



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:58 PM UTC

PDB ID : 5E70 / pdb_00005e70
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 ⓘ 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:

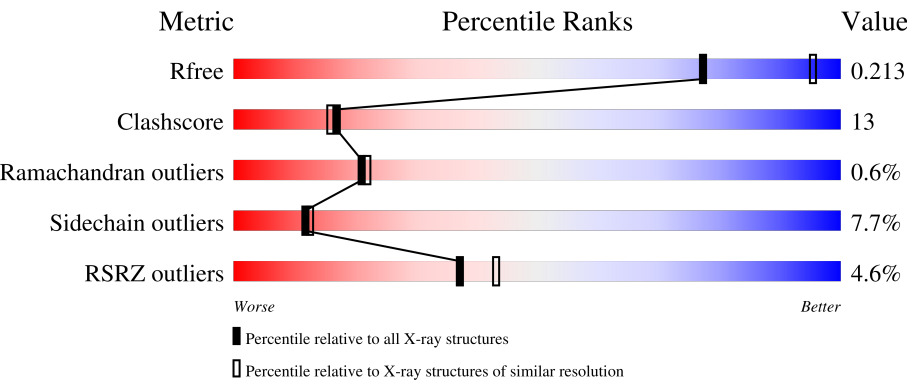
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 $\leq 5\%$. 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	612	4% 71% 21% . .
1	B	612	% 77% 17% . .
1	C	612	12% 70% 20% . 6%
1	D	612	% 73% 18% 5% .
2	E	8	100%

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Mol	Chain	Length	Quality of chain
2	F	8	 88% 12%
2	G	8	 50% 38% 12%
2	H	8	 12% 62% 25%
2	I	8	 50% 38% 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 Entry composition [i](#)

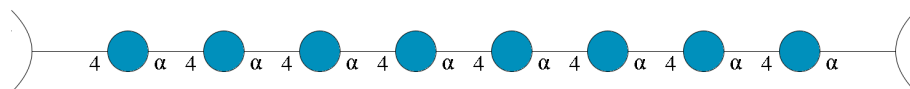
There are 4 unique types of molecules in this entry. The entry contains 21132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

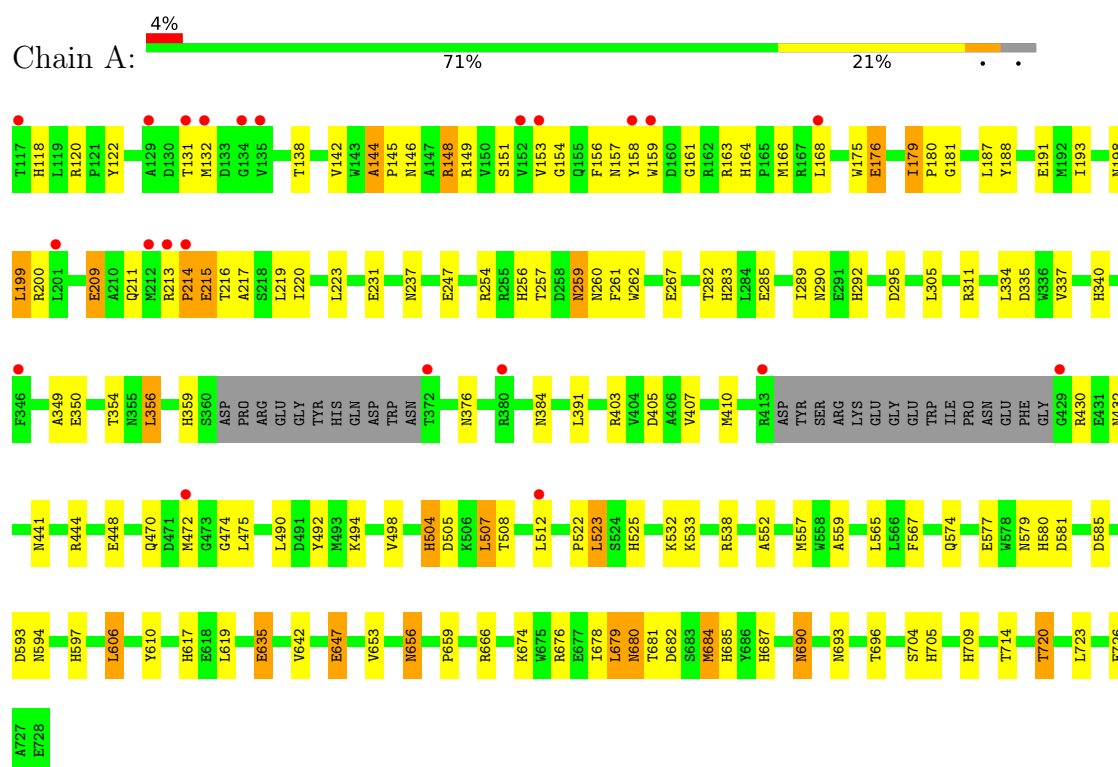
- Molecule 4 is water.

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

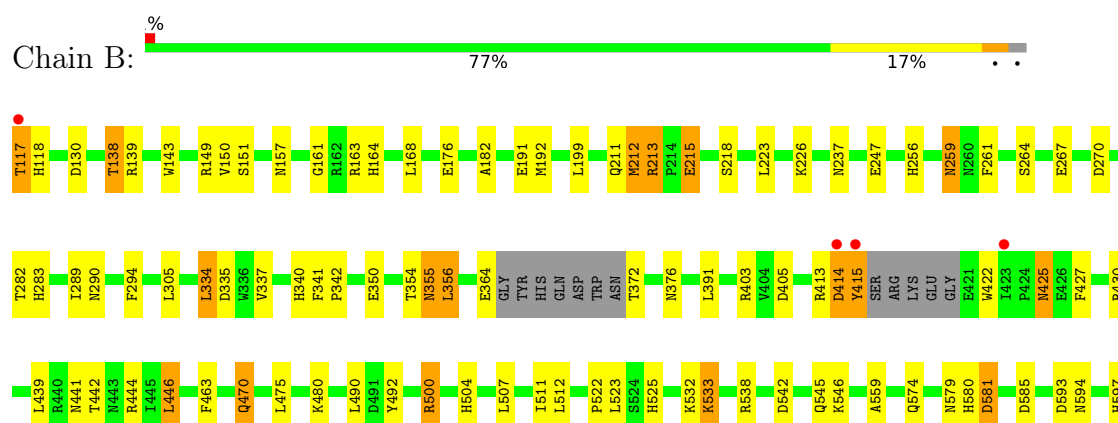
3 Residue-property plots

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: 1,4-alpha-glucan branching enzyme GlgB

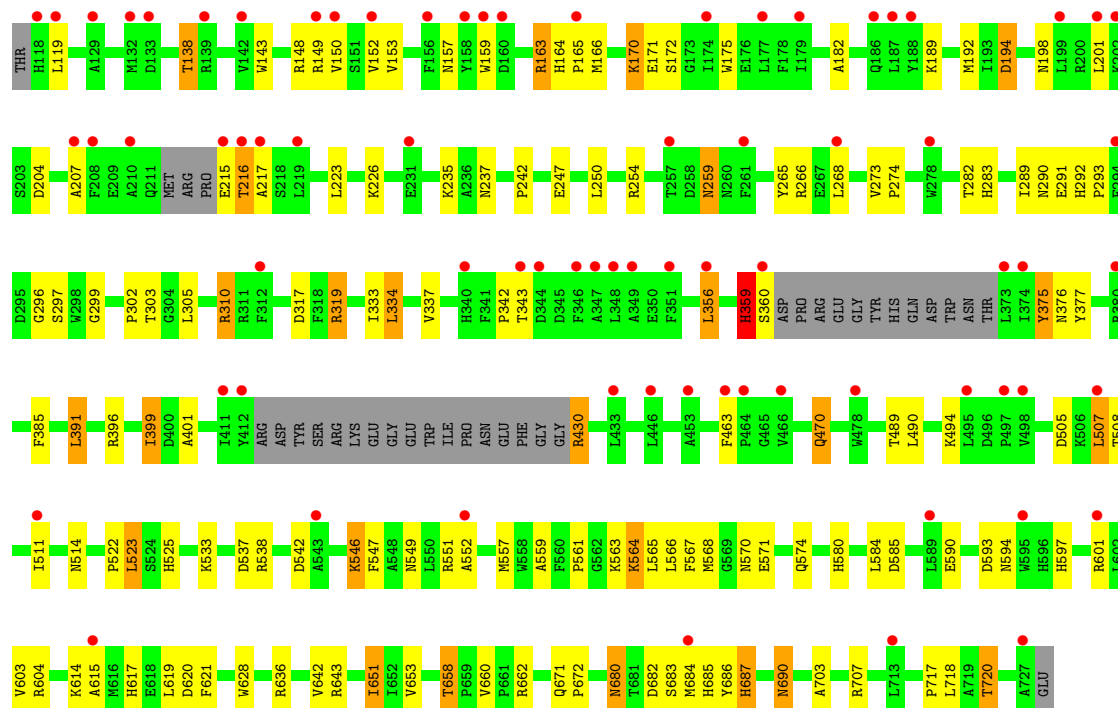


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

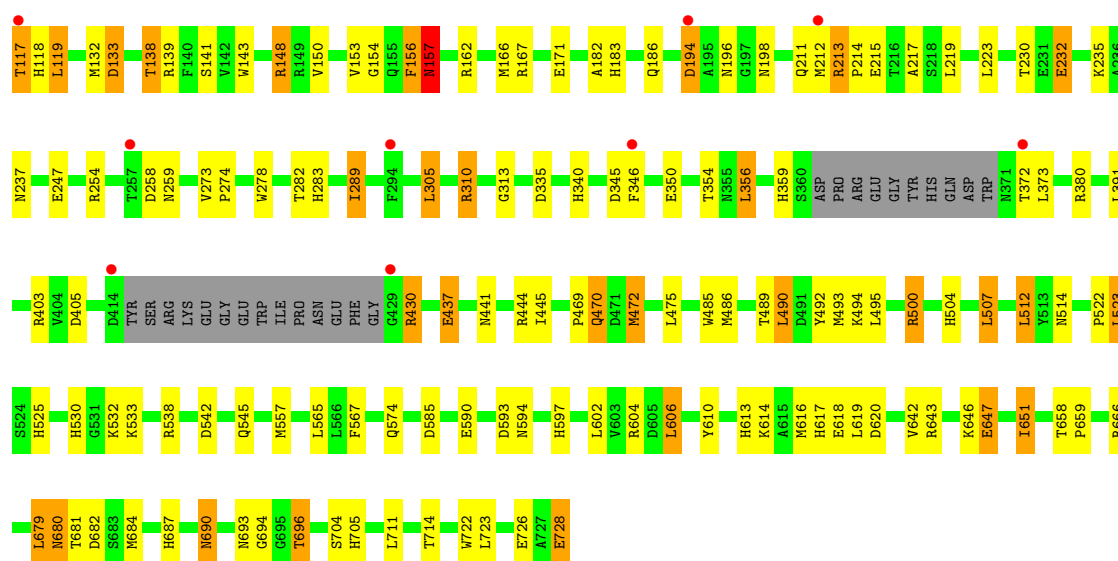
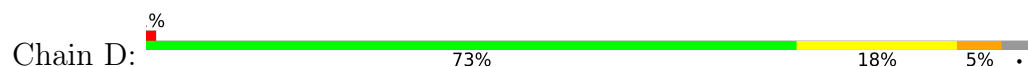




- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



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



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

Chain E:  100%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

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

Chain F:  88% 12%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

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

Chain G:  50% 38% 12%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

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

Chain H:  12% 62% 25%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

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

Chain I:  50% 38% 12%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

4 Data and refinement statistics

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 50.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.33) 94.6 (50.00-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (9.46%)	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 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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: 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	0.77	0/5028	0.90	9/6827 (0.1%)
1	B	0.91	1/5120 (0.0%)	0.95	3/6953 (0.0%)
1	C	0.51	0/4918	0.82	6/6677 (0.1%)
1	D	0.76	0/5006	0.92	1/6796 (0.0%)
All	All	0.75	1/20072 (0.0%)	0.90	19/27253 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	716	PRO	CA-C	5.51	1.54	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	HIS	N-CA-C	7.74	115.12	108.78
1	A	474	GLY	N-CA-C	6.77	121.21	112.54
1	A	144	ALA	CA-C-N	6.24	125.73	119.24
1	A	144	ALA	C-N-CA	6.24	125.73	119.24
1	B	463	PHE	CA-C-N	-6.15	113.61	119.76
1	B	463	PHE	C-N-CA	-6.15	113.61	119.76
1	B	355	ASN	CB-CA-C	-6.00	98.48	110.42
1	C	217	ALA	N-CA-C	5.91	117.95	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ASN	N-CA-CB	-5.68	100.89	110.49
1	A	659	PRO	CA-C-N	-5.60	118.56	122.59
1	A	659	PRO	C-N-CA	-5.60	118.56	122.59
1	A	257	THR	N-CA-C	5.57	117.43	111.36
1	C	463	PHE	CA-C-N	5.55	125.72	119.90
1	C	463	PHE	C-N-CA	5.55	125.72	119.90
1	C	359	HIS	CB-CA-C	-5.45	109.22	117.07
1	C	359	HIS	CA-C-O	5.37	121.05	117.94
1	A	678	ILE	N-CA-C	-5.34	107.92	113.10
1	A	179	ILE	N-CA-C	5.33	113.31	107.60
1	A	176	GLU	N-CA-C	5.18	116.40	108.42

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 ⓘ

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	135	0
1	B	4960	0	4666	113	0
1	C	4768	0	4505	115	0
1	D	4852	0	4584	123	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	18	0
4	C	75	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	340	0	0	19	0
All	All	21132	0	18759	493	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 13.

All (493) 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:D:132:MET:HE3	1:D:139:ARG:NH1	1.78	0.98
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:430:ARG:HE	1:C:430:ARG:HA	1.46	0.79
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:B:415:TYR:CD1	1:B:415:TYR:C	2.64	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:B:415:TYR:C	1:B:415:TYR:HD1	1.95	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:166:MET:HE2	1:A:176:GLU:HA	1.69	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:C:684[A]:MET:HE1	1:D:684:MET:HG3	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ASN:HD21	1:A:714:THR:H	1.39	0.71
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
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.27	0.70
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:D:469:PRO:HG2	1:D:472:MET:HE2	1.74	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:C	1:A:159:TRP:N	2.54	0.65
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:132:MET:HE3	1:D:139:ARG:HH12	1.62	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:A:157:ASN:C	1:A:159:TRP:H	2.04	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:680:ASN:C	1:B:680:ASN:HD22	2.05	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
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:226:LYS:NZ	4:B:905:HOH:O	2.33	0.61
1:C:680:ASN:C	1:C:680:ASN:HD22	2.09	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:D:680:ASN:HD22	1:D:680:ASN:C	2.07	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:D:237:ASN:ND2	1:D:283:HIS:HE1	1.98	0.61
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:C:684[A]:MET:HE1	1:D:684:MET:CG	2.32	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:199:LEU:HD13	1:B:199:LEU:C	2.29	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:A:635:GLU:H	1:A:635:GLU:CD	2.10	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
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: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:A:680:ASN:HD22	1:A:680:ASN:C	2.14	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:D:258:ASP:O	1:D:259:ASN:CG	2.50	0.55
1:A:213:ARG:HA	1:A:214:PRO:C	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:563:LYS:C	1:C:564:LYS:HD3	2.33	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
1:A:337:VAL:HG23	1:A:337:VAL:O	2.07	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:407:VAL:HA	1:A:410:MET:HE2	1.90	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:B:425:ASN:HD22	1:B:425:ASN:C	2.17	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:148:ARG:O	1:A:148:ARG:HG2	2.08	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:415:TYR:C	1:B:430:ARG:HB3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:166:MET:HE3	1:C:175:TRP:HB3	1.90	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:ALA:O	1:A:350:GLU:C	2.56	0.49
1:A:685[A]:HIS:CE1	1:B:685[A]:HIS:CE1	3.00	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
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:647:GLU:CD	4:D:947:HOH:O	2.56	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:C:636:ARG:HG2	1:C:662:ARG:CZ	2.44	0.48
1:D:728:GLU:OXT	1:D:728:GLU:HG2	2.13	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:D:211:GLN:NE2	1:D:217:ALA:H	2.12	0.47
1:A:656:ASN:C	1:A:656:ASN:HD22	2.22	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:A:376:ASN:C	1:A:376:ASN:HD22	2.21	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:B:532:LYS:NZ	4:B:923:HOH:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:656:ASN:C	1:B:656:ASN:HD22	2.24	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:D:469:PRO:CG	1:D:472:MET:HE2	2.42	0.46
1:B:635:GLU:HA	1:B:635:GLU:OE2	2.15	0.46
1:D:132:MET:HE3	1:D:139:ARG:HH11	1.73	0.46
1:D:345:ASP:O	1:D:346:PHE:C	2.58	0.46
1:C:684[A]:MET:H	1:C:690:ASN:HD22	1.64	0.46
1:D:138:THR:CG2	1:D:182:ALA:C	2.89	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:B:211:GLN:CD	1:B:215:GLU:HB2	2.42	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
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: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:C:171:GLU:CG	1:C:172:SER:N	2.80	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:289:ILE:C	1:B:289:ILE:HD12	2.42	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:B:579:ASN:HD22	1:B:579:ASN:C	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:579:ASN:C	1:A:579:ASN:HD22	2.25	0.43
1:C:297:SER:C	1:C:299:GLY:H	2.26	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: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:565:LEU:HD23	1:D:565:LEU:C	2.43	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:D:289:ILE:C	1:D:289:ILE:HD12	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:THR:HB	1:B:118:HIS:H	1.25	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:259:ASN:HD22	1:A:259:ASN:C	2.27	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:565:LEU:C	1:A:565:LEU:HD23	2.43	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
1:C:289:ILE:HD12	1:C:289:ILE:C	2.45	0.42
1:C:671:GLN:HA	1:C:672:PRO:HD2	1.87	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: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:C:565:LEU:C	1:C:565:LEU:HD23	2.45	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:399:ILE:C	1:C:399:ILE:HD12	2.45	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:A:432:ASN:OD1	1:A:432:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:376:ASN:C	1:B:376:ASN:HD22	2.29	0.41
1:C:150:VAL:HG12	1:C:166:MET:HE2	2.03	0.41
1:C:549:ASN:OD1	1:C:718:LEU:HD22	2.21	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
1:A:574:GLN:HE21	1:A:585:ASP:H	1.60	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
1:D:680:ASN:C	1:D:680:ASN:ND2	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:717:PRO:O	1:C:718:LEU:C	2.65	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%)	18	18
1	B	596/612 (97%)	580 (97%)	13 (2%)	3 (0%)	24	26
1	C	572/612 (94%)	538 (94%)	30 (5%)	4 (1%)	18	18
1	D	584/612 (95%)	558 (96%)	22 (4%)	4 (1%)	18	18
All	All	2338/2448 (96%)	2233 (96%)	90 (4%)	15 (1%)	21	22

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%)	468 (93%)	36 (7%)	13	14
1	B	512/521 (98%)	472 (92%)	40 (8%)	11	12
1	C	492/521 (94%)	455 (92%)	37 (8%)	12	13
1	D	501/521 (96%)	460 (92%)	41 (8%)	10	11
All	All	2009/2084 (96%)	1855 (92%)	154 (8%)	12	12

All (154) 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	209	GLU

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Mol	Chain	Res	Type
1	A	216	THR
1	A	223	LEU
1	A	231	GLU
1	A	259	ASN
1	A	305	LEU
1	A	356	LEU
1	A	359	HIS
1	A	391	LEU
1	A	441	ASN
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	606	LEU
1	A	619	LEU
1	A	635	GLU
1	A	642	VAL
1	A	647	GLU
1	A	656	ASN
1	A	679	LEU
1	A	680	ASN
1	A	684	MET
1	A	690	ASN
1	A	720	THR
1	A	723	LEU
1	B	117	THR
1	B	138	THR
1	B	151	SER
1	B	163	ARG
1	B	168	LEU
1	B	176	GLU
1	B	192	MET
1	B	212	MET
1	B	213	ARG
1	B	215	GLU
1	B	218	SER
1	B	223	LEU
1	B	259	ASN

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Mol	Chain	Res	Type
1	B	290	ASN
1	B	305	LEU
1	B	334	LEU
1	B	356	LEU
1	B	364	GLU
1	B	372	THR
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	500	ARG
1	B	507	LEU
1	B	512	LEU
1	B	523	LEU
1	B	533	LYS
1	B	546	LYS
1	B	581	ASP
1	B	606	LEU
1	B	619	LEU
1	B	642	VAL
1	B	658	THR
1	B	679	LEU
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	170	LYS
1	C	223	LEU
1	C	226	LYS
1	C	235	LYS
1	C	259	ASN
1	C	266	ARG
1	C	290	ASN
1	C	310	ARG
1	C	319	ARG
1	C	334	LEU
1	C	343	THR

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Mol	Chain	Res	Type
1	C	356	LEU
1	C	359	HIS
1	C	375	TYR
1	C	391	LEU
1	C	399	ILE
1	C	430	ARG
1	C	470	GLN
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	614	LYS
1	C	619	LEU
1	C	642	VAL
1	C	651	ILE
1	C	658	THR
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	289	ILE
1	D	305	LEU
1	D	310	ARG
1	D	356	LEU
1	D	359	HIS
1	D	373	LEU
1	D	391	LEU
1	D	430	ARG

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Mol	Chain	Res	Type
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	500	ARG
1	D	507	LEU
1	D	512	LEU
1	D	523	LEU
1	D	606	LEU
1	D	619	LEU
1	D	642	VAL
1	D	647	GLU
1	D	651	ILE
1	D	679	LEU
1	D	680	ASN
1	D	690	ASN
1	D	696	THR
1	D	723	LEU
1	D	728	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	157	ASN
1	A	183	HIS
1	A	198	ASN
1	A	237	ASN
1	A	256	HIS
1	A	259	ASN
1	A	283	HIS
1	A	326	HIS
1	A	331	ASN
1	A	340	HIS
1	A	376	ASN
1	A	501	GLN
1	A	504	HIS
1	A	514	ASN
1	A	525	HIS
1	A	530	HIS

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Mol	Chain	Res	Type
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	663	HIS
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
1	B	259	ASN
1	B	271	GLN
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	501	GLN
1	B	504	HIS
1	B	514	ASN
1	B	525	HIS
1	B	545	GLN
1	B	570	ASN
1	B	579	ASN
1	B	580	HIS
1	B	597	HIS
1	B	617	HIS
1	B	656	ASN
1	B	680	ASN
1	B	687	HIS
1	B	690	ASN

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Mol	Chain	Res	Type
1	B	705	HIS
1	B	709	HIS
1	C	146	ASN
1	C	164	HIS
1	C	237	ASN
1	C	238	GLN
1	C	256	HIS
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	376	ASN
1	C	470	GLN
1	C	501	GLN
1	C	514	ASN
1	C	525	HIS
1	C	530	HIS
1	C	545	GLN
1	C	570	ASN
1	C	574	GLN
1	C	579	ASN
1	C	580	HIS
1	C	597	HIS
1	C	600	GLN
1	C	617	HIS
1	C	656	ASN
1	C	671	GLN
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	256	HIS
1	D	283	HIS
1	D	290	ASN

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Mol	Chain	Res	Type
1	D	331	ASN
1	D	340	HIS
1	D	441	ASN
1	D	443	ASN
1	D	470	GLN
1	D	487	HIS
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 ⓘ

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 ⓘ

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	2.17	3 (20%)
2	GLC	E	2	2	11,11,12	0.49	0	15,15,17	1.15	2 (13%)
2	GLC	E	3	2	11,11,12	0.58	0	15,15,17	1.58	2 (13%)
2	GLC	E	4	2	11,11,12	0.14	0	15,15,17	0.92	1 (6%)
2	GLC	E	5	2	11,11,12	0.54	0	15,15,17	2.00	3 (20%)
2	GLC	E	6	2	11,11,12	0.58	0	15,15,17	1.27	1 (6%)
2	GLC	E	7	2	11,11,12	0.55	0	15,15,17	0.92	1 (6%)
2	GLC	E	8	2	11,11,12	0.54	0	15,15,17	1.56	1 (6%)
2	GLC	F	1	2	11,11,12	0.65	0	15,15,17	1.10	1 (6%)
2	GLC	F	2	2	11,11,12	0.42	0	15,15,17	0.97	1 (6%)
2	GLC	F	3	2	11,11,12	0.52	0	15,15,17	1.67	4 (26%)
2	GLC	F	4	2	11,11,12	0.38	0	15,15,17	0.75	1 (6%)
2	GLC	F	5	2	11,11,12	0.49	0	15,15,17	1.36	3 (20%)
2	GLC	F	6	2	11,11,12	0.64	0	15,15,17	1.11	1 (6%)
2	GLC	F	7	2	11,11,12	0.53	0	15,15,17	1.02	1 (6%)
2	GLC	F	8	2	11,11,12	0.32	0	15,15,17	1.40	2 (13%)
2	GLC	G	1	2	11,11,12	0.34	0	15,15,17	1.06	1 (6%)
2	GLC	G	2	2	11,11,12	0.57	0	15,15,17	1.15	1 (6%)
2	GLC	G	3	2	11,11,12	0.24	0	15,15,17	0.53	0
2	GLC	G	4	2	11,11,12	0.38	0	15,15,17	0.71	0
2	GLC	G	5	2	11,11,12	0.26	0	15,15,17	0.65	0
2	GLC	G	6	2	11,11,12	0.31	0	15,15,17	1.02	0
2	GLC	G	7	2	11,11,12	0.34	0	15,15,17	0.77	1 (6%)
2	GLC	G	8	2	11,11,12	0.37	0	15,15,17	0.82	0
2	GLC	H	1	2	11,11,12	0.42	0	15,15,17	1.14	1 (6%)
2	GLC	H	2	2	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
2	GLC	H	3	2	11,11,12	0.42	0	15,15,17	1.36	2 (13%)
2	GLC	H	4	2	11,11,12	0.28	0	15,15,17	0.86	0
2	GLC	H	5	2	11,11,12	0.59	0	15,15,17	0.97	1 (6%)
2	GLC	H	6	2	11,11,12	0.62	0	15,15,17	1.61	2 (13%)
2	GLC	H	7	2	11,11,12	0.40	0	15,15,17	0.92	1 (6%)
2	GLC	H	8	2	11,11,12	0.39	0	15,15,17	1.16	2 (13%)
2	GLC	I	1	2	11,11,12	0.36	0	15,15,17	0.95	0
2	GLC	I	2	2	11,11,12	0.55	0	15,15,17	0.90	1 (6%)
2	GLC	I	3	2	11,11,12	0.29	0	15,15,17	0.82	1 (6%)
2	GLC	I	4	2	11,11,12	0.35	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.37	0	15,15,17	1.07	1 (6%)
2	GLC	I	7	2	11,11,12	0.50	0	15,15,17	0.99	0
2	GLC	I	8	2	11,11,12	0.48	0	15,15,17	0.83	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	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLC	C1-O5-C5	6.82	121.33	112.19
2	E	5	GLC	C1-O5-C5	5.80	119.96	112.19
2	I	5	GLC	C1-O5-C5	5.52	119.58	112.19
2	E	8	GLC	C1-O5-C5	5.40	119.42	112.19
2	H	6	GLC	C1-O5-C5	5.25	119.23	112.19
2	E	3	GLC	C1-C2-C3	4.24	115.83	109.64
2	F	3	GLC	C1-O5-C5	3.92	117.44	112.19
2	E	6	GLC	C1-O5-C5	3.64	117.07	112.19
2	F	8	GLC	C1-O5-C5	3.60	117.01	112.19
2	F	5	GLC	C1-C2-C3	3.52	114.77	109.64
2	H	1	GLC	C1-O5-C5	3.30	116.61	112.19
2	H	3	GLC	O5-C5-C6	3.07	113.65	107.66
2	E	3	GLC	C2-C3-C4	3.03	116.18	110.86
2	F	1	GLC	C1-O5-C5	2.81	115.96	112.19
2	F	7	GLC	C1-O5-C5	2.79	115.92	112.19
2	G	1	GLC	C1-C2-C3	2.69	113.56	109.64
2	E	7	GLC	C1-O5-C5	2.55	115.61	112.19
2	E	2	GLC	C1-O5-C5	2.51	115.56	112.19
2	H	2	GLC	C1-O5-C5	2.44	115.46	112.19
2	G	2	GLC	C1-C2-C3	2.43	113.18	109.64
2	E	1	GLC	C2-C3-C4	-2.39	106.66	110.86
2	F	5	GLC	C1-O5-C5	-2.39	108.98	112.19
2	H	7	GLC	O5-C1-C2	-2.38	105.11	110.79
2	E	1	GLC	O5-C5-C6	2.37	112.28	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GLC	C2-C3-C4	-2.36	106.72	110.86
2	F	3	GLC	C1-C2-C3	-2.34	106.24	109.64
2	E	4	GLC	C2-C3-C4	-2.33	106.77	110.86
2	H	6	GLC	C6-C5-C4	-2.32	107.31	113.02
2	E	5	GLC	O5-C5-C4	2.32	116.48	110.83
2	H	5	GLC	C1-C2-C3	2.29	112.98	109.64
2	F	8	GLC	C2-C3-C4	-2.26	106.88	110.86
2	I	3	GLC	C1-O5-C5	2.26	115.22	112.19
2	F	4	GLC	C1-O5-C5	2.23	115.18	112.19
2	E	5	GLC	C6-C5-C4	-2.20	107.61	113.02
2	I	2	GLC	C1-O5-C5	2.19	115.12	112.19
2	I	6	GLC	C2-C3-C4	2.16	114.66	110.86
2	F	6	GLC	C1-C2-C3	2.12	112.74	109.64
2	H	8	GLC	C1-O5-C5	2.12	115.03	112.19
2	F	5	GLC	C2-C3-C4	2.09	114.54	110.86
2	F	3	GLC	C2-C3-C4	-2.09	107.19	110.86
2	G	7	GLC	C1-C2-C3	2.08	112.67	109.64
2	F	3	GLC	O5-C5-C4	2.07	115.86	110.83
2	F	2	GLC	C1-O5-C5	2.06	114.95	112.19
2	H	3	GLC	C3-C4-C5	-2.06	106.50	110.23
2	H	8	GLC	O3-C3-C2	-2.00	105.97	110.05

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	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	F	6	GLC	O5-C5-C6-O6
2	I	5	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	G	6	GLC	C4-C5-C6-O6
2	I	8	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	7	GLC	O5-C5-C6-O6
2	F	4	GLC	C4-C5-C6-O6
2	G	1	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
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

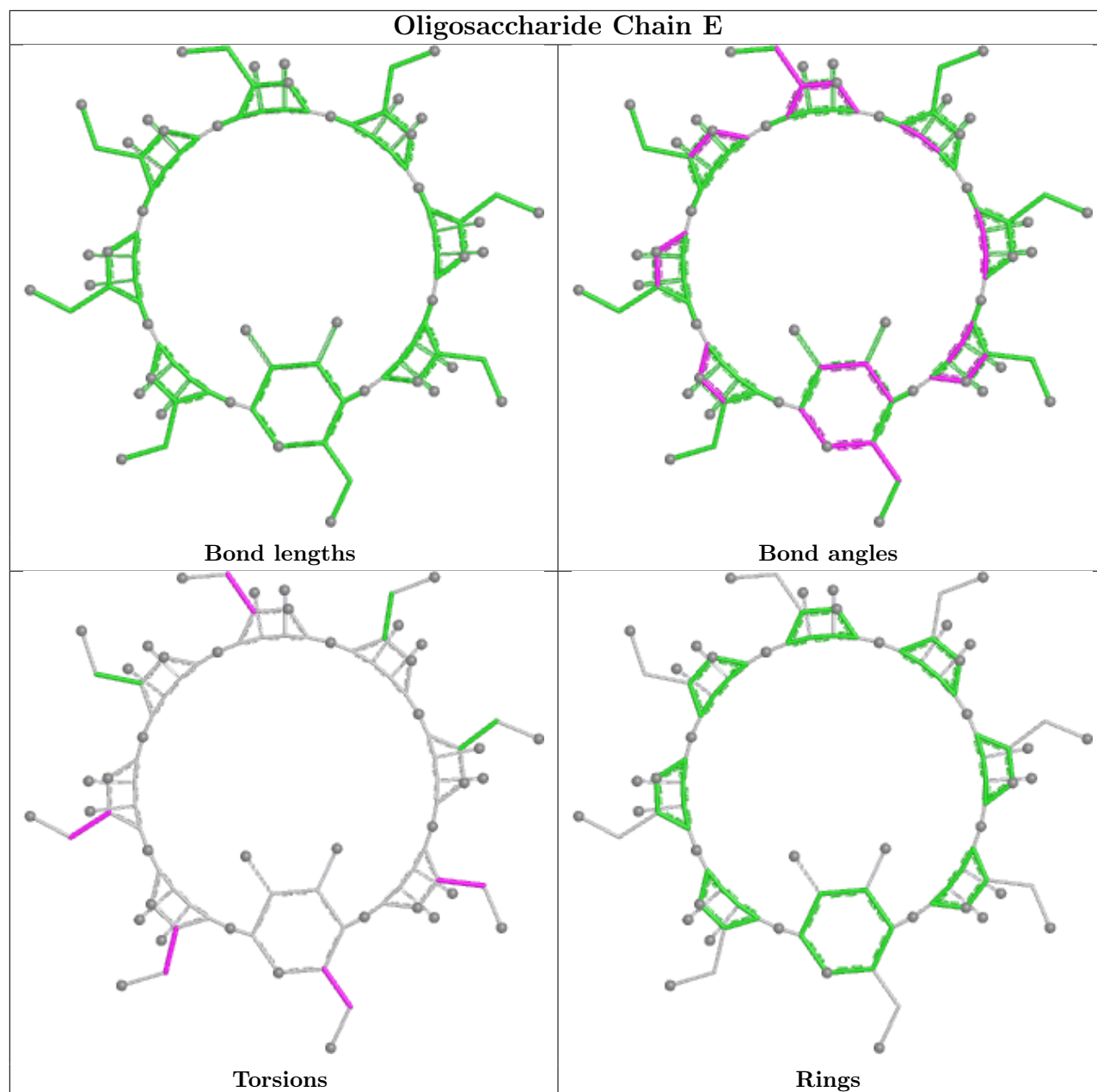
There are no ring outliers.

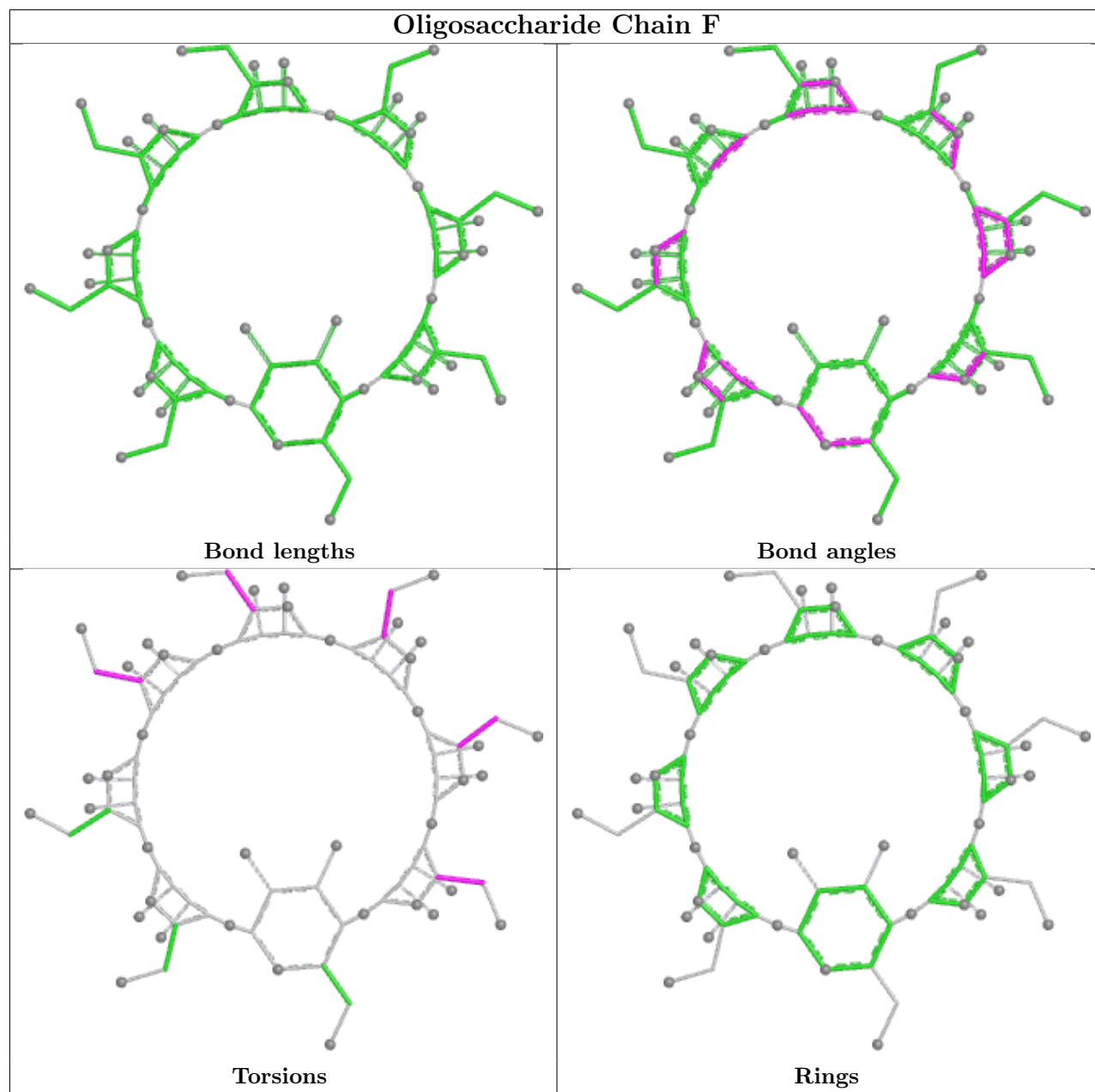
14 monomers are involved in 19 short contacts:

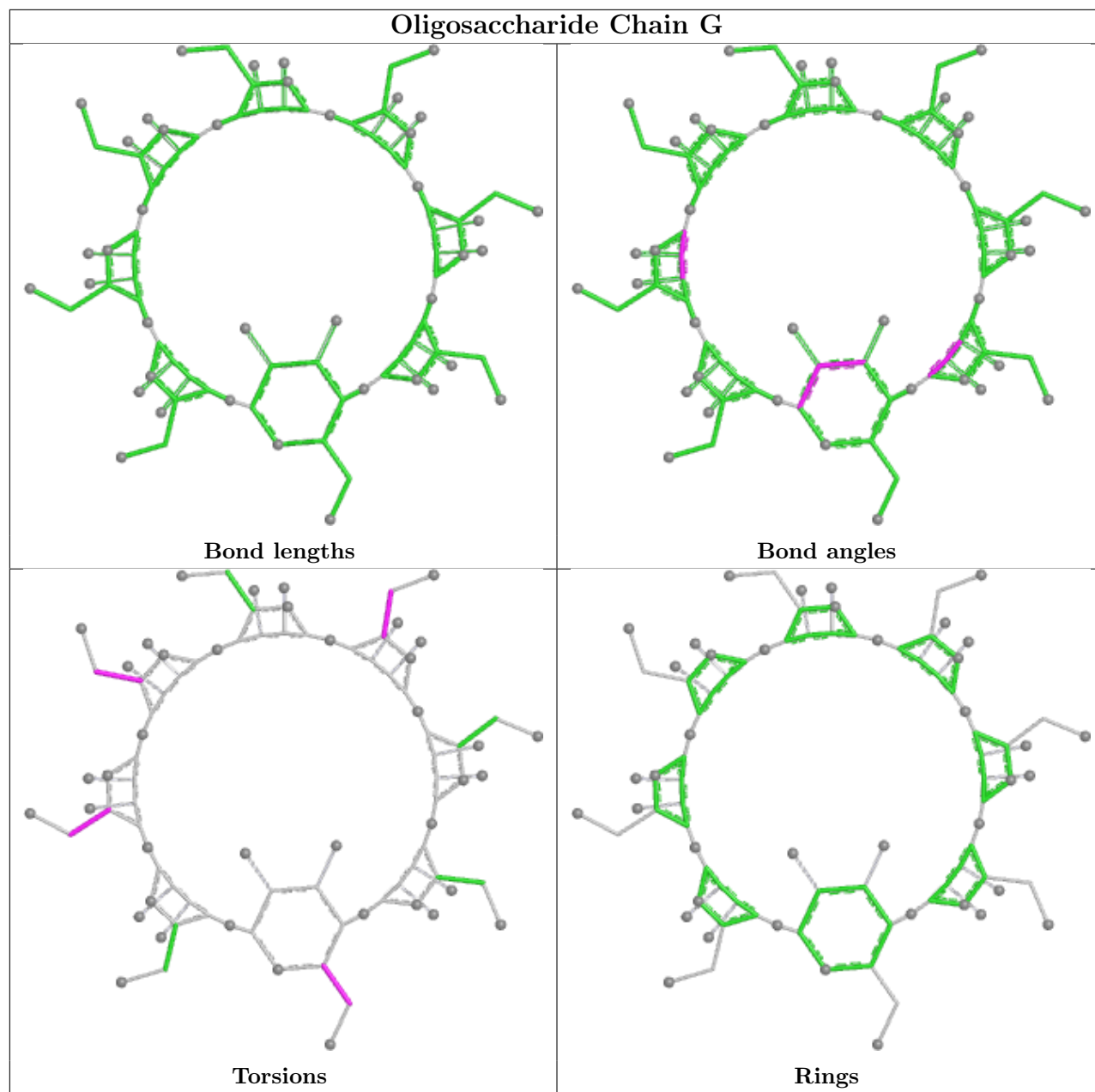
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	GLC	1	0
2	E	6	GLC	1	0
2	E	1	GLC	4	0
2	H	5	GLC	0	1
2	G	8	GLC	1	0
2	E	8	GLC	2	0
2	E	2	GLC	6	0
2	E	3	GLC	4	0
2	G	7	GLC	1	0
2	E	7	GLC	1	0
2	I	2	GLC	2	0
2	E	5	GLC	1	0
2	E	4	GLC	3	0
2	F	4	GLC	1	0

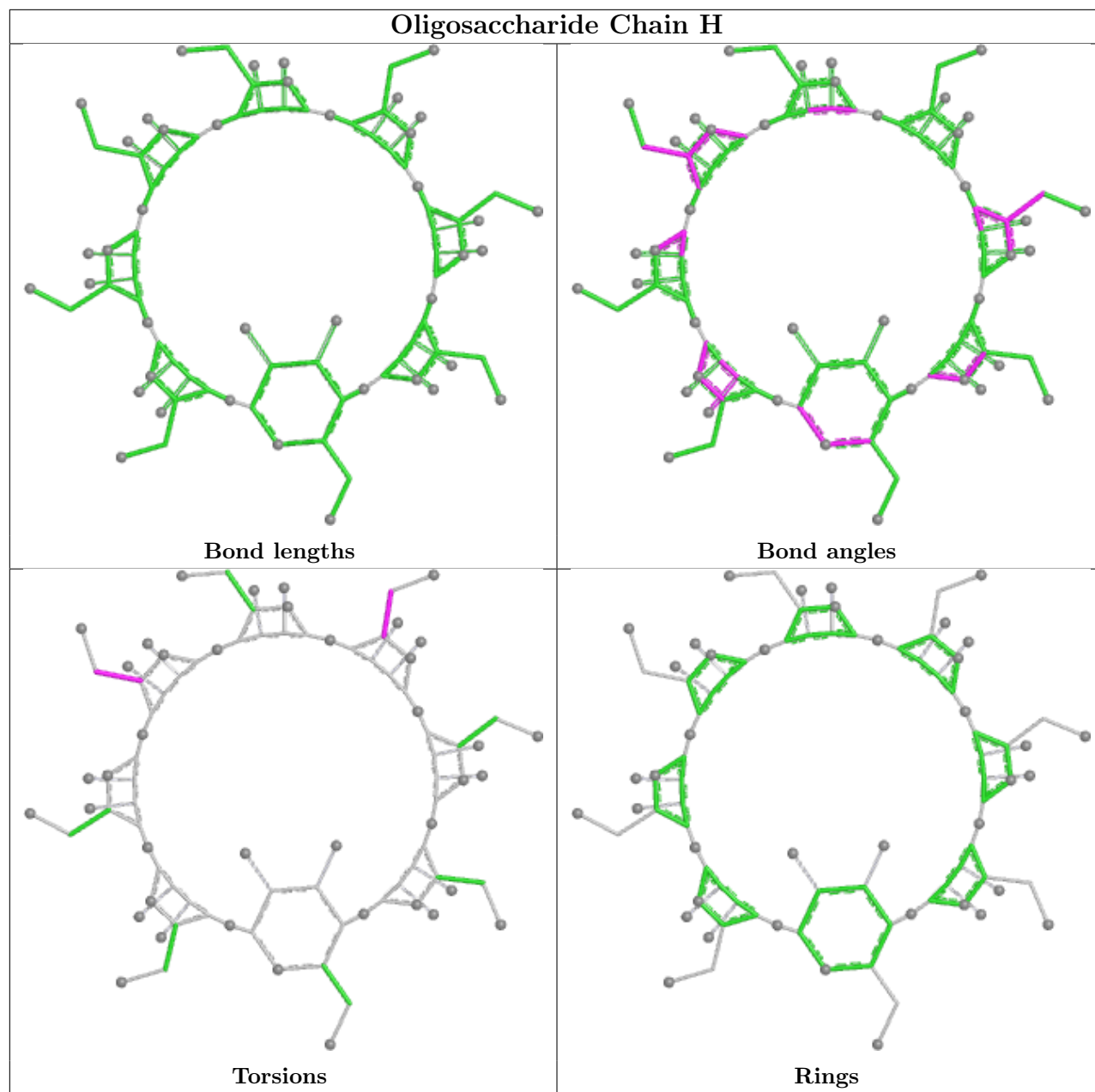
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

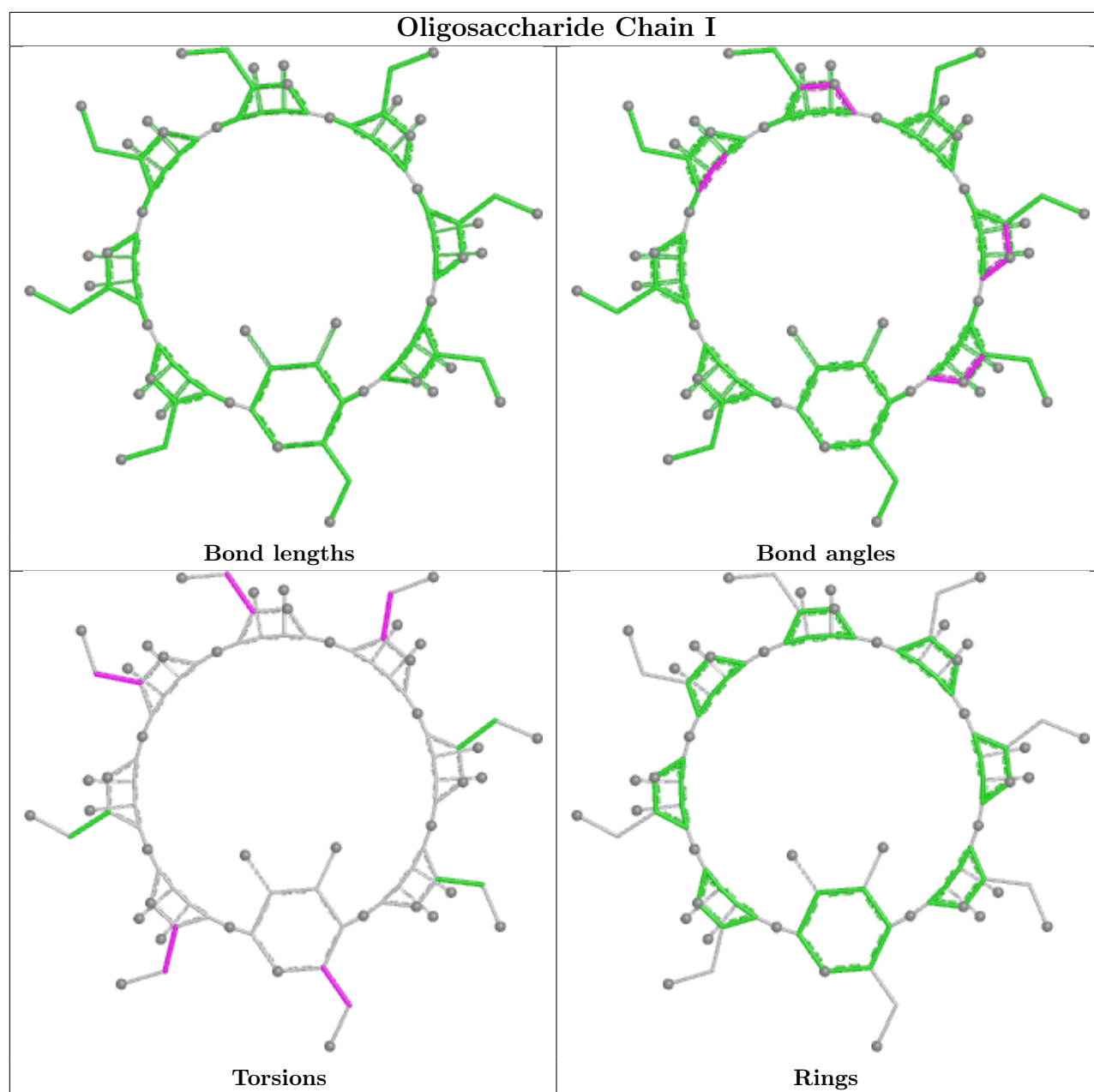
bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [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	A	802	-	5,5,5	0.31	0	5,5,5	1.37	1 (20%)
3	GOL	A	803	-	5,5,5	0.44	0	5,5,5	0.68	0
3	GOL	D	803	-	5,5,5	0.37	0	5,5,5	0.60	0
3	GOL	D	804	-	5,5,5	0.45	0	5,5,5	0.38	0
3	GOL	B	803	-	5,5,5	0.50	0	5,5,5	0.56	0
3	GOL	B	802	-	5,5,5	0.40	0	5,5,5	0.67	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
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	D	803	-	-	0/4/4/4	-
3	GOL	D	804	-	-	2/4/4/4	-
3	GOL	B	803	-	-	3/4/4/4	-
3	GOL	B	802	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	GOL	C3-C2-C1	-2.52	102.57	111.80

There are no chirality outliers.

All (9) 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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

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	586/612 (95%)	-0.04	22 (3%) 44 50	12, 38, 105, 134	13 (2%)
1	B	600/612 (98%)	-0.43	4 (0%) 84 87	12, 31, 55, 75	8 (1%)
1	C	578/612 (94%)	1.05	74 (12%) 7 9	27, 79, 117, 140	4 (0%)
1	D	588/612 (96%)	-0.26	9 (1%) 72 76	16, 38, 60, 84	6 (1%)
All	All	2352/2448 (96%)	0.07	109 (4%) 37 43	12, 41, 102, 140	31 (1%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	498	VAL	4.6
1	A	117	THR	4.3
1	B	415	TYR	4.2
1	C	118	HIS	4.2
1	C	261	PHE	4.1
1	D	414	ASP	4.0
1	C	278	TRP	4.0
1	A	158	TYR	4.0
1	A	346	PHE	3.9
1	C	601[A]	ARG	3.9
1	C	346	PHE	3.8
1	C	199	LEU	3.8
1	C	219	LEU	3.7
1	C	373	LEU	3.7
1	C	412	TYR	3.7
1	A	212	MET	3.6
1	C	174	ILE	3.4
1	A	135	VAL	3.4
1	C	595	TRP	3.3
1	C	713	LEU	3.2
1	C	374	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	413	ARG	3.2
1	C	343	THR	3.1
1	C	158	TYR	3.1
1	C	495	LEU	3.0
1	C	466	VAL	3.0
1	C	187	LEU	2.9
1	C	132	MET	2.9
1	C	217	ALA	2.9
1	C	294	PHE	2.9
1	A	152	VAL	2.9
1	D	372	THR	2.9
1	A	429	GLY	2.9
1	A	131	THR	2.8
1	B	117	THR	2.8
1	C	231	GLU	2.8
1	C	347	ALA	2.8
1	C	433	LEU	2.7
1	C	160	ASP	2.7
1	C	684[A]	MET	2.7
1	B	414	ASP	2.7
1	C	348	LEU	2.7
1	C	351	PHE	2.7
1	D	294[A]	PHE	2.7
1	C	511	ILE	2.6
1	C	497	PRO	2.6
1	C	159	TRP	2.6
1	A	153	VAL	2.6
1	C	727	ALA	2.6
1	C	142	VAL	2.6
1	C	207	ALA	2.5
1	C	349	ALA	2.5
1	C	257	THR	2.5
1	C	165	PRO	2.5
1	C	356	LEU	2.5
1	C	360	SER	2.4
1	C	478	TRP	2.4
1	A	201	LEU	2.4
1	C	268	LEU	2.4
1	A	380	ARG	2.4
1	C	208	PHE	2.4
1	A	512	LEU	2.4
1	C	215	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	552	ALA	2.4
1	D	117	THR	2.4
1	B	423	ILE	2.4
1	C	411	ILE	2.4
1	C	463	PHE	2.3
1	C	589	LEU	2.3
1	C	464	PRO	2.3
1	A	134	GLY	2.3
1	C	188	TYR	2.3
1	D	429	GLY	2.3
1	D	257	THR	2.3
1	A	213	ARG	2.3
1	C	202	LYS	2.3
1	C	507	LEU	2.3
1	A	132	MET	2.3
1	A	472	MET	2.3
1	C	210	ALA	2.3
1	C	150	VAL	2.3
1	C	152	VAL	2.3
1	C	156	PHE	2.2
1	D	194	ASP	2.2
1	A	129	ALA	2.2
1	C	216	THR	2.2
1	A	214	PRO	2.2
1	C	453	ALA	2.2
1	C	201	LEU	2.2
1	C	133	ASP	2.2
1	C	344	ASP	2.2
1	D	346	PHE	2.2
1	C	129	ALA	2.2
1	C	615	ALA	2.2
1	A	168	LEU	2.1
1	C	179	ILE	2.1
1	A	159	TRP	2.1
1	C	340	HIS	2.1
1	C	543	ALA	2.1
1	C	119	LEU	2.1
1	C	177	LEU	2.1
1	C	186	GLN	2.1
1	C	312	PHE	2.1
1	C	139	ARG	2.1
1	A	372	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	446	LEU	2.1
1	C	149	ARG	2.0
1	D	212	MET	2.0
1	C	380	ARG	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	0.54	0.26	102,103,103,103	11
2	GLC	G	2	11/12	0.57	0.23	102,104,104,104	0
2	GLC	E	7	11/12	0.61	0.22	73,74,75,77	11
2	GLC	I	5	11/12	0.61	0.22	90,90,91,91	11
2	GLC	E	1	11/12	0.64	0.17	78,79,79,79	11
2	GLC	E	2	11/12	0.65	0.16	74,78,79,79	0
2	GLC	I	6	11/12	0.68	0.19	91,92,92,92	11
2	GLC	I	7	11/12	0.70	0.15	89,91,92,92	0
2	GLC	G	5	11/12	0.71	0.23	99,99,99,100	11
2	GLC	G	6	11/12	0.71	0.20	100,100,100,100	11
2	GLC	I	3	11/12	0.71	0.13	83,84,85,86	1
2	GLC	G	7	11/12	0.72	0.22	100,101,101,101	11
2	GLC	E	8	11/12	0.74	0.22	78,78,79,79	11
2	GLC	G	8	11/12	0.75	0.20	101,102,102,102	11
2	GLC	F	4	11/12	0.76	0.14	72,72,73,73	10
2	GLC	H	6	11/12	0.76	0.12	54,59,61,61	0
2	GLC	F	5	11/12	0.78	0.17	69,71,72,72	10
2	GLC	I	8	11/12	0.79	0.14	80,84,86,87	1
2	GLC	I	4	11/12	0.80	0.17	87,88,88,89	11
2	GLC	G	4	11/12	0.82	0.15	96,98,98,98	11
2	GLC	E	6	11/12	0.82	0.15	62,65,67,70	1
2	GLC	F	6	11/12	0.83	0.11	57,64,66,67	0
2	GLC	E	3	11/12	0.83	0.11	60,66,71,71	0
2	GLC	F	3	11/12	0.83	0.13	67,70,71,71	0

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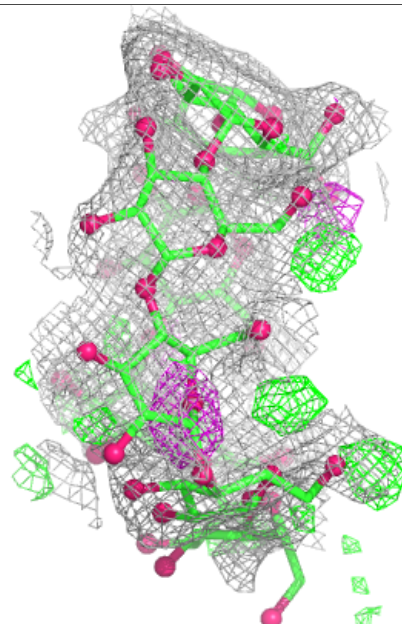
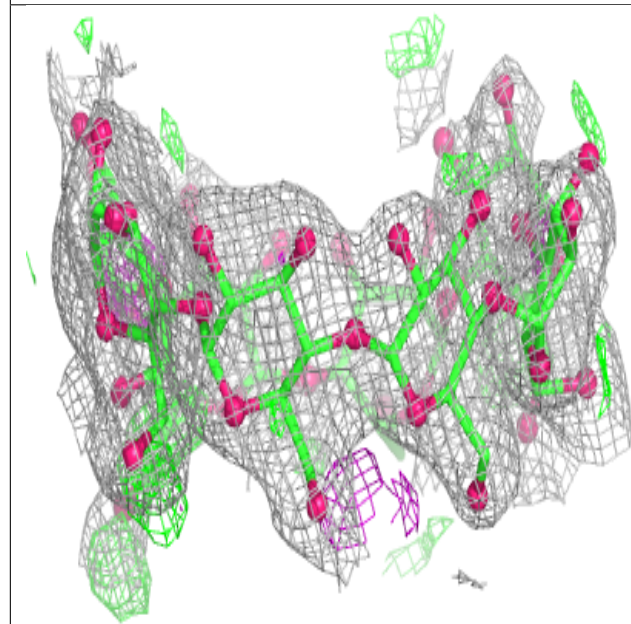
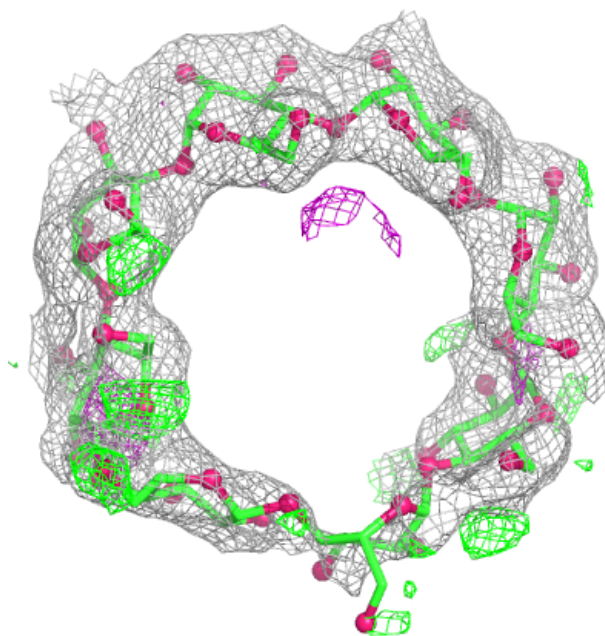
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	H	2	11/12	0.84	0.10	67,68,68,69	0
2	GLC	H	3	11/12	0.85	0.11	68,69,70,70	0
2	GLC	H	1	11/12	0.86	0.11	59,62,63,65	0
2	GLC	F	2	11/12	0.86	0.11	53,58,60,64	0
2	GLC	H	5	11/12	0.88	0.10	61,63,65,66	0
2	GLC	H	4	11/12	0.88	0.10	66,67,68,68	0
2	GLC	I	2	11/12	0.89	0.15	77,78,79,81	0
2	GLC	F	7	11/12	0.90	0.10	43,48,52,53	0
2	GLC	H	7	11/12	0.90	0.09	42,47,50,50	0
2	GLC	G	3	11/12	0.90	0.15	98,99,100,100	11
2	GLC	E	5	11/12	0.94	0.09	49,52,55,58	0
2	GLC	I	1	11/12	0.94	0.13	75,76,76,78	0
2	GLC	E	4	11/12	0.94	0.09	45,50,53,54	0
2	GLC	H	8	11/12	0.95	0.08	46,48,50,55	0
2	GLC	F	1	11/12	0.97	0.05	34,39,42,47	0
2	GLC	F	8	11/12	0.97	0.06	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.

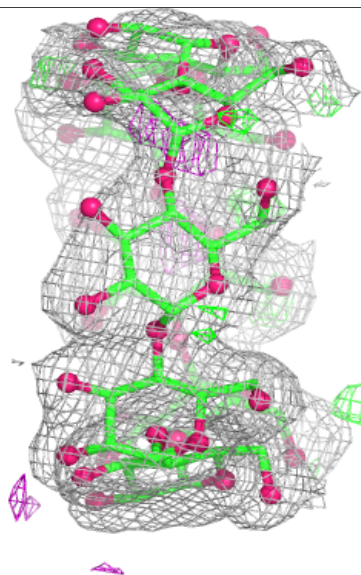
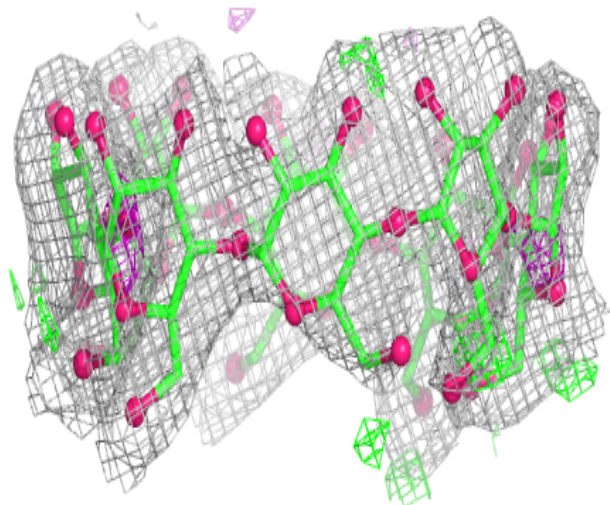
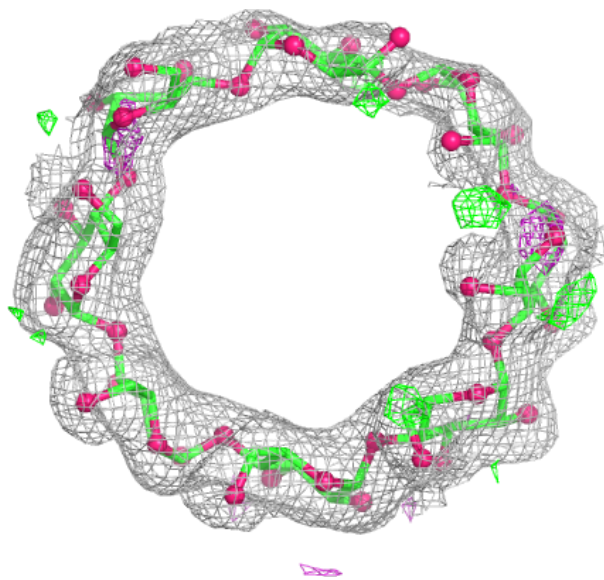
Electron density around Chain E:

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



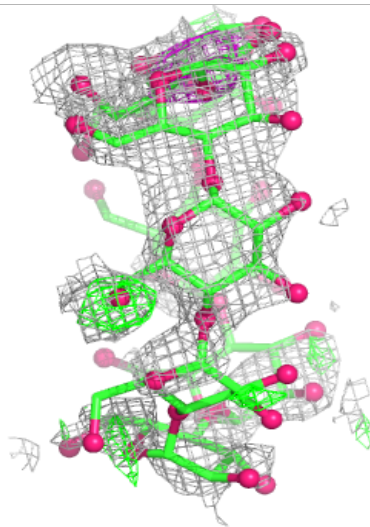
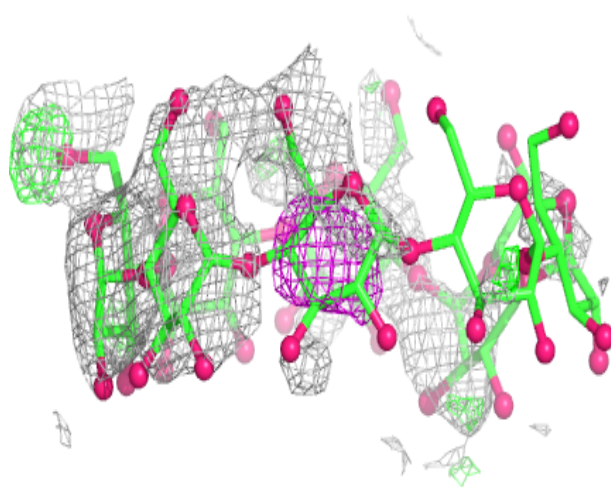
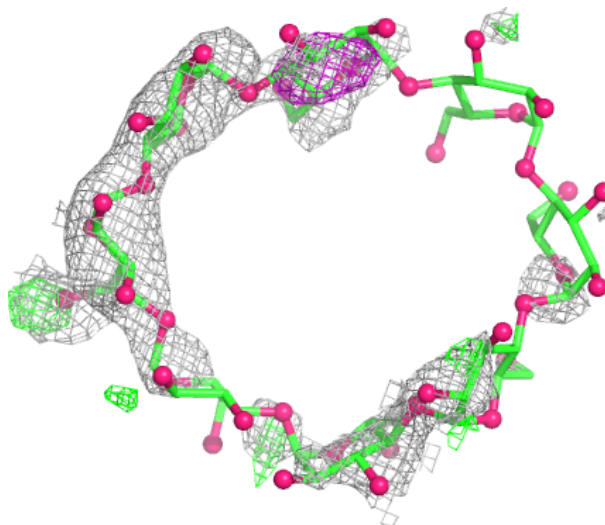
Electron density around Chain F:

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



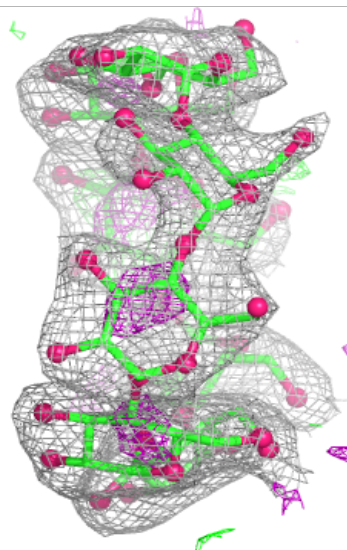
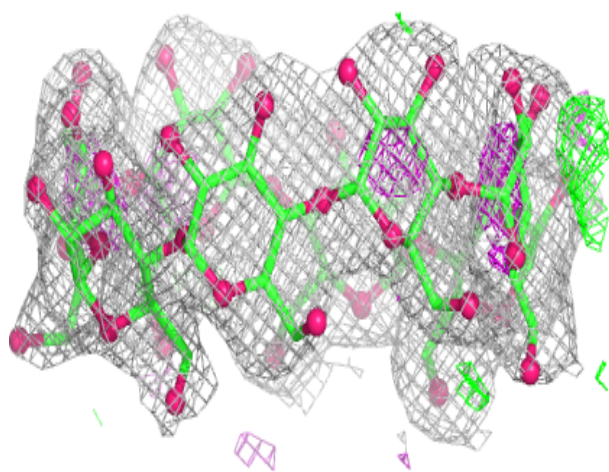
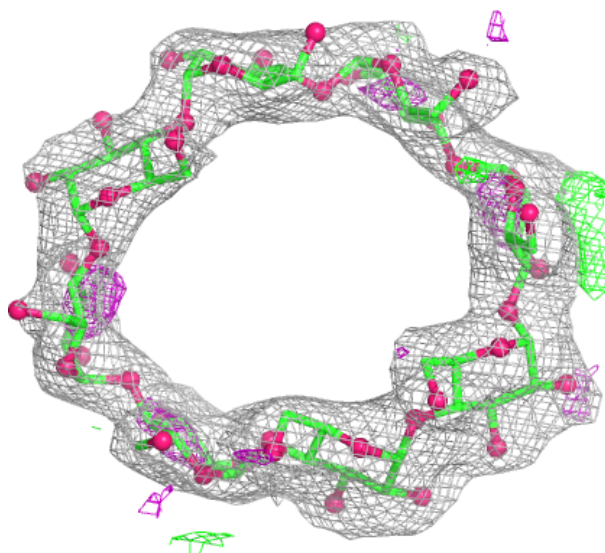
Electron density around Chain G:

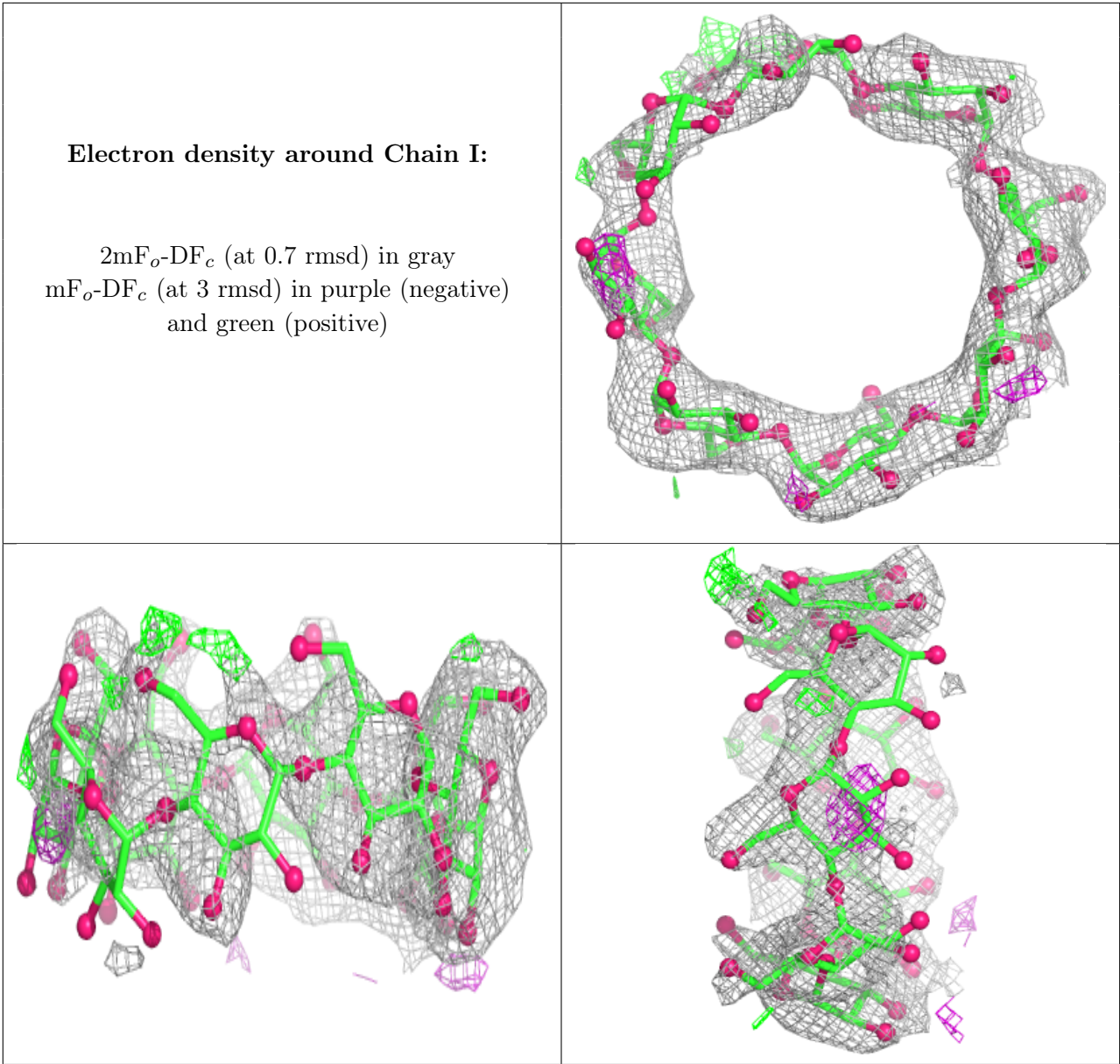
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	802	6/6	0.89	0.11	42,44,44,46	0
3	GOL	B	802	6/6	0.93	0.11	30,34,35,36	0
3	GOL	A	803	6/6	0.94	0.08	27,31,32,34	0
3	GOL	B	803	6/6	0.94	0.08	45,45,45,46	0
3	GOL	D	803	6/6	0.94	0.10	50,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	804	6/6	0.95	0.07	45,45,46,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.