:ASP:HB2	1.93	0.68
1:B:282:THR:OG1	1:B:283:HIS:HD2	1.75	0.68
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.76	0.68
1:A:594:ASN:H	1:A:597:HIS:CD2	2.11	0.68
1:D:696:THR:OG1	1:D:726:GLU:OE1	2.11	0.68
1:D:574:GLN:NE2	1:D:585:ASP:H	1.93	0.67
1:B:237:ASN:ND2	1:B:283:HIS:HE1	1.93	0.67
1:A:214:PRO:O	1:A:215:GLU:O	2.13	0.66
1:B:684:MET:H	1:B:690:ASN:HD22	1.43	0.66
1:A:340:HIS:HE1	1:A:405:ASP:OD2	1.78	0.66
1:A:508:THR:OG1	2:E:5:GLC:H61	1.95	0.66
1:D:194:ASP:HB3	1:D:196:ASN:H	1.60	0.66
1:D:684:MET:H	1:D:690:ASN:HD22	1.41	0.66
1:A:237:ASN:ND2	1:A:283:HIS:HE1	1.94	0.66
1:A:157:ASN:HD21	1:A:164:HIS:HB2	1.61	0.65
1:D:441:ASN:O	4:D:901:HOH:O	2.13	0.65
2:E:1:GLC:H3	2:E:2:GLC:O5	1.96	0.65
1:B:414:ASP:O	1:B:422:TRP:CD1	2.49	0.65
1:D:213:ARG:HB3	1:D:214:PRO:HA	1.78	0.65
1:D:156:PHE:CD2	1:D:157:ASN:HB2	2.32	0.65
1:B:480:LYS:HE3	4:B:910:HOH:O	1.96	0.65
1:B:594:ASN:H	1:B:597:HIS:CD2	2.16	0.64
1:D:494[A]:LYS:HG2	1:D:538:ARG:HB3	1.80	0.64
1:D:530:HIS:HE1	4:D:1208:HOH:O	1.81	0.64
1:B:149:ARG:HD2	1:B:150:VAL:N	2.12	0.63
1:A:209:GLU:HG2	1:A:219:LEU:CD2	2.29	0.63
1:D:183:HIS:CE1	1:D:186:GLN:HE21	2.16	0.63
1:A:148:ARG:O	1:A:193:ILE:HB	1.98	0.63
1:A:704:SER:OG	1:A:705:HIS:HD2	1.82	0.62
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.34	0.62
4:B:1329:HOH:O	2:F:4:GLC:H62	1.99	0.62
1:D:117:THR:HA	1:D:119:LEU:N	2.15	0.62
1:D:616:MET:SD	1:D:651:ILE:HG12	2.40	0.62
1:B:602:LEU:HG	1:B:606:LEU:HD22	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:HIS:HD2	4:D:1217:HOH:O	1.83	0.62
1:A:350:GLU:HA	1:A:354:THR:O	2.00	0.61
1:B:340:HIS:HE1	1:B:405:ASP:OD2	1.82	0.61
1:D:235:LYS:HG3	4:D:1030:HOH:O	2.01	0.61
1:A:213:ARG:CG	1:A:214:PRO:HA	2.31	0.61
1:A:666:ARG:N	3:A:802:GOL:H31	2.09	0.61
1:D:237:ASN:HD22	1:D:283:HIS:HE1	1.47	0.61
1:D:680:ASN:ND2	1:D:682:ASP:H	1.98	0.61
1:A:157:ASN:C	1:A:159:TRP:N	2.54	0.61
1:D:237:ASN:ND2	1:D:283:HIS:HE1	1.98	0.61
1:A:157:ASN:C	1:A:159:TRP:H	2.04	0.60
1:A:704:SER:OG	1:A:705:HIS:CD2	2.53	0.60
1:B:117:THR:HB	1:B:118:HIS:HD2	1.66	0.60
1:C:684[A]:MET:H	1:C:690:ASN:ND2	1.98	0.60
1:B:259:ASN:HD22	1:B:261:PHE:H	1.48	0.60
1:A:512:LEU:CD2	2:E:4:GLC:H61	2.30	0.60
1:D:167:ARG:NH2	4:D:905:HOH:O	2.35	0.60
2:G:7:GLC:H62	2:G:8:GLC:C1	2.31	0.60
1:B:644:ARG:CG	1:B:650:GLU:HG2	2.33	0.59
1:B:138:THR:HG23	1:B:182:ALA:HB3	1.84	0.59
1:B:680:ASN:C	1:B:680:ASN:HD22	2.05	0.59
1:B:259:ASN:HB2	1:B:261:PHE:CE2	2.37	0.59
1:B:335:ASP:OD1	1:B:403:ARG:HD3	2.02	0.59
1:B:593:ASP:OD2	1:B:687:HIS:CE1	2.55	0.59
1:D:156:PHE:CD1	1:D:186:GLN:OE1	2.53	0.59
1:C:296:GLY:HA2	1:C:580:HIS:CE1	2.38	0.59
1:C:138:THR:HG22	1:C:182:ALA:O	2.03	0.59
1:A:504:HIS:HD2	4:A:1010:HOH:O	1.85	0.58
1:A:680:ASN:HD22	1:A:682:ASP:H	1.50	0.58
1:B:579:ASN:ND2	1:B:581:ASP:H	2.00	0.58
1:D:651:ILE:CD1	1:D:722:TRP:HB3	2.32	0.58
1:D:680:ASN:HD22	1:D:680:ASN:C	2.07	0.58
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.51	0.58
1:C:157:ASN:HD22	1:C:164:HIS:HD2	1.50	0.58
1:C:163:ARG:CG	1:C:163:ARG:NH1	2.56	0.58
1:B:213:ARG:H	1:B:213:ARG:HE	1.52	0.58
1:B:574:GLN:NE2	1:B:585:ASP:H	2.01	0.58
1:C:684[B]:MET:H	1:C:690:ASN:ND2	2.01	0.58
1:A:209:GLU:HG2	1:A:219:LEU:HD23	1.85	0.58
1:D:232:GLU:N	1:D:232:GLU:OE1	2.37	0.58
1:B:441:ASN:OD1	1:B:444:ARG:NH1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:ASN:H	1:D:597:HIS:HD2	1.53	0.57
1:B:671:GLN:OE1	1:B:725:ARG:NH1	2.38	0.57
1:C:680:ASN:C	1:C:680:ASN:HD22	2.09	0.57
1:A:512:LEU:N	1:A:512:LEU:HD22	2.20	0.57
1:B:425:ASN:ND2	1:B:427:PHE:H	2.02	0.56
1:D:273:VAL:HB	1:D:274:PRO:HD3	1.87	0.56
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.87	0.56
1:B:658:THR:CG2	1:B:660:VAL:H	2.19	0.56
1:B:213:ARG:H	1:B:213:ARG:NE	2.04	0.56
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.89	0.56
1:D:148:ARG:HG3	1:D:194:ASP:O	2.06	0.56
1:B:674:LYS:NZ	4:B:904:HOH:O	2.30	0.56
1:A:579:ASN:ND2	1:A:581:ASP:H	2.04	0.55
1:B:684:MET:H	1:B:690:ASN:ND2	2.03	0.55
1:B:593:ASP:OD2	1:B:687:HIS:HE1	1.90	0.55
1:B:247:GLU:OE1	1:B:525:HIS:CD2	2.57	0.55
1:C:237:ASN:HD21	1:C:283:HIS:HE1	1.52	0.55
1:C:430:ARG:HA	1:C:430:ARG:NE	2.12	0.55
1:C:552:ALA:O	1:C:720:THR:HG21	2.07	0.55
1:A:247:GLU:OE1	1:A:525:HIS:CD2	2.60	0.55
1:A:709:HIS:CD2	4:A:1059:HOH:O	2.51	0.55
1:D:132:MET:CE	1:D:139:ARG:NH1	2.70	0.55
1:D:514:ASN:ND2	4:D:915:HOH:O	2.40	0.55
1:B:606:LEU:HD13	1:B:679:LEU:HD11	1.88	0.55
1:C:310:ARG:O	1:C:310:ARG:HD3	2.06	0.55
1:C:564:LYS:HD3	1:C:564:LYS:N	2.22	0.55
1:C:568:MET:HG3	1:C:584:LEU:HD11	1.89	0.55
1:A:580:HIS:HD2	4:A:1116:HOH:O	1.89	0.54
1:C:604:ARG:NH2	4:C:903:HOH:O	2.39	0.54
1:C:703:ALA:HA	1:C:707:ARG:O	2.06	0.54
1:A:151:SER:HB2	1:A:164:HIS:O	2.06	0.54
1:D:694:GLY:N	4:D:906:HOH:O	2.35	0.54
1:D:444:ARG:NE	4:D:901:HOH:O	2.39	0.54
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.42	0.54
1:C:337:VAL:HG23	1:C:337:VAL:O	2.08	0.54
1:C:508:THR:O	1:C:511:ILE:HG22	2.07	0.54
1:C:574:GLN:NE2	1:C:585:ASP:H	2.06	0.54
1:D:211:GLN:HE22	1:D:215:GLU:HG3	1.72	0.54
1:A:148:ARG:O	1:A:148:ARG:HG2	2.08	0.54
1:A:430:ARG:NH1	4:A:910:HOH:O	2.39	0.54
1:A:470:GLN:O	1:A:472:MET:O	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:HD13	1:B:199:LEU:C	2.29	0.54
1:A:337:VAL:HG23	1:A:337:VAL:O	2.07	0.53
1:A:635:GLU:H	1:A:635:GLU:CD	2.10	0.53
1:C:684[A]:MET:SD	1:C:685:HIS:ND1	2.80	0.53
1:A:213:ARG:HG3	1:A:214:PRO:HA	1.91	0.53
1:B:259:ASN:HB2	1:B:261:PHE:CD2	2.43	0.53
1:D:613:HIS:HB3	3:D:803:GOL:H12	1.89	0.53
1:A:187:LEU:HD22	1:A:211:GLN:HE21	1.73	0.53
1:C:150:VAL:HG13	1:C:192:MET:HB2	1.91	0.53
1:C:601[B]:ARG:HH11	1:C:601[B]:ARG:CG	2.22	0.53
1:A:593:ASP:OD2	1:A:687:HIS:HE1	1.91	0.53
1:B:270:ASP:OD2	4:B:901:HOH:O	2.19	0.53
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.90	0.53
1:A:606:LEU:HD13	1:A:679:LEU:HD11	1.91	0.53
1:B:403:ARG:NH2	4:B:913:HOH:O	2.41	0.53
1:C:265:TYR:HB2	1:C:317:ASP:HB3	1.91	0.52
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.38	0.52
1:A:532:LYS:O	1:A:533:LYS:HB2	2.09	0.52
1:B:579:ASN:HD22	1:B:581:ASP:H	1.58	0.52
1:D:490:LEU:O	1:D:494[A]:LYS:HG3	2.10	0.52
1:A:403:ARG:NH1	4:A:913:HOH:O	2.40	0.52
1:B:594:ASN:N	1:B:597:HIS:HD2	2.03	0.52
1:D:680:ASN:HD22	1:D:682:ASP:H	1.57	0.52
1:B:161:GLY:HA3	1:B:191:GLU:OE2	2.10	0.52
1:B:504:HIS:HD2	4:B:1005:HOH:O	1.92	0.52
1:C:194:ASP:HB2	1:C:198:ASN:O	2.09	0.52
1:A:680:ASN:ND2	1:A:682:ASP:H	2.07	0.52
1:D:148:ARG:CG	1:D:194:ASP:O	2.57	0.52
1:D:532:LYS:O	1:D:533:LYS:HB2	2.09	0.52
1:D:523:LEU:HD22	1:D:557:MET:SD	2.50	0.52
1:A:494:LYS:HD3	1:A:538:ARG:HG2	1.92	0.52
1:C:163:ARG:NH1	1:C:163:ARG:HG3	2.25	0.51
1:D:542:ASP:H	1:D:545:GLN:HE21	1.59	0.51
1:A:157:ASN:O	1:A:159:TRP:N	2.44	0.51
1:A:259:ASN:HD22	1:A:260:ASN:N	2.09	0.51
1:D:444:ARG:HB3	4:D:901:HOH:O	2.10	0.51
1:C:305:LEU:HD12	1:C:385:PHE:CE2	2.45	0.51
1:C:375:TYR:HB2	1:C:377:TYR:CZ	2.46	0.51
1:C:658:THR:HB	4:C:913:HOH:O	2.11	0.51
1:D:658:THR:HB	1:D:659:PRO:HD2	1.92	0.51
1:D:437:GLU:CG	4:D:924:HOH:O	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:HIS:HB2	1:A:259:ASN:HD21	1.75	0.51
1:A:335:ASP:OD1	1:A:403:ARG:HD3	2.09	0.51
1:A:552:ALA:O	1:A:720:THR:CG2	2.58	0.51
1:A:680:ASN:HD22	1:A:680:ASN:C	2.14	0.51
1:B:580:HIS:HD2	4:B:1294:HOH:O	1.93	0.51
2:E:1:GLC:O2	2:E:8:GLC:C3	2.58	0.51
1:B:118:HIS:H	1:B:118:HIS:CD2	2.29	0.51
1:C:552:ALA:O	1:C:720:THR:CG2	2.59	0.51
1:D:651:ILE:HD11	1:D:722:TRP:HB3	1.92	0.51
1:D:258:ASP:O	1:D:259:ASN:CG	2.50	0.51
1:A:213:ARG:HA	1:A:214:PRO:C	2.29	0.51
1:B:130:ASP:OD1	1:B:139:ARG:NH1	2.30	0.50
1:C:273:VAL:HB	1:C:274:PRO:HD3	1.93	0.50
1:D:215:GLU:HG2	2:I:2:GLC:O2	2.11	0.50
1:B:674:LYS:CE	4:B:904:HOH:O	2.60	0.50
1:A:256:HIS:HD2	1:B:728:GLU:O	1.93	0.50
1:B:350:GLU:HA	1:B:354:THR:O	2.11	0.50
1:C:189:LYS:HD2	1:C:201:LEU:HD12	1.94	0.50
1:C:523:LEU:HD22	1:C:557:MET:SD	2.52	0.50
1:A:213:ARG:HG2	1:A:214:PRO:HA	1.94	0.50
1:A:617:HIS:HE1	4:A:1129:HOH:O	1.93	0.50
1:A:647:GLU:HG2	4:A:1102:HOH:O	2.12	0.50
1:B:337:VAL:HG22	4:B:955:HOH:O	2.12	0.49
1:C:170:LYS:HE2	1:C:170:LYS:CA	2.41	0.49
1:C:684[A]:MET:HE2	1:D:684:MET:SD	2.51	0.49
1:C:291:GLU:HA	1:C:291:GLU:OE1	2.11	0.49
2:E:1:GLC:C3	2:E:2:GLC:O5	2.55	0.49
1:A:577:GLU:OE2	4:A:901:HOH:O	2.20	0.49
1:B:680:ASN:HD22	1:B:682:ASP:H	1.59	0.49
1:A:593:ASP:OD2	1:A:687:HIS:CE1	2.66	0.49
1:B:680:ASN:ND2	1:B:682:ASP:H	2.11	0.49
1:A:181:GLY:N	4:A:917:HOH:O	2.44	0.49
1:A:198:ASN:ND2	1:A:200:ARG:HH21	2.10	0.49
1:A:254:ARG:NE	4:A:922:HOH:O	2.46	0.49
1:A:685[A]:HIS:CE1	1:B:685[A]:HIS:CE1	3.00	0.49
1:C:563:LYS:C	1:C:564:LYS:HD3	2.33	0.49
2:E:2:GLC:H61	2:E:3:GLC:C5	2.43	0.49
1:D:445:ILE:HG13	4:D:901:HOH:O	2.11	0.49
1:C:559:ALA:HB1	1:C:653:VAL:HG21	1.94	0.48
1:D:606:LEU:HD13	1:D:679:LEU:HD11	1.95	0.48
2:E:2:GLC:H61	2:E:3:GLC:H5	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:THR:HB	1:B:118:HIS:CD2	2.48	0.48
1:D:594:ASN:H	1:D:597:HIS:CD2	2.30	0.48
1:D:728:GLU:OXT	1:D:728:GLU:HG2	2.13	0.48
1:B:294:PHE:HB3	4:B:1353:HOH:O	2.13	0.48
1:C:680:ASN:HD22	1:C:682:ASP:H	1.61	0.48
1:B:425:ASN:HD22	1:B:425:ASN:C	2.17	0.48
1:C:636:ARG:HG2	1:C:662:ARG:CZ	2.44	0.48
1:A:681:THR:HG23	1:A:720:THR:O	2.14	0.48
1:B:256:HIS:HE1	1:B:267:GLU:OE2	1.97	0.48
1:C:533:LYS:HE2	1:C:537:ASP:HB3	1.96	0.48
1:C:680:ASN:ND2	1:C:682:ASP:H	2.12	0.48
1:A:594:ASN:N	1:A:597:HIS:HD2	2.02	0.48
4:A:1092:HOH:O	1:B:685[B]:HIS:HE1	1.96	0.48
1:D:486:MET:O	1:D:490:LEU:HB2	2.13	0.48
1:B:415:TYR:C	1:B:430:ARG:HB3	2.34	0.47
1:D:211:GLN:NE2	1:D:217:ALA:H	2.12	0.47
1:B:644:ARG:HG2	1:B:650:GLU:HG2	1.96	0.47
1:D:614:LYS:O	1:D:618:GLU:HB2	2.14	0.47
1:B:559:ALA:HB1	1:B:653:VAL:HG21	1.95	0.47
1:D:162:ARG:HH21	1:D:162:ARG:HG2	1.78	0.47
1:D:350:GLU:HA	1:D:354:THR:O	2.14	0.47
1:A:290[B]:ASN:HD21	1:A:337:VAL:HG21	1.78	0.47
1:B:138:THR:CG2	1:B:182:ALA:O	2.55	0.47
1:D:680:ASN:HD22	1:D:681:THR:N	2.13	0.47
1:A:512:LEU:CD2	2:E:4:GLC:C6	2.93	0.47
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.95	0.47
1:A:693:ASN:ND2	1:A:714:THR:H	2.08	0.46
1:D:684:MET:N	1:D:690:ASN:HD22	2.12	0.46
1:B:542:ASP:OD2	1:B:545:GLN:HG3	2.14	0.46
1:A:209:GLU:HG2	1:A:219:LEU:HD22	1.98	0.46
1:A:684:MET:H	1:A:690:ASN:HD22	1.62	0.46
2:E:1:GLC:O2	2:E:8:GLC:O3	2.28	0.46
1:C:282:THR:OG1	1:C:283:HIS:HD2	1.98	0.46
1:D:602:LEU:HG	1:D:606:LEU:HD22	1.97	0.46
1:B:635:GLU:HA	1:B:635:GLU:OE2	2.15	0.46
1:C:684[A]:MET:H	1:C:690:ASN:HD22	1.64	0.46
2:E:2:GLC:H61	2:E:3:GLC:H62	1.97	0.46
1:D:211:GLN:HE21	1:D:217:ALA:HB3	1.81	0.45
1:A:154:GLY:HA2	1:A:188:TYR:HA	1.98	0.45
1:C:170:LYS:HA	1:C:170:LYS:CE	2.41	0.45
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:GLC:H61	2:E:3:GLC:C6	2.46	0.45
1:A:285:GLU:OE1	1:A:403:ARG:HD2	2.17	0.45
1:B:660:VAL:HA	1:B:661:PRO:HD3	1.86	0.45
1:A:259:ASN:ND2	1:A:261:PHE:H	2.15	0.45
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.99	0.45
1:C:215:GLU:CG	4:C:968:HOH:O	2.64	0.45
1:B:212:MET:HG2	4:B:1291:HOH:O	2.16	0.45
1:A:523:LEU:HD22	1:A:557:MET:SD	2.56	0.45
1:B:422:TRP:HZ2	1:B:430:ARG:HH21	1.65	0.45
1:C:171:GLU:CG	1:C:172:SER:N	2.80	0.45
1:C:620:ASP:OD2	1:C:643:ARG:NH2	2.31	0.45
1:C:247:GLU:OE1	1:C:525:HIS:CD2	2.70	0.45
1:D:138:THR:HG23	1:D:182:ALA:HB3	1.99	0.45
1:D:150:VAL:HG12	1:D:166:MET:SD	2.57	0.45
1:D:310:ARG:NE	4:D:904:HOH:O	2.34	0.45
1:D:620:ASP:OD2	1:D:643:ARG:NH2	2.43	0.45
1:B:644:ARG:HG3	1:B:650:GLU:HG2	1.98	0.45
1:B:658:THR:HG23	1:B:659:PRO:HD2	1.99	0.45
1:C:375:TYR:O	1:C:376:ASN:HB3	2.17	0.44
1:A:512:LEU:HD22	1:A:512:LEU:H	1.82	0.44
1:C:559:ALA:HA	1:C:616:MET:HE3	1.99	0.44
1:A:349:ALA:O	1:A:350:GLU:C	2.56	0.44
1:A:676[B]:ARG:NE	1:A:726:GLU:OE1	2.51	0.44
1:C:490:LEU:HD12	1:C:490:LEU:HA	1.90	0.44
1:C:547:PHE:O	1:C:551:ARG:HG3	2.18	0.44
1:A:154:GLY:HA3	1:A:156:PHE:CZ	2.52	0.44
1:C:615:ALA:HB3	1:C:651:ILE:HD13	1.99	0.44
1:D:693:ASN:ND2	1:D:714:THR:H	2.10	0.44
1:B:164:HIS:CE1	4:B:1282:HOH:O	2.45	0.44
1:B:439:LEU:HD23	1:B:439:LEU:HA	1.82	0.44
1:C:247:GLU:OE1	1:C:525:HIS:HD2	2.00	0.44
1:A:684:MET:HG3	1:A:685[B]:HIS:N	2.32	0.44
1:B:533:LYS:O	1:B:538:ARG:NH2	2.51	0.44
1:C:237:ASN:ND2	1:C:283:HIS:CE1	2.74	0.44
1:B:215:GLU:H	1:B:215:GLU:HG2	1.59	0.43
1:D:335:ASP:OD1	1:D:403:ARG:HD3	2.18	0.43
1:A:237:ASN:HD22	1:A:283:HIS:HE1	1.62	0.43
1:A:289:ILE:HG13	1:A:334:LEU:HD11	1.99	0.43
1:C:511:ILE:HG21	1:C:628:TRP:HE1	1.83	0.43
1:C:571:GLU:HA	1:C:603:VAL:HG21	2.00	0.43
1:D:647:GLU:CD	4:D:947:HOH:O	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:HG13	1:B:334:LEU:CD1	2.46	0.43
1:B:425:ASN:HD22	1:B:427:PHE:N	2.13	0.43
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.64	0.43
1:D:646:LYS:HB2	1:D:646:LYS:HE3	1.75	0.43
1:A:138:THR:HG21	1:A:220:ILE:HG21	1.99	0.43
1:A:292:HIS:O	1:A:311:ARG:NH1	2.39	0.43
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.80	0.43
1:B:256:HIS:CE1	1:B:267:GLU:OE2	2.72	0.43
1:C:621:PHE:N	4:C:905:HOH:O	2.46	0.43
1:C:684[A]:MET:CE	1:D:684:MET:CG	2.97	0.43
1:B:414:ASP:O	1:B:422:TRP:CG	2.72	0.43
1:D:380:ARG:HD2	1:D:380:ARG:HA	1.82	0.43
1:B:601:ARG:HD2	1:B:685[A]:HIS:CE1	2.53	0.43
1:D:430:ARG:HA	1:D:430:ARG:HD2	1.63	0.43
1:B:709:HIS:HE1	4:D:902:HOH:O	2.01	0.43
1:C:359:HIS:HB3	1:C:360:SER:H	1.42	0.43
1:A:512:LEU:HA	1:A:512:LEU:HD13	1.80	0.43
1:B:117:THR:HB	1:B:118:HIS:H	1.25	0.43
1:B:226:LYS:NZ	4:B:905:HOH:O	2.33	0.43
1:A:168:LEU:HB2	1:A:175:TRP:CD2	2.53	0.42
1:C:293:PRO:HD3	1:C:303:THR:HG23	2.02	0.42
1:C:593:ASP:OD2	1:C:687:HIS:HE1	2.02	0.42
1:C:594:ASN:N	1:C:597:HIS:HD2	2.01	0.42
1:D:143:TRP:CH2	1:D:356:LEU:HD22	2.54	0.42
1:D:525:HIS:HB3	1:D:567:PHE:CE1	2.54	0.42
1:A:410:MET:HE1	1:A:439:LEU:HD21	2.01	0.42
1:C:204:ASP:HB3	1:C:207:ALA:HB2	2.01	0.42
1:C:489:THR:HG22	1:C:507:LEU:HD12	2.01	0.42
1:C:514:ASN:ND2	4:C:907:HOH:O	2.52	0.42
1:A:376:ASN:C	1:A:376:ASN:HD22	2.21	0.42
1:B:138:THR:HG23	1:B:182:ALA:CB	2.49	0.42
1:A:684:MET:HG3	1:A:685[A]:HIS:N	2.33	0.42
1:C:242:PRO:HD3	1:C:617:HIS:CE1	2.54	0.42
1:C:143:TRP:CH2	1:C:356:LEU:HD22	2.54	0.42
1:C:254:ARG:HG3	4:C:960:HOH:O	2.19	0.42
1:A:187:LEU:HD13	1:A:211:GLN:NE2	2.34	0.42
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.74	0.42
1:B:666:ARG:O	3:B:803:GOL:C3	2.56	0.42
1:C:601[B]:ARG:CG	1:C:601[B]:ARG:NH1	2.81	0.42
1:A:290[B]:ASN:HD21	1:A:337:VAL:CG2	2.33	0.42
1:A:290[B]:ASN:ND2	1:A:337:VAL:CG2	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:GLN:HA	1:C:672:PRO:HD2	1.87	0.42
1:A:407:VAL:HA	1:A:410:MET:HE2	2.01	0.42
1:D:211:GLN:NE2	1:D:217:ALA:HB3	2.35	0.42
1:C:215:GLU:HG2	4:C:968:HOH:O	2.20	0.42
1:D:132:MET:HE3	1:D:139:ARG:NH1	2.34	0.42
1:D:194:ASP:HB2	1:D:198:ASN:H	1.85	0.42
1:A:525:HIS:HB3	1:A:567:PHE:CE1	2.55	0.41
1:B:511:ILE:HD12	1:B:511:ILE:HG23	1.81	0.41
1:C:153:VAL:HB	1:C:159:TRP:HA	2.02	0.41
1:D:143:TRP:CZ3	1:D:356:LEU:HD13	2.55	0.41
1:C:152:VAL:HG23	1:C:166:MET:SD	2.61	0.41
1:C:259:ASN:HD22	1:C:259:ASN:H	1.67	0.41
1:C:525:HIS:HB3	1:C:567:PHE:CE1	2.55	0.41
1:A:256:HIS:HE1	1:A:267:GLU:OE2	2.03	0.41
1:A:552:ALA:O	1:A:720:THR:HG23	2.20	0.41
1:A:290[B]:ASN:OD1	1:A:290[B]:ASN:O	2.38	0.41
1:B:656:ASN:C	1:B:656:ASN:HD22	2.24	0.41
1:C:566:LEU:HG	1:C:570:ASN:HB2	2.01	0.41
1:B:606:LEU:HD13	1:B:679:LEU:CD1	2.50	0.41
1:D:215:GLU:CG	2:I:2:GLC:O2	2.69	0.41
1:D:704:SER:OG	1:D:705:HIS:HD2	2.04	0.41
1:A:144:ALA:HA	1:A:145:PRO:HD2	1.89	0.41
1:A:163:ARG:HE	1:A:163:ARG:HB2	1.77	0.41
1:A:179:ILE:HA	1:A:180:PRO:HD2	1.88	0.41
1:A:656:ASN:C	1:A:656:ASN:HD22	2.22	0.41
1:B:376:ASN:ND2	4:B:935:HOH:O	2.53	0.41
1:C:215:GLU:O	1:C:216:THR:CB	2.68	0.41
1:C:494:LYS:HD3	1:C:538:ARG:HG2	2.03	0.41
1:D:153:VAL:HA	1:D:157:ASN:ND2	2.35	0.41
1:D:230:THR:OG1	1:D:232:GLU:HG2	2.20	0.41
1:D:254:ARG:NE	4:D:941:HOH:O	2.53	0.41
1:D:489:THR:O	1:D:493:MET:HG2	2.21	0.41
1:D:610:TYR:O	1:D:617:HIS:HD2	2.03	0.41
1:A:120:ARG:HG2	1:A:122:TYR:OH	2.21	0.41
1:D:305:LEU:HD13	1:D:305:LEU:HA	1.78	0.41
1:D:345:ASP:O	1:D:346:PHE:C	2.58	0.41
1:C:549:ASN:OD1	1:C:718:LEU:HD22	2.21	0.41
1:C:684[A]:MET:HE1	1:D:684:MET:CG	2.50	0.41
1:D:138:THR:CG2	1:D:182:ALA:C	2.89	0.41
1:D:666:ARG:HA	1:D:711:LEU:O	2.21	0.41
1:A:118:HIS:O	1:A:384:ASN:ND2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLN:HE21	1:A:585:ASP:H	1.60	0.41
1:B:211:GLN:CD	1:B:215:GLU:HB2	2.42	0.41
1:C:237:ASN:HD22	1:C:283:HIS:HE1	1.65	0.41
1:C:292:HIS:CG	1:C:299:GLY:HA2	2.56	0.41
1:C:523:LEU:HD12	1:C:523:LEU:HA	1.90	0.41
1:C:684[B]:MET:H	1:C:690:ASN:HD22	1.68	0.41
1:D:213:ARG:HB3	4:D:1225:HOH:O	2.21	0.41
1:D:485:TRP:CE2	1:D:489:THR:HG21	2.56	0.41
1:D:492:TYR:CZ	1:D:507:LEU:HD22	2.56	0.41
4:D:1187:HOH:O	2:H:1:GLC:H3	2.21	0.41
1:A:444:ARG:O	1:A:448:GLU:HG3	2.21	0.41
1:D:542:ASP:H	1:D:545:GLN:NE2	2.19	0.41
1:B:259:ASN:ND2	1:B:259:ASN:H	2.18	0.40
1:C:561:PRO:HA	1:C:643:ARG:NH2	2.35	0.40
1:D:310:ARG:HD2	1:D:313:GLY:O	2.20	0.40
1:A:198:ASN:HD22	1:A:200:ARG:HH21	1.69	0.40
1:A:492:TYR:CZ	1:A:507:LEU:HD22	2.57	0.40
1:A:610:TYR:O	1:A:617:HIS:HD2	2.04	0.40
1:D:133:ASP:OD2	1:D:133:ASP:N	2.54	0.40
1:A:181:GLY:HA2	4:A:917:HOH:O	2.20	0.40
1:A:674:LYS:HB3	1:A:696:THR:HG23	2.03	0.40
1:B:264:SER:HB2	4:B:1214:HOH:O	2.20	0.40
1:B:341:PHE:HA	1:B:342:PRO:HD3	1.91	0.40
1:B:442:THR:HG22	1:B:446:LEU:HD22	2.03	0.40
1:C:149:ARG:NH1	1:C:165:PRO:HB3	2.36	0.40
1:D:211:GLN:NE2	1:D:215:GLU:HG3	2.36	0.40
1:D:512:LEU:HD23	1:D:512:LEU:HA	1.80	0.40
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ASP:OD1	2:H:5:GLC:O6[2_655]	2.18	0.02

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	586/612 (96%)	557 (95%)	25 (4%)	4 (1%)	22	22
1	B	596/612 (97%)	580 (97%)	13 (2%)	3 (0%)	29	31
1	C	572/612 (94%)	538 (94%)	30 (5%)	4 (1%)	22	22
1	D	584/612 (95%)	558 (96%)	22 (4%)	4 (1%)	22	22
All	All	2338/2448 (96%)	2233 (96%)	90 (4%)	15 (1%)	25	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	PRO
1	A	215	GLU
1	C	216	THR
1	D	194	ASP
1	B	355	ASN
1	B	414	ASP
1	B	522	PRO
1	C	194	ASP
1	D	157	ASN
1	D	372	THR
1	A	522	PRO
1	C	687	HIS
1	D	522	PRO
1	A	158	TYR
1	C	522	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	504/521 (97%)	467 (93%)	37 (7%)	14	14
1	B	512/521 (98%)	470 (92%)	42 (8%)	11	11
1	C	492/521 (94%)	451 (92%)	41 (8%)	11	11
1	D	501/521 (96%)	459 (92%)	42 (8%)	11	10
All	All	2009/2084 (96%)	1847 (92%)	162 (8%)	11	11

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	THR
1	A	132	MET
1	A	142	VAL
1	A	146	ASN
1	A	148	ARG
1	A	199	LEU
1	A	216	THR
1	A	223	LEU
1	A	231	GLU
1	A	259	ASN
1	A	305	LEU
1	A	315	ARG
1	A	331	ASN
1	A	356	LEU
1	A	359	HIS
1	A	376	ASN
1	A	391	LEU
1	A	462	ASP
1	A	475	LEU
1	A	490	LEU
1	A	498	VAL
1	A	504	HIS
1	A	505[A]	ASP
1	A	505[B]	ASP
1	A	507	LEU
1	A	523	LEU
1	A	579	ASN
1	A	606	LEU
1	A	619	LEU
1	A	642	VAL
1	A	647	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	656	ASN
1	A	679	LEU
1	A	680	ASN
1	A	684	MET
1	A	720	THR
1	A	723	LEU
1	B	117	THR
1	B	133	ASP
1	B	138	THR
1	B	151	SER
1	B	163	ARG
1	B	168	LEU
1	B	212	MET
1	B	213	ARG
1	B	215	GLU
1	B	218	SER
1	B	223	LEU
1	B	259	ASN
1	B	290	ASN
1	B	305	LEU
1	B	315	ARG
1	B	331	ASN
1	B	334	LEU
1	B	356	LEU
1	B	363	ARG
1	B	364	GLU
1	B	372	THR
1	B	376	ASN
1	B	391	LEU
1	B	415	TYR
1	B	425	ASN
1	B	446	LEU
1	B	470	GLN
1	B	475	LEU
1	B	490	LEU
1	B	507	LEU
1	B	512	LEU
1	B	523	LEU
1	B	546	LYS
1	B	579	ASN
1	B	581	ASP
1	B	606	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	619	LEU
1	B	642	VAL
1	B	656	ASN
1	B	658	THR
1	B	680	ASN
1	B	723	LEU
1	C	119	LEU
1	C	138	THR
1	C	148	ARG
1	C	163	ARG
1	C	223	LEU
1	C	226	LYS
1	C	235	LYS
1	C	259	ASN
1	C	266	ARG
1	C	278	TRP
1	C	290	ASN
1	C	291	GLU
1	C	310	ARG
1	C	315	ARG
1	C	319	ARG
1	C	331	ASN
1	C	334	LEU
1	C	343	THR
1	C	356	LEU
1	C	359	HIS
1	C	375	TYR
1	C	391	LEU
1	C	430	ARG
1	C	458	GLU
1	C	470	GLN
1	C	472	MET
1	C	496	ASP
1	C	505	ASP
1	C	507	LEU
1	C	523	LEU
1	C	546	LYS
1	C	564	LYS
1	C	590	GLU
1	C	619	LEU
1	C	642	VAL
1	C	643	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	676	ARG
1	C	680	ASN
1	C	683	SER
1	C	690	ASN
1	C	720	THR
1	D	117	THR
1	D	119	LEU
1	D	133	ASP
1	D	138	THR
1	D	141	SER
1	D	148	ARG
1	D	171	GLU
1	D	212	MET
1	D	213	ARG
1	D	219	LEU
1	D	223	LEU
1	D	232	GLU
1	D	310	ARG
1	D	315	ARG
1	D	331	ASN
1	D	356	LEU
1	D	359	HIS
1	D	373	LEU
1	D	391	LEU
1	D	430	ARG
1	D	437	GLU
1	D	470	GLN
1	D	472	MET
1	D	475	LEU
1	D	490	LEU
1	D	495	LEU
1	D	507	LEU
1	D	512	LEU
1	D	523	LEU
1	D	581	ASP
1	D	595	TRP
1	D	606	LEU
1	D	619	LEU
1	D	642	VAL
1	D	647	GLU
1	D	651	ILE
1	D	656	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	679	LEU
1	D	680	ASN
1	D	690	ASN
1	D	723	LEU
1	D	728	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	157	ASN
1	A	198	ASN
1	A	237	ASN
1	A	256	HIS
1	A	259	ASN
1	A	283	HIS
1	A	331	ASN
1	A	340	HIS
1	A	359	HIS
1	A	376	ASN
1	A	504	HIS
1	A	514	ASN
1	A	525	HIS
1	A	530	HIS
1	A	570	ASN
1	A	574	GLN
1	A	579	ASN
1	A	597	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	687	HIS
1	A	690	ASN
1	A	693	ASN
1	A	705	HIS
1	A	709	HIS
1	B	118	HIS
1	B	164	HIS
1	B	183	HIS
1	B	198	ASN
1	B	237	ASN
1	B	256	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	259	ASN
1	B	283	HIS
1	B	331	ASN
1	B	340	HIS
1	B	359	HIS
1	B	376	ASN
1	B	425	ASN
1	B	470	GLN
1	B	504	HIS
1	B	514	ASN
1	B	525	HIS
1	B	545	GLN
1	B	570	ASN
1	B	574	GLN
1	B	579	ASN
1	B	597	HIS
1	B	617	HIS
1	B	656	ASN
1	B	680	ASN
1	B	687	HIS
1	B	690	ASN
1	B	705	HIS
1	B	709	HIS
1	C	164	HIS
1	C	237	ASN
1	C	259	ASN
1	C	283	HIS
1	C	290	ASN
1	C	301	GLN
1	C	331	ASN
1	C	355	ASN
1	C	470	GLN
1	C	501	GLN
1	C	525	HIS
1	C	530	HIS
1	C	545	GLN
1	C	570	ASN
1	C	574	GLN
1	C	580	HIS
1	C	597	HIS
1	C	617	HIS
1	C	656	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	680	ASN
1	C	687	HIS
1	C	690	ASN
1	C	693	ASN
1	C	708	GLN
1	D	157	ASN
1	D	164	HIS
1	D	186	GLN
1	D	211	GLN
1	D	237	ASN
1	D	238	GLN
1	D	283	HIS
1	D	290	ASN
1	D	331	ASN
1	D	340	HIS
1	D	441	ASN
1	D	443	ASN
1	D	470	GLN
1	D	504	HIS
1	D	514	ASN
1	D	525	HIS
1	D	545	GLN
1	D	570	ASN
1	D	574	GLN
1	D	597	HIS
1	D	617	HIS
1	D	656	ASN
1	D	680	ASN
1	D	685	HIS
1	D	687	HIS
1	D	690	ASN
1	D	693	ASN
1	D	705	HIS
1	D	708	GLN

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)

40 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	E	1	2	11,11,12	0.69	0	15,15,17	2.25	4 (26%)
2	GLC	E	2	2	11,11,12	0.51	0	15,15,17	1.17	2 (13%)
2	GLC	E	3	2	11,11,12	0.60	0	15,15,17	1.76	2 (13%)
2	GLC	E	4	2	11,11,12	0.15	0	15,15,17	1.02	1 (6%)
2	GLC	E	5	2	11,11,12	0.56	0	15,15,17	2.01	3 (20%)
2	GLC	E	6	2	11,11,12	0.59	0	15,15,17	1.31	1 (6%)
2	GLC	E	7	2	11,11,12	0.56	0	15,15,17	1.03	1 (6%)
2	GLC	E	8	2	11,11,12	0.54	0	15,15,17	1.61	2 (13%)
2	GLC	F	1	2	11,11,12	0.67	0	15,15,17	1.15	1 (6%)
2	GLC	F	2	2	11,11,12	0.43	0	15,15,17	1.08	1 (6%)
2	GLC	F	3	2	11,11,12	0.51	0	15,15,17	1.84	5 (33%)
2	GLC	F	4	2	11,11,12	0.39	0	15,15,17	0.78	1 (6%)
2	GLC	F	5	2	11,11,12	0.51	0	15,15,17	1.50	3 (20%)
2	GLC	F	6	2	11,11,12	0.65	0	15,15,17	1.27	2 (13%)
2	GLC	F	7	2	11,11,12	0.53	0	15,15,17	1.05	1 (6%)
2	GLC	F	8	2	11,11,12	0.32	0	15,15,17	1.49	3 (20%)
2	GLC	G	1	2	11,11,12	0.35	0	15,15,17	1.19	1 (6%)
2	GLC	G	2	2	11,11,12	0.59	0	15,15,17	1.33	2 (13%)
2	GLC	G	3	2	11,11,12	0.25	0	15,15,17	0.70	0
2	GLC	G	4	2	11,11,12	0.38	0	15,15,17	0.80	0
2	GLC	G	5	2	11,11,12	0.26	0	15,15,17	0.71	0
2	GLC	G	6	2	11,11,12	0.32	0	15,15,17	1.16	1 (6%)
2	GLC	G	7	2	11,11,12	0.35	0	15,15,17	0.87	1 (6%)
2	GLC	G	8	2	11,11,12	0.38	0	15,15,17	0.97	0
2	GLC	H	1	2	11,11,12	0.43	0	15,15,17	1.15	1 (6%)
2	GLC	H	2	2	11,11,12	0.62	0	15,15,17	1.02	1 (6%)
2	GLC	H	3	2	11,11,12	0.42	0	15,15,17	1.65	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	H	4	2	11,11,12	0.29	0	15,15,17	1.04	1 (6%)
2	GLC	H	5	2	11,11,12	0.61	0	15,15,17	1.10	1 (6%)
2	GLC	H	6	2	11,11,12	0.63	0	15,15,17	1.62	2 (13%)
2	GLC	H	7	2	11,11,12	0.40	0	15,15,17	1.22	1 (6%)
2	GLC	H	8	2	11,11,12	0.41	0	15,15,17	1.25	3 (20%)
2	GLC	I	1	2	11,11,12	0.37	0	15,15,17	1.12	2 (13%)
2	GLC	I	2	2	11,11,12	0.56	0	15,15,17	0.98	1 (6%)
2	GLC	I	3	2	11,11,12	0.29	0	15,15,17	0.95	1 (6%)
2	GLC	I	4	2	11,11,12	0.35	0	15,15,17	0.84	0
2	GLC	I	5	2	11,11,12	0.41	0	15,15,17	1.64	1 (6%)
2	GLC	I	6	2	11,11,12	0.38	0	15,15,17	1.19	2 (13%)
2	GLC	I	7	2	11,11,12	0.51	0	15,15,17	1.14	1 (6%)
2	GLC	I	8	2	11,11,12	0.48	0	15,15,17	0.99	1 (6%)

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	E	1	2	-	2/2/19/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	2/2/19/22	0/1/1/1
2	GLC	E	6	2	-	0/2/19/22	0/1/1/1
2	GLC	E	7	2	-	2/2/19/22	0/1/1/1
2	GLC	E	8	2	-	2/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	GLC	F	4	2	-	2/2/19/22	0/1/1/1
2	GLC	F	5	2	-	1/2/19/22	0/1/1/1
2	GLC	F	6	2	-	2/2/19/22	0/1/1/1
2	GLC	F	7	2	-	0/2/19/22	0/1/1/1
2	GLC	F	8	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	1/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	G	6	2	-	2/2/19/22	0/1/1/1
2	GLC	G	7	2	-	2/2/19/22	0/1/1/1
2	GLC	G	8	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/19/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	2/2/19/22	0/1/1/1
2	GLC	H	5	2	-	0/2/19/22	0/1/1/1
2	GLC	H	6	2	-	1/2/19/22	0/1/1/1
2	GLC	H	7	2	-	0/2/19/22	0/1/1/1
2	GLC	H	8	2	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	1/2/19/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	1/2/19/22	0/1/1/1
2	GLC	I	5	2	-	2/2/19/22	0/1/1/1
2	GLC	I	6	2	-	2/2/19/22	0/1/1/1
2	GLC	I	7	2	-	0/2/19/22	0/1/1/1
2	GLC	I	8	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	GLC	C1-O5-C5	6.75	121.33	112.19
2	E	5	GLC	C1-O5-C5	5.73	119.96	112.19
2	I	5	GLC	C1-O5-C5	5.45	119.58	112.19
2	E	8	GLC	C1-O5-C5	5.34	119.42	112.19
2	H	6	GLC	C1-O5-C5	5.19	119.23	112.19
2	E	3	GLC	C1-C2-C3	5.01	115.83	109.67
2	F	5	GLC	C1-C2-C3	4.15	114.77	109.67
2	H	3	GLC	O5-C5-C6	4.11	113.65	107.20
2	F	3	GLC	C1-O5-C5	3.88	117.44	112.19
2	H	7	GLC	O5-C1-C2	-3.67	105.11	110.77
2	E	6	GLC	C1-O5-C5	3.60	117.07	112.19
2	F	8	GLC	C1-O5-C5	3.56	117.01	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	GLC	C1-O5-C5	3.26	116.61	112.19
2	E	1	GLC	O5-C5-C6	3.23	112.28	107.20
2	G	1	GLC	C1-C2-C3	3.16	113.56	109.67
2	E	3	GLC	C2-C3-C4	3.06	116.18	110.89
2	F	3	GLC	O5-C1-C2	-2.93	106.25	110.77
2	G	2	GLC	C1-C2-C3	2.86	113.18	109.67
2	F	3	GLC	C1-C2-C3	-2.79	106.24	109.67
2	F	1	GLC	C1-O5-C5	2.78	115.96	112.19
2	F	7	GLC	C1-O5-C5	2.75	115.92	112.19
2	H	3	GLC	O5-C1-C2	-2.71	106.58	110.77
2	H	5	GLC	C1-C2-C3	2.70	112.98	109.67
2	H	4	GLC	O5-C1-C2	-2.60	106.77	110.77
2	F	6	GLC	O5-C5-C6	2.55	111.20	107.20
2	E	7	GLC	C1-O5-C5	2.52	115.61	112.19
2	F	6	GLC	C1-C2-C3	2.50	112.74	109.67
2	I	1	GLC	O5-C1-C2	-2.49	106.92	110.77
2	E	2	GLC	C1-O5-C5	2.48	115.56	112.19
2	E	1	GLC	C2-C3-C4	-2.45	106.66	110.89
2	I	7	GLC	O5-C5-C6	2.44	111.04	107.20
2	G	7	GLC	C1-C2-C3	2.44	112.67	109.67
2	H	6	GLC	C6-C5-C4	-2.43	107.31	113.00
2	E	2	GLC	C2-C3-C4	-2.41	106.72	110.89
2	H	2	GLC	C1-O5-C5	2.41	115.46	112.19
2	E	4	GLC	C2-C3-C4	-2.38	106.77	110.89
2	G	2	GLC	O5-C5-C6	2.38	110.94	107.20
2	F	5	GLC	C1-O5-C5	-2.37	108.98	112.19
2	I	8	GLC	O5-C1-C2	-2.36	107.13	110.77
2	G	6	GLC	C1-C2-C3	2.34	112.54	109.67
2	E	5	GLC	O5-C5-C4	2.32	116.48	110.83
2	F	8	GLC	C2-C3-C4	-2.32	106.88	110.89
2	F	8	GLC	O5-C5-C6	2.32	110.84	107.20
2	E	5	GLC	C6-C5-C4	-2.30	107.61	113.00
2	I	6	GLC	C1-C2-C3	2.27	112.46	109.67
2	I	3	GLC	C1-O5-C5	2.23	115.22	112.19
2	F	4	GLC	C1-O5-C5	2.21	115.18	112.19
2	I	6	GLC	C2-C3-C4	2.18	114.66	110.89
2	I	1	GLC	C1-C2-C3	2.16	112.32	109.67
2	I	2	GLC	C1-O5-C5	2.16	115.12	112.19
2	F	3	GLC	C2-C3-C4	-2.14	107.19	110.89
2	H	8	GLC	O5-C5-C6	2.11	110.51	107.20
2	F	5	GLC	C2-C3-C4	2.11	114.54	110.89
2	H	8	GLC	O3-C3-C2	-2.10	105.97	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	3	GLC	C3-C4-C5	-2.10	106.50	110.24
2	H	8	GLC	C1-O5-C5	2.09	115.03	112.19
2	F	3	GLC	O5-C5-C4	2.07	115.86	110.83
2	F	2	GLC	C1-O5-C5	2.04	114.95	112.19
2	E	8	GLC	O5-C5-C6	2.04	110.39	107.20
2	E	1	GLC	O2-C2-C1	2.02	113.29	109.15

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	GLC	O5-C5-C6-O6
2	G	6	GLC	O5-C5-C6-O6
2	E	8	GLC	O5-C5-C6-O6
2	E	8	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	G	7	GLC	O5-C5-C6-O6
2	F	6	GLC	O5-C5-C6-O6
2	I	6	GLC	O5-C5-C6-O6
2	E	5	GLC	C4-C5-C6-O6
2	F	3	GLC	C4-C5-C6-O6
2	G	7	GLC	C4-C5-C6-O6
2	E	5	GLC	O5-C5-C6-O6
2	I	5	GLC	O5-C5-C6-O6
2	I	8	GLC	O5-C5-C6-O6
2	F	4	GLC	C4-C5-C6-O6
2	E	7	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6
2	G	6	GLC	C4-C5-C6-O6
2	E	7	GLC	C4-C5-C6-O6
2	I	8	GLC	C4-C5-C6-O6
2	F	6	GLC	C4-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	I	6	GLC	C4-C5-C6-O6
2	F	4	GLC	O5-C5-C6-O6
2	H	6	GLC	O5-C5-C6-O6
2	I	4	GLC	O5-C5-C6-O6
2	I	5	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	F	5	GLC	C4-C5-C6-O6
2	H	4	GLC	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	I	1	GLC	C4-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	G	4	GLC	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	H	4	GLC	O5-C5-C6-O6

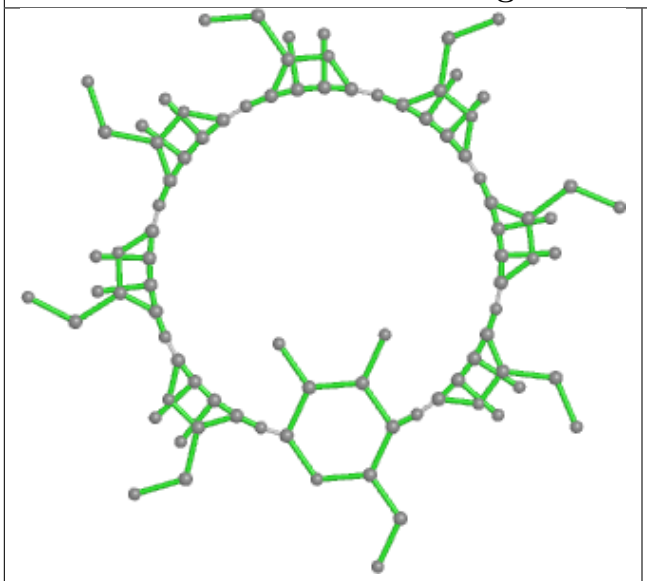
There are no ring outliers.

14 monomers are involved in 19 short contacts:

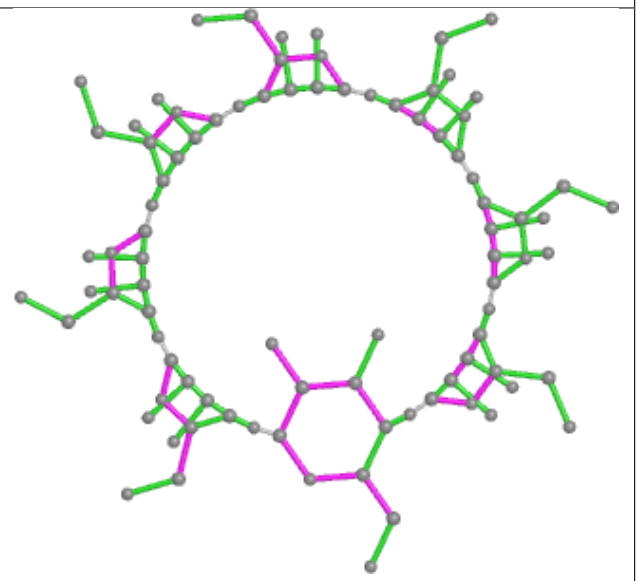
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GLC	6	0
2	E	5	GLC	1	0
2	I	2	GLC	2	0
2	E	1	GLC	4	0
2	H	5	GLC	0	1
2	F	4	GLC	1	0
2	G	7	GLC	1	0
2	H	1	GLC	1	0
2	E	3	GLC	4	0
2	G	8	GLC	1	0
2	E	8	GLC	2	0
2	E	7	GLC	1	0
2	E	6	GLC	1	0
2	E	4	GLC	3	0

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

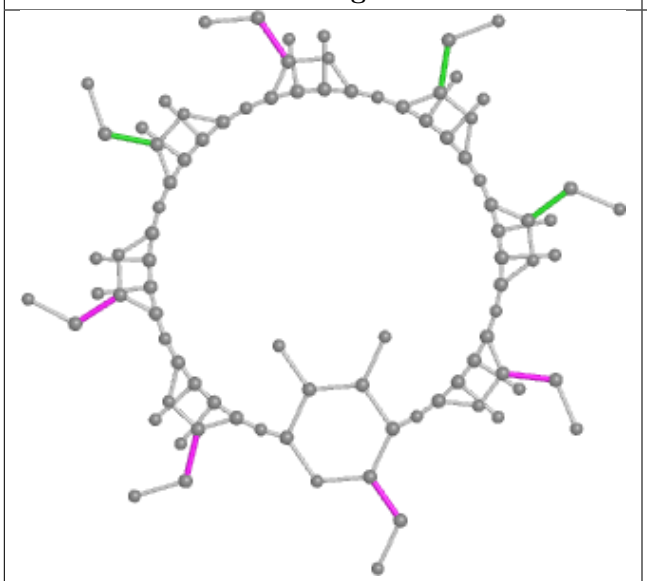
Oligosaccharide Chain E



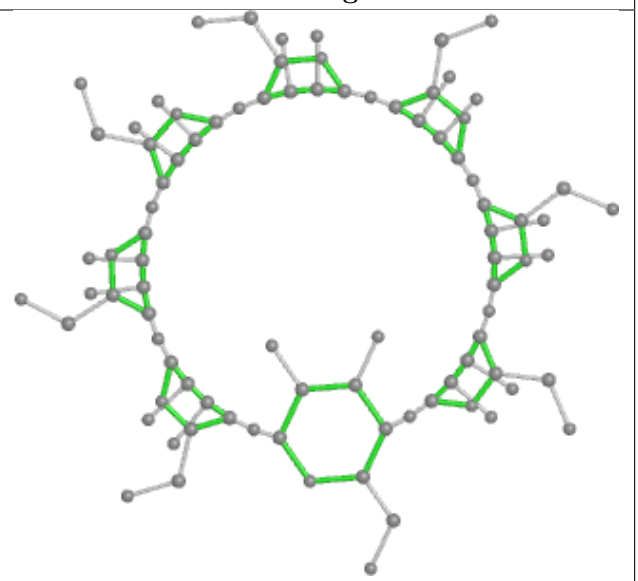
Bond lengths



Bond angles

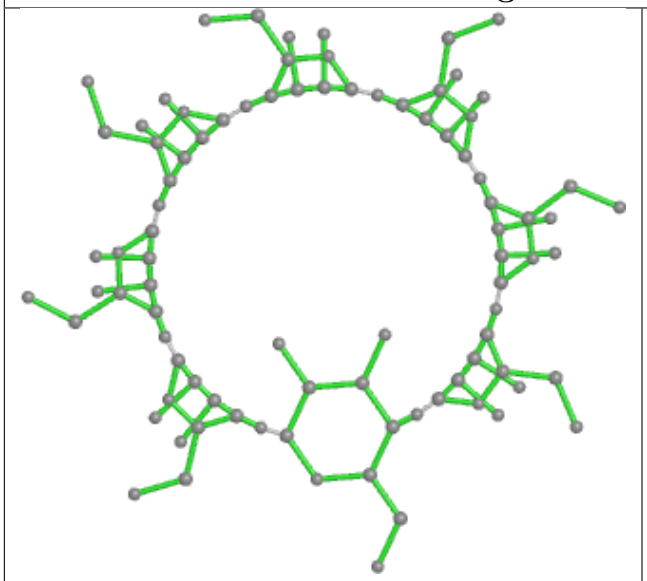


Torsions

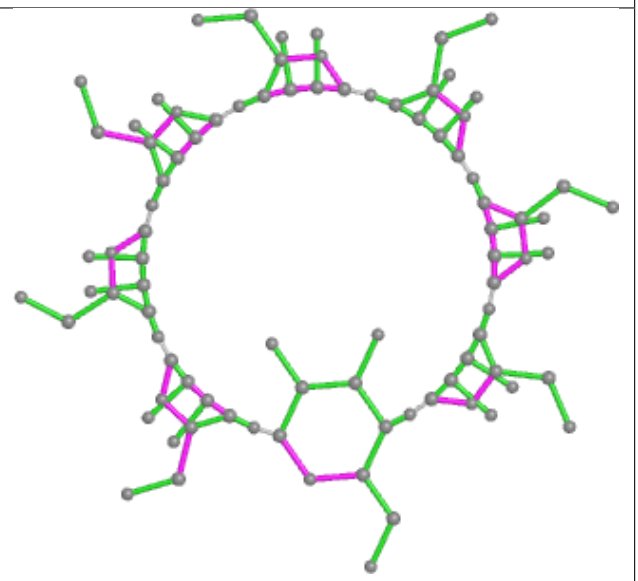


Rings

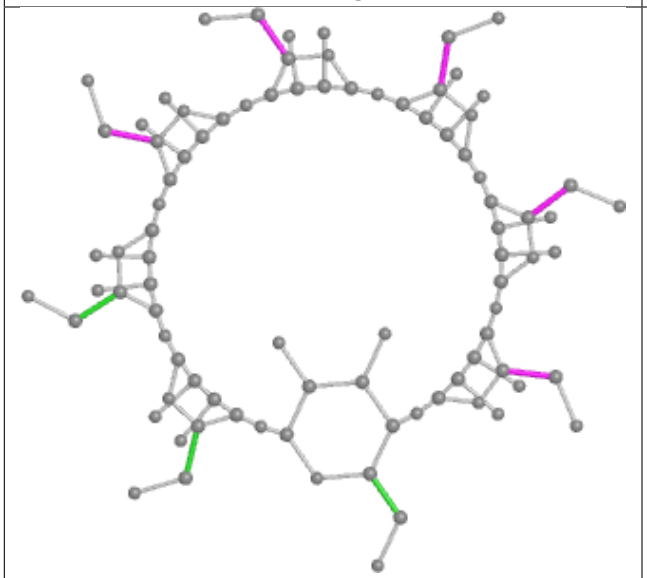
Oligosaccharide Chain F



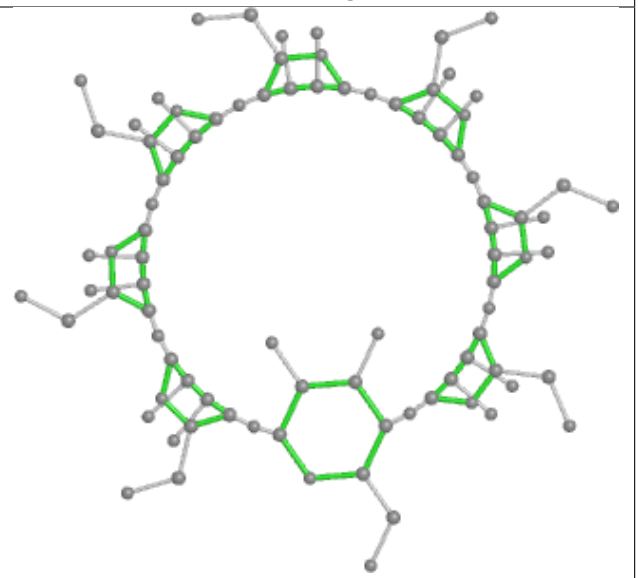
Bond lengths



Bond angles

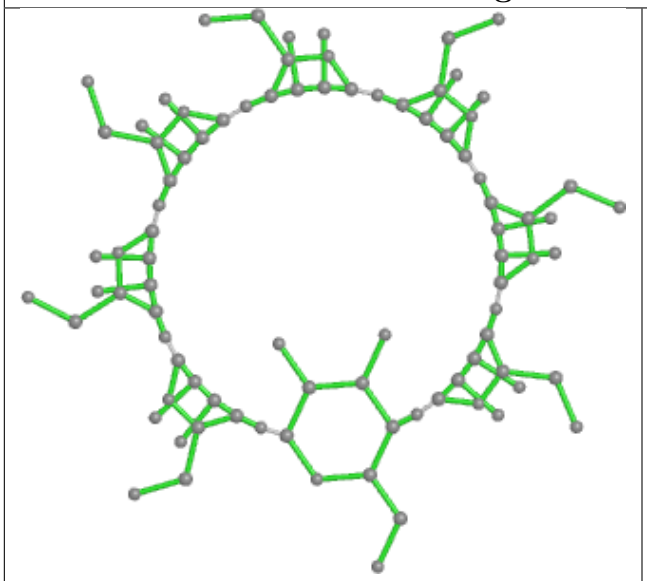


Torsions

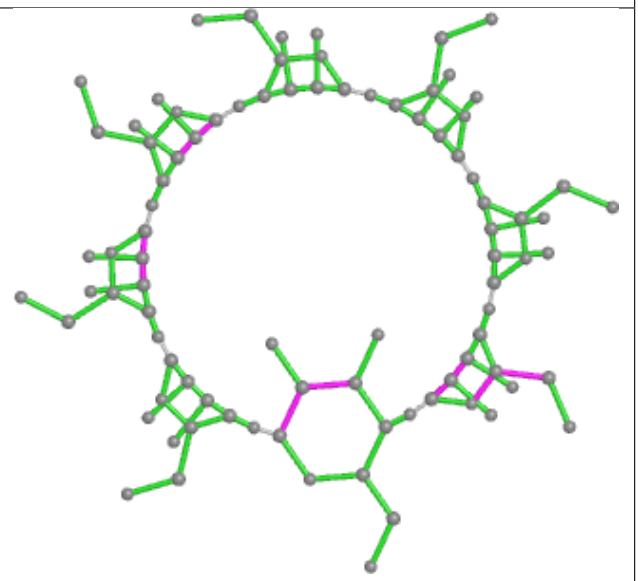


Rings

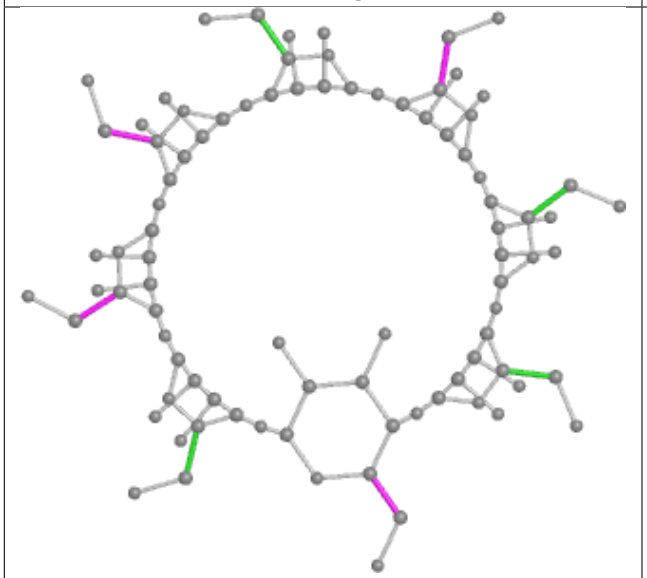
Oligosaccharide Chain G



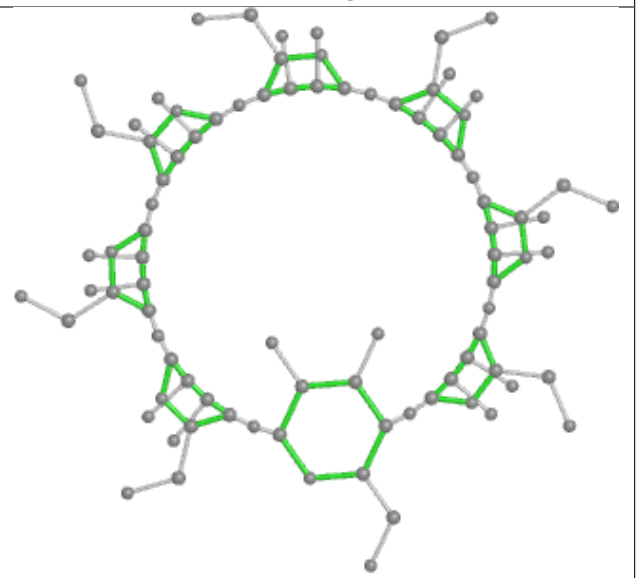
Bond lengths



Bond angles

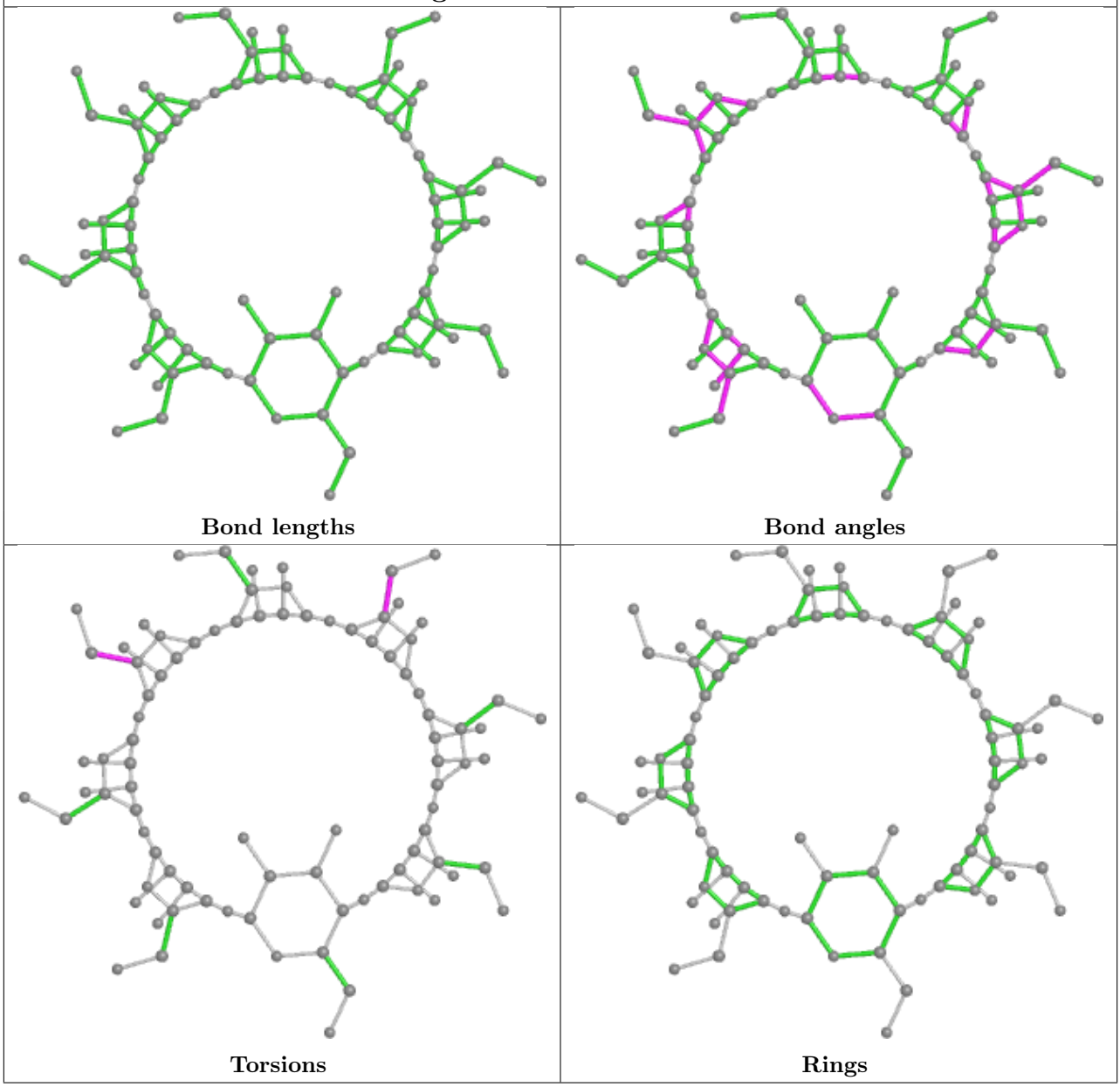


Torsions

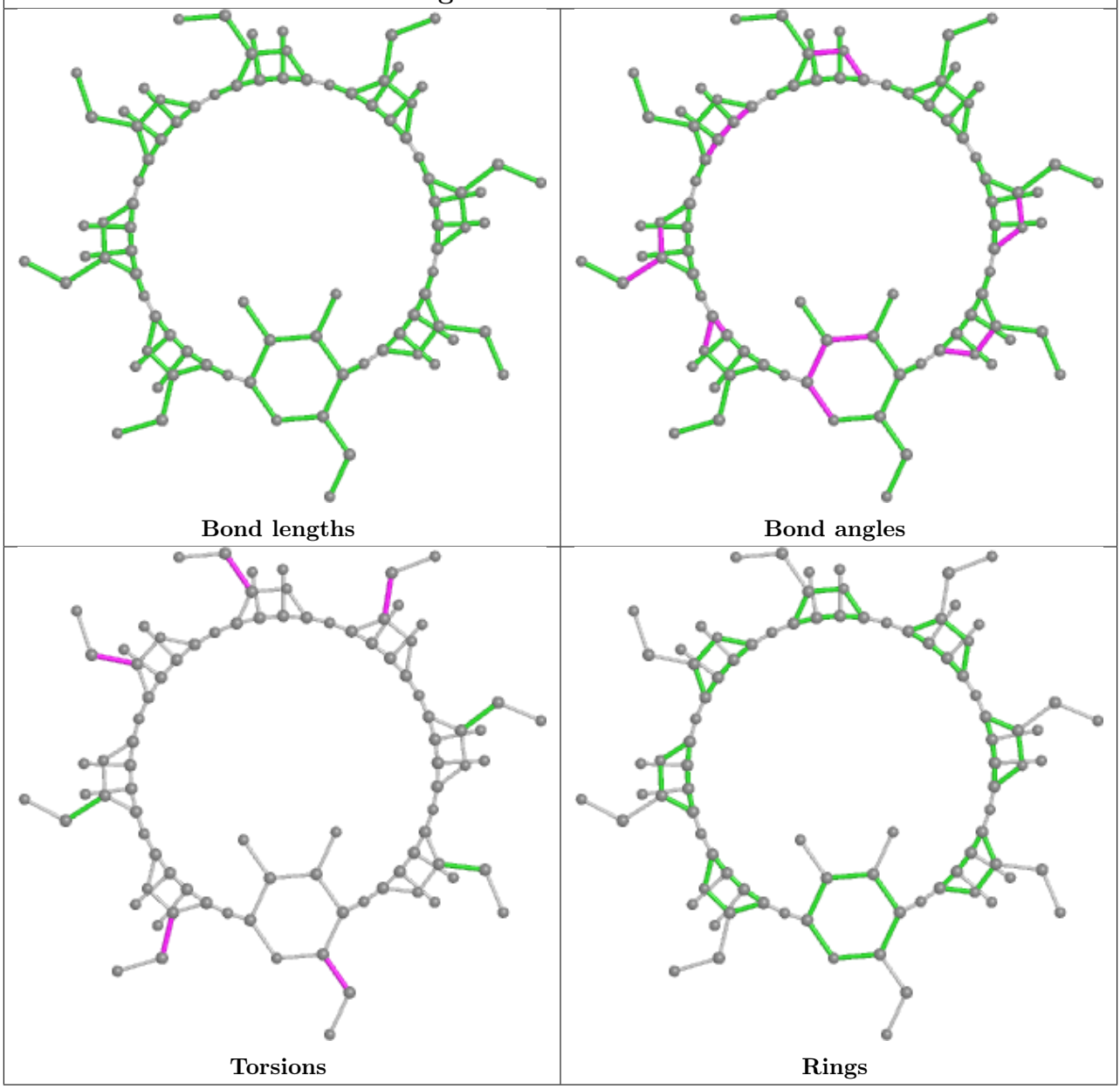


Rings

Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
3	GOL	B	803	-	5,5,5	0.49	0	5,5,5	0.50	0
3	GOL	A	803	-	5,5,5	0.44	0	5,5,5	0.66	0
3	GOL	B	802	-	5,5,5	0.38	0	5,5,5	0.65	0
3	GOL	D	803	-	5,5,5	0.37	0	5,5,5	0.57	0
3	GOL	D	804	-	5,5,5	0.44	0	5,5,5	0.35	0
3	GOL	A	802	-	5,5,5	0.30	0	5,5,5	1.28	1 (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
3	GOL	B	803	-	-	4/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	B	802	-	-	2/4/4/4	-
3	GOL	D	803	-	-	0/4/4/4	-
3	GOL	D	804	-	-	2/4/4/4	-
3	GOL	A	802	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	GOL	C3-C2-C1	-2.35	102.57	111.70

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	O1-C1-C2-C3
3	B	802	GOL	O1-C1-C2-C3
3	B	803	GOL	C1-C2-C3-O3
3	D	804	GOL	O1-C1-C2-C3
3	A	803	GOL	O1-C1-C2-O2
3	B	803	GOL	O2-C2-C3-O3
3	B	802	GOL	O1-C1-C2-O2
3	D	804	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	GOL	2	0
3	D	803	GOL	1	0
3	A	802	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	586/612 (95%)	0.38	66 (11%) 5 8	19, 38, 105, 134	7 (1%)
1	B	600/612 (98%)	-0.01	4 (0%) 87 92	16, 31, 56, 75	6 (1%)
1	C	578/612 (94%)	1.59	196 (33%) 0 0	49, 79, 117, 140	2 (0%)
1	D	588/612 (96%)	-0.07	12 (2%) 65 74	24, 38, 60, 84	4 (0%)
All	All	2352/2448 (96%)	0.46	278 (11%) 4 8	16, 41, 102, 140	19 (0%)

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	SER	9.3
1	C	133	ASP	9.0
1	C	132	MET	8.2
1	C	343	THR	7.9
1	C	499	TYR	7.4
1	C	200	ARG	6.8
1	A	429	GLY	6.6
1	C	150	VAL	6.6
1	C	159	TRP	6.5
1	C	199	LEU	6.4
1	C	258	ASP	6.2
1	C	190	TYR	6.1
1	C	257	THR	6.1
1	C	261	PHE	6.1
1	C	216	THR	5.7
1	C	502	TYR	5.6
1	C	660	VAL	5.6
1	A	149	ARG	5.6
1	C	201	LEU	5.5
1	C	464	PRO	5.4
1	A	195	ALA	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	131	THR	5.3
1	C	294	PHE	5.2
1	A	380	ARG	5.1
1	A	158	TYR	5.0
1	C	341	PHE	5.0
1	B	415	TYR	5.0
1	C	350	GLU	5.0
1	C	196	ASN	4.9
1	C	134	GLY	4.9
1	C	357	TYR	4.9
1	C	210	ALA	4.9
1	C	355	ASN	4.8
1	C	543	ALA	4.8
1	C	509	PHE	4.7
1	C	512	LEU	4.7
1	C	170	LYS	4.7
1	A	131	THR	4.7
1	C	127	ALA	4.7
1	C	708	GLN	4.7
1	C	155	GLN	4.6
1	C	595	TRP	4.6
1	C	144	ALA	4.5
1	C	702	ILE	4.5
1	C	168	LEU	4.5
1	A	162	ARG	4.5
1	A	144	ALA	4.5
1	C	222	GLY	4.4
1	B	133	ASP	4.3
1	C	511	ILE	4.3
1	A	147	ALA	4.3
1	C	587	HIS	4.3
1	C	207	ALA	4.3
1	C	211	GLN	4.3
1	A	199	LEU	4.3
1	C	189	LYS	4.2
1	C	496	ASP	4.2
1	A	168	LEU	4.2
1	C	124	THR	4.2
1	C	259	ASN	4.2
1	C	208	PHE	4.2
1	C	263	LEU	4.2
1	C	194	ASP	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	4.2
1	A	175	TRP	4.2
1	C	433	LEU	4.2
1	C	148	ARG	4.1
1	C	631	VAL	4.1
1	C	709	HIS	4.1
1	A	472	MET	4.1
1	C	260	ASN	4.1
1	C	187	LEU	4.1
1	C	156	PHE	4.1
1	C	147	ALA	4.1
1	C	175	TRP	4.1
1	C	203	SER	4.1
1	C	498	VAL	4.0
1	A	201	LEU	4.0
1	A	196	ASN	4.0
1	C	378	GLY	3.9
1	C	379	ARG	3.9
1	C	145	PRO	3.9
1	C	188	TYR	3.9
1	A	354	THR	3.9
1	C	154	GLY	3.9
1	C	172	SER	3.9
1	C	698	HIS	3.9
1	C	346	PHE	3.9
1	C	463	PHE	3.8
1	C	121	PRO	3.8
1	A	145	PRO	3.8
1	A	166	MET	3.8
1	C	344	ASP	3.8
1	C	217	ALA	3.8
1	C	375	TYR	3.8
1	C	192	MET	3.7
1	C	223	LEU	3.7
1	C	592	GLY	3.7
1	C	347	ALA	3.7
1	C	374	ILE	3.7
1	C	484	GLY	3.7
1	C	262	TRP	3.7
1	A	146	ASN	3.7
1	C	373	LEU	3.6
1	A	150	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	584	LEU	3.6
1	C	544	TRP	3.6
1	C	495	LEU	3.6
1	C	356	LEU	3.6
1	C	345	ASP	3.6
1	C	181	GLY	3.6
1	A	159	TRP	3.5
1	C	202	LYS	3.5
1	C	503	HIS	3.5
1	C	126	GLY	3.5
1	C	408	ALA	3.5
1	D	413	ARG	3.5
1	C	348	LEU	3.5
1	C	380	ARG	3.5
1	C	118	HIS	3.5
1	C	601[A]	ARG	3.5
1	C	497	PRO	3.5
1	A	193	ILE	3.4
1	C	171	GLU	3.4
1	D	728	GLU	3.4
1	A	212	MET	3.4
1	A	148	ARG	3.4
1	C	149	ARG	3.4
1	C	536	LEU	3.4
1	A	152	VAL	3.3
1	C	353	GLY	3.3
1	C	658	THR	3.3
1	C	540	PRO	3.3
1	C	206	TYR	3.3
1	C	256	HIS	3.3
1	D	371	ASN	3.3
1	A	167	ARG	3.3
1	C	635	GLU	3.3
1	C	359	HIS	3.2
1	C	505	ASP	3.2
1	C	122	TYR	3.2
1	A	192	MET	3.2
1	C	412	TYR	3.2
1	C	542	ASP	3.2
1	C	541	GLY	3.1
1	A	165	PRO	3.1
1	C	710	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	ASP	3.1
1	C	352	ASP	3.1
1	C	672	PRO	3.1
1	C	228	VAL	3.1
1	C	590	GLU	3.1
1	C	582	ALA	3.1
1	C	135	VAL	3.0
1	C	354	THR	3.0
1	C	193	ILE	3.0
1	C	487	HIS	3.0
1	C	158	TYR	3.0
1	A	160	ASP	3.0
1	A	471	ASP	3.0
1	A	374	ILE	3.0
1	C	445	ILE	3.0
1	A	200	ARG	3.0
1	C	169	ARG	3.0
1	C	703	ALA	3.0
1	A	194	ASP	3.0
1	C	581	ASP	3.0
1	C	300	TYR	2.9
1	C	157	ASN	2.9
1	C	278	TRP	2.9
1	C	387	VAL	2.9
1	C	140	PHE	2.9
1	D	372	THR	2.9
1	C	143	TRP	2.9
1	A	171	GLU	2.9
1	C	221	CYS	2.9
1	A	190	TYR	2.9
1	A	161	GLY	2.8
1	C	142	VAL	2.8
1	C	342	PRO	2.8
1	C	198	ASN	2.8
1	C	141	SER	2.8
1	C	529	VAL	2.8
1	C	636	ARG	2.8
1	D	414	ASP	2.8
1	D	257	THR	2.7
1	A	170	LYS	2.7
1	C	545	GLN	2.7
1	C	139	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	2.7
1	D	346	PHE	2.7
1	C	119	LEU	2.7
1	A	169	ARG	2.7
1	C	338	PRO	2.7
1	A	164	HIS	2.7
1	B	132	MET	2.7
1	A	133	ASP	2.6
1	A	117	THR	2.6
1	C	632	ASP	2.6
1	A	129	ALA	2.6
1	A	360	SER	2.6
1	C	339	GLY	2.6
1	C	120	ARG	2.6
1	C	255	ARG	2.6
1	A	163	ARG	2.5
1	C	205	PRO	2.5
1	C	586	TRP	2.5
1	C	183	HIS	2.5
1	C	176	GLU	2.5
1	C	351	PHE	2.5
1	C	130	ASP	2.5
1	C	472	MET	2.5
1	C	267	GLU	2.5
1	C	637	SER	2.4
1	C	195	ALA	2.4
1	A	346	PHE	2.4
1	C	659	PRO	2.4
1	C	713	LEU	2.4
1	C	197	GLY	2.4
1	C	634	LYS	2.4
1	C	128	HIS	2.4
1	C	471	ASP	2.4
1	A	177	LEU	2.4
1	C	530	HIS	2.4
1	A	352	ASP	2.3
1	A	142	VAL	2.3
1	A	156	PHE	2.3
1	C	589	LEU	2.3
1	D	212	MET	2.3
1	C	220	ILE	2.3
1	C	474	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	172	SER	2.3
1	A	176	GLU	2.3
1	C	700	ASP	2.3
1	A	151	SER	2.3
1	C	151	SER	2.2
1	C	583	SER	2.2
1	B	276	ALA	2.2
1	C	488	ASP	2.2
1	D	279	MET	2.2
1	C	707	ARG	2.2
1	C	591	GLY	2.2
1	C	301	GLN	2.2
1	A	197	GLY	2.2
1	C	531	GLY	2.2
1	C	358	GLU	2.2
1	A	174	ILE	2.1
1	D	360	SER	2.1
1	A	355	ASN	2.1
1	C	633	ASP	2.1
1	C	146	ASN	2.1
1	C	180	PRO	2.1
1	C	182	ALA	2.1
1	A	475	LEU	2.1
1	C	125	LEU	2.1
1	C	160	ASP	2.1
1	A	372	THR	2.1
1	C	701	GLU	2.1
1	A	373	LEU	2.1
1	A	359	HIS	2.1
1	C	594	ASN	2.1
1	C	293	PRO	2.1
1	C	508	THR	2.1
1	A	135	VAL	2.1
1	A	353	GLY	2.1
1	C	434	GLU	2.0
1	C	608	LEU	2.0
1	C	383	SER	2.0
1	C	409	SER	2.0
1	C	539	MET	2.0
1	D	727	ALA	2.0
1	D	603	VAL	2.0
1	A	143	TRP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	209	GLU	2.0
1	C	711	LEU	2.0
1	A	134	GLY	2.0
1	C	465	GLY	2.0
1	C	712	SER	2.0

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

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

6.3 Carbohydrates (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(Å^2)	Q<0.9
2	GLC	G	1	11/12	0.42	0.82	102,103,103,103	11
2	GLC	G	2	11/12	0.43	0.56	102,104,104,104	0
2	GLC	G	7	11/12	0.45	0.53	100,101,101,101	11
2	GLC	G	6	11/12	0.55	0.55	100,100,100,100	11
2	GLC	E	7	11/12	0.56	0.32	73,74,75,77	11
2	GLC	I	5	11/12	0.60	0.30	90,90,91,91	11
2	GLC	G	5	11/12	0.62	0.69	99,99,99,100	11
2	GLC	E	2	11/12	0.66	0.36	74,78,79,79	0
2	GLC	E	1	11/12	0.66	0.35	78,79,79,79	11
2	GLC	G	8	11/12	0.71	0.76	101,102,102,102	11
2	GLC	I	6	11/12	0.71	0.47	91,92,92,92	11
2	GLC	I	7	11/12	0.72	0.45	89,91,92,92	0
2	GLC	G	4	11/12	0.78	0.26	96,98,98,98	11
2	GLC	E	8	11/12	0.78	0.48	78,78,79,79	11
2	GLC	I	3	11/12	0.80	0.22	83,84,85,86	1
2	GLC	F	5	11/12	0.80	0.27	69,71,72,72	10
2	GLC	E	6	11/12	0.81	0.17	62,65,67,70	1
2	GLC	F	3	11/12	0.81	0.29	67,70,71,71	0
2	GLC	I	8	11/12	0.81	0.36	80,84,86,87	1
2	GLC	I	2	11/12	0.82	0.27	77,78,79,81	0
2	GLC	I	4	11/12	0.83	0.29	87,88,88,89	11
2	GLC	G	3	11/12	0.84	0.21	98,99,100,100	11
2	GLC	F	4	11/12	0.87	0.32	72,72,73,73	10

Continued on next page...

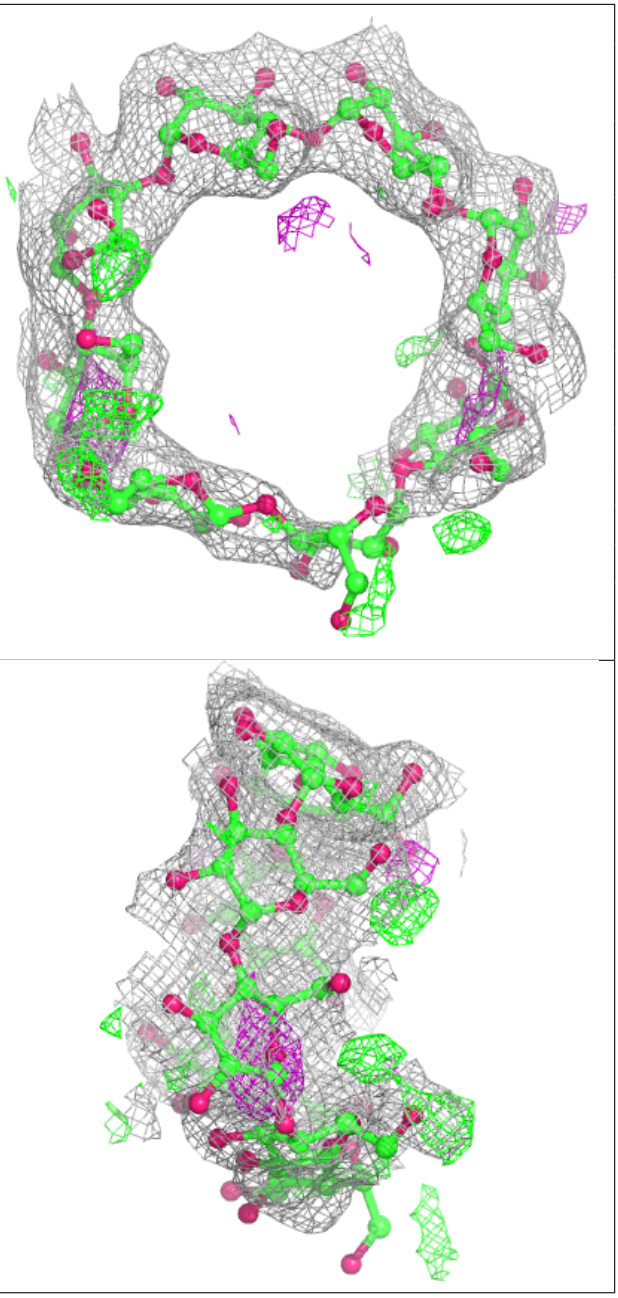
Continued from previous page...

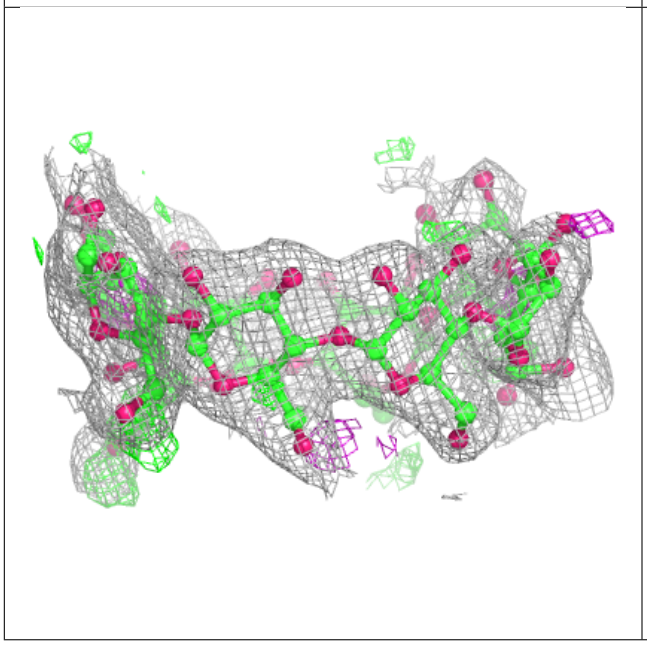
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	H	2	11/12	0.88	0.30	67,68,68,69	0
2	GLC	H	6	11/12	0.88	0.20	54,59,61,61	0
2	GLC	F	6	11/12	0.88	0.22	57,64,66,67	0
2	GLC	E	3	11/12	0.89	0.15	60,66,71,71	0
2	GLC	H	5	11/12	0.89	0.22	61,63,65,66	0
2	GLC	H	1	11/12	0.90	0.22	59,62,63,65	0
2	GLC	F	2	11/12	0.91	0.23	53,58,60,64	0
2	GLC	F	7	11/12	0.91	0.15	43,48,52,53	0
2	GLC	H	3	11/12	0.91	0.26	68,69,70,70	0
2	GLC	H	4	11/12	0.93	0.16	66,67,68,68	0
2	GLC	H	7	11/12	0.95	0.11	42,47,50,50	0
2	GLC	I	1	11/12	0.95	0.15	75,76,76,78	0
2	GLC	E	5	11/12	0.95	0.13	49,52,55,58	0
2	GLC	H	8	11/12	0.96	0.12	46,48,50,55	0
2	GLC	E	4	11/12	0.97	0.13	45,50,53,54	0
2	GLC	F	1	11/12	0.97	0.12	34,39,42,47	0
2	GLC	F	8	11/12	0.98	0.09	32,37,39,39	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 E:

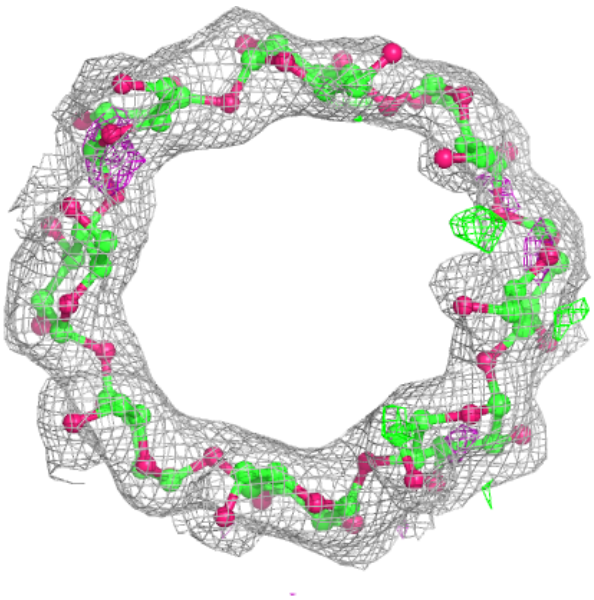
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

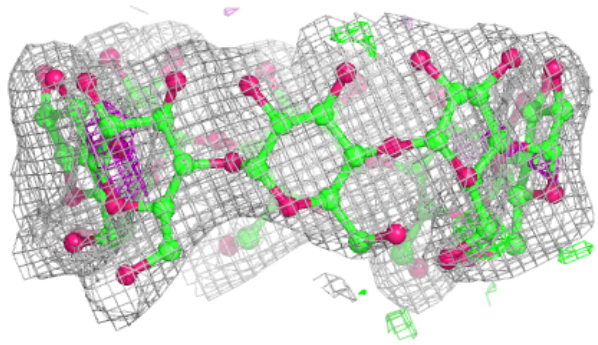


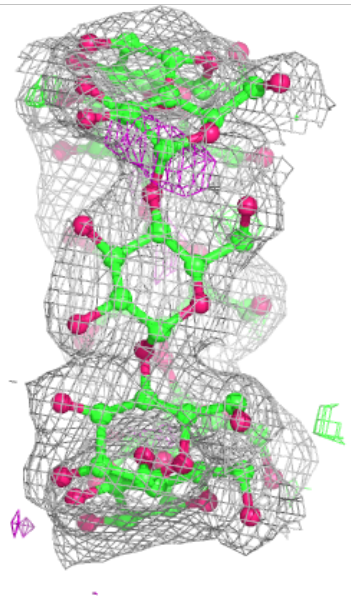


Electron density around Chain F:

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

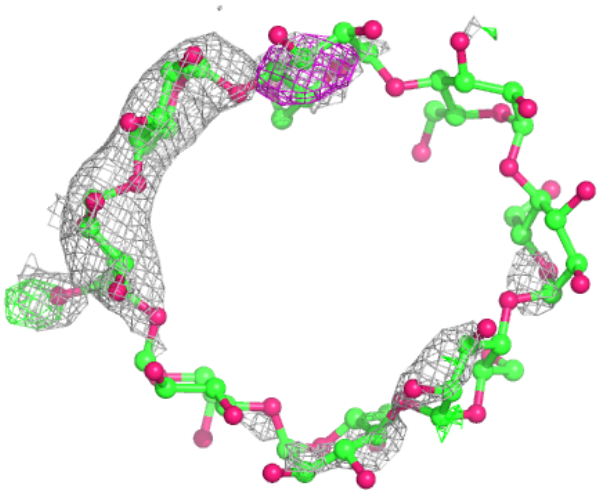


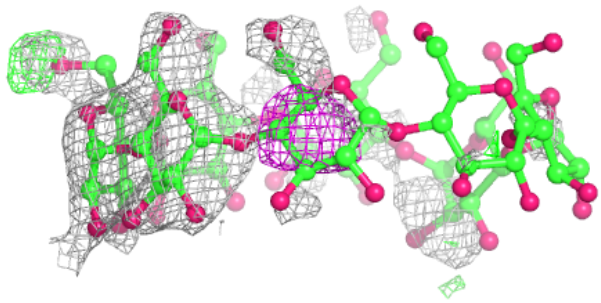


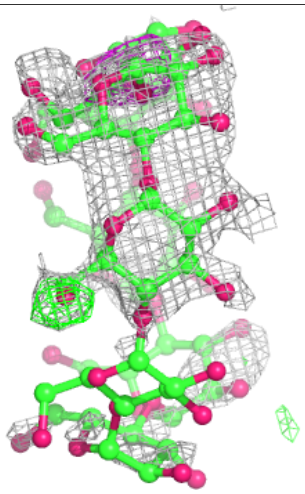


Electron density around Chain G:

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

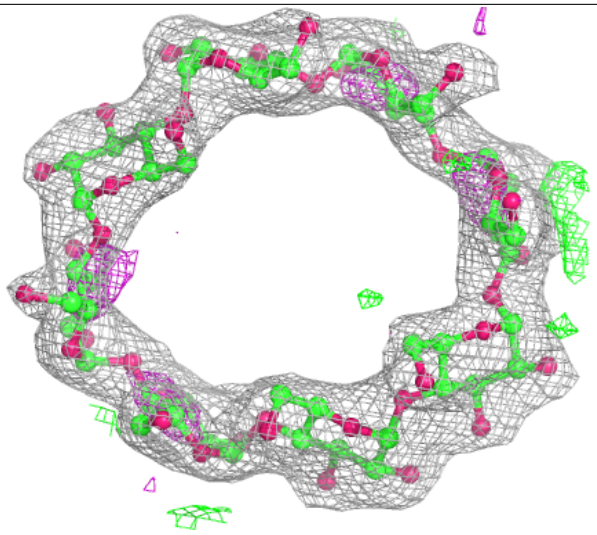


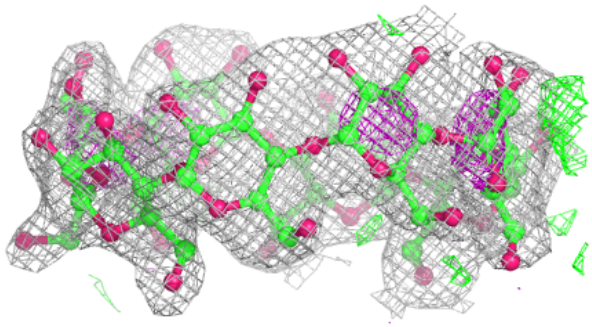


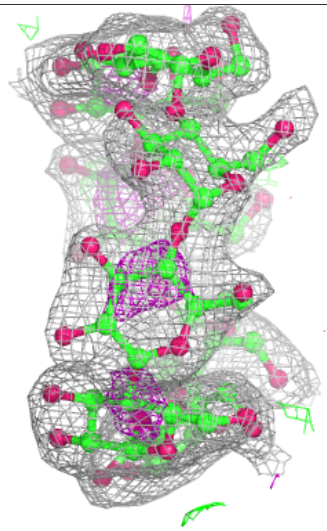


Electron density around Chain H:

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

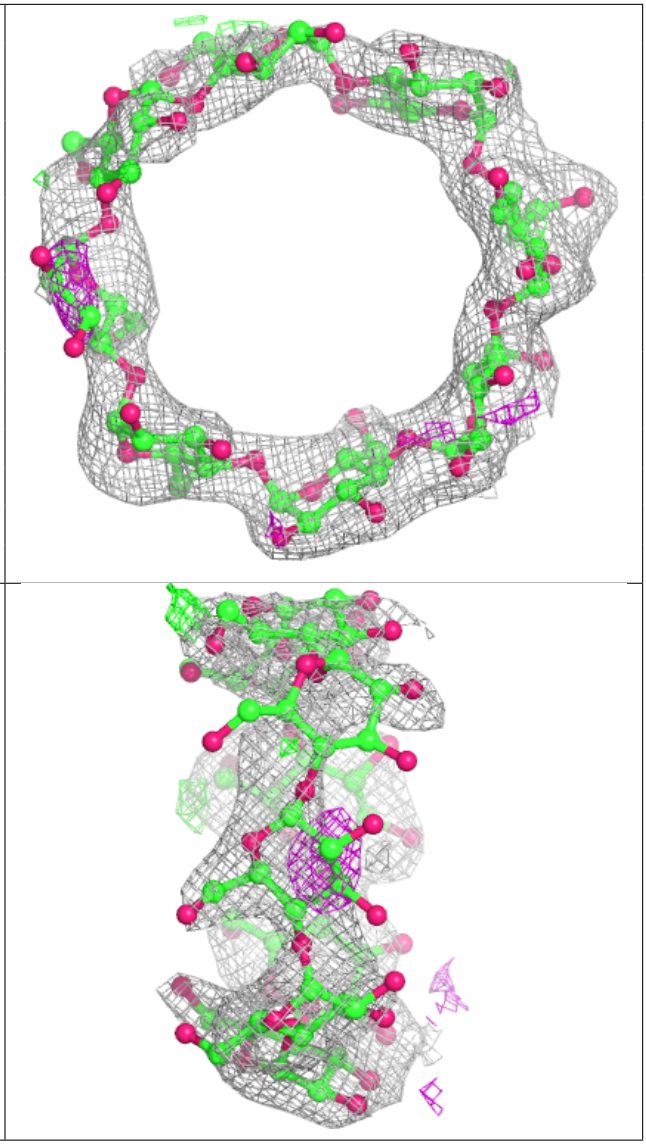






Electron density around Chain I:

$2mF_o$-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(Å^2)	Q<0.9
3	GOL	A	802	6/6	0.92	0.20	42,44,44,46	0
3	GOL	B	803	6/6	0.94	0.14	45,45,45,46	0
3	GOL	D	803	6/6	0.94	0.16	50,53,53,53	0
3	GOL	B	802	6/6	0.95	0.17	30,34,35,36	0
3	GOL	A	803	6/6	0.96	0.19	27,31,32,34	0
3	GOL	D	804	6/6	0.96	0.13	45,45,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.