



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:59 PM BST

PDB ID : 4LPC  
Title : Crystal Structure of E.Coli Branching Enzyme in complex with maltoheptaose  
Authors : Feng, L.; Geiger, J.H.  
Deposited on : 2013-07-16  
Resolution : 2.39 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

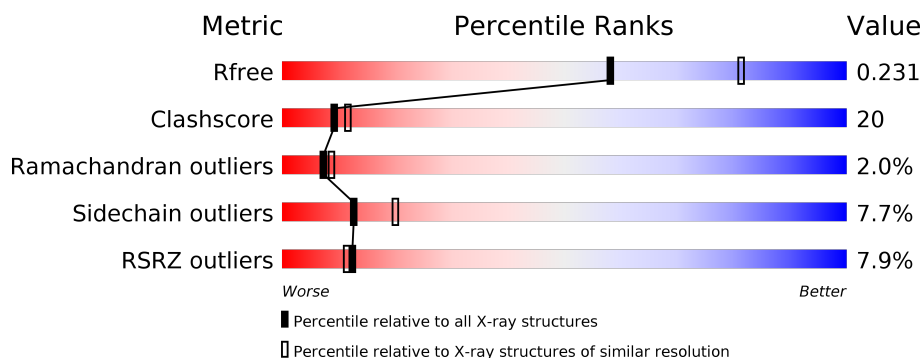
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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.




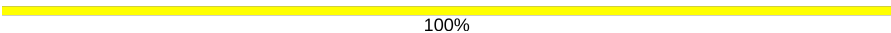
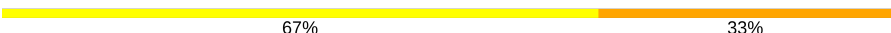



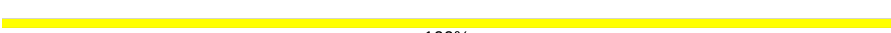


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>9%</div> <div>60%</div> <div>30%</div> <div>5%</div> <div>.</div> </div>
1	B	612	<div> <div>2%</div> <div>67%</div> <div>24%</div> <div>6%</div> <div>..</div> </div>
1	C	612	<div> <div>17%</div> <div>62%</div> <div>29%</div> <div>5%</div> <div>.</div> </div>
1	D	612	<div> <div>2%</div> <div>68%</div> <div>23%</div> <div>.</div> <div>.</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	2	 50% 50%
2	M	2	 100%
3	G	3	 67% 33%
4	H	2	 100%
4	J	2	 50% 50%
4	N	2	 50% 50%
4	O	2	 100%
5	I	7	 14% 86%
6	L	4	 75% 25%

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
4	BGC	N	1	-	-	X	-
5	GLC	I	3	-	-	-	X
5	GLC	I	4	-	-	-	X
6	GLC	L	1	-	-	-	X
7	GOL	A	807	-	-	X	-
7	GOL	B	815	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 20728 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	587	Total	C	N	O	S	0	5	0
			4870	3109	867	878	16			
1	B	598	Total	C	N	O	S	0	2	0
			4935	3149	880	890	16			
1	C	582	Total	C	N	O	S	0	1	0
			4795	3068	850	861	16			
1	D	588	Total	C	N	O	S	0	4	0
			4867	3108	865	877	17			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			

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



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	H	2	Total	C	O	0	0	0
			23	12	11			
4	J	2	Total	C	O	0	0	0
			23	12	11			
4	N	2	Total	C	O	0	0	0
			23	12	11			
4	O	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



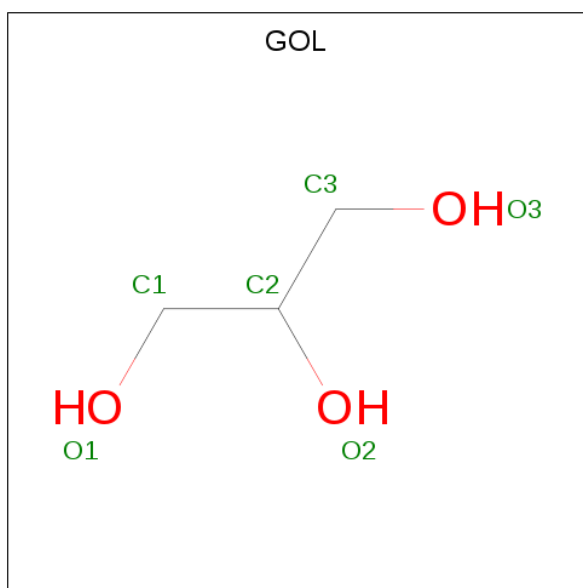
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	I	7	Total	C	O	0	0	0
			78	42	36			

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



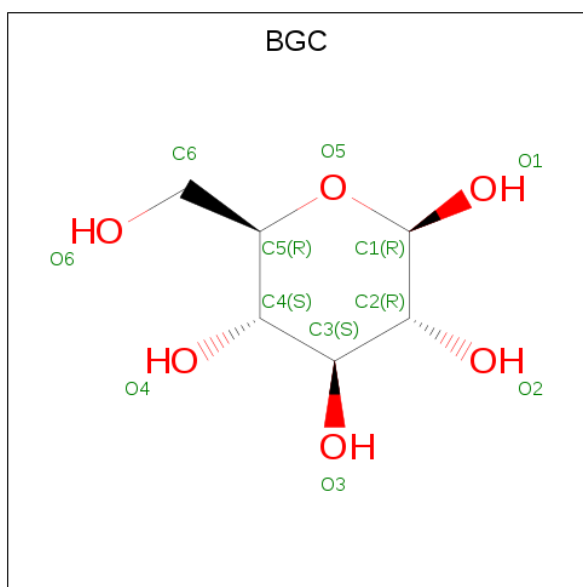
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	L	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is beta-D-glucopyranose (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	220	Total	O	0	0
			220	220		
9	B	329	Total	O	0	0
			329	329		
9	C	72	Total	O	0	0
			72	72		
9	D	221	Total	O	0	0
			221	221		

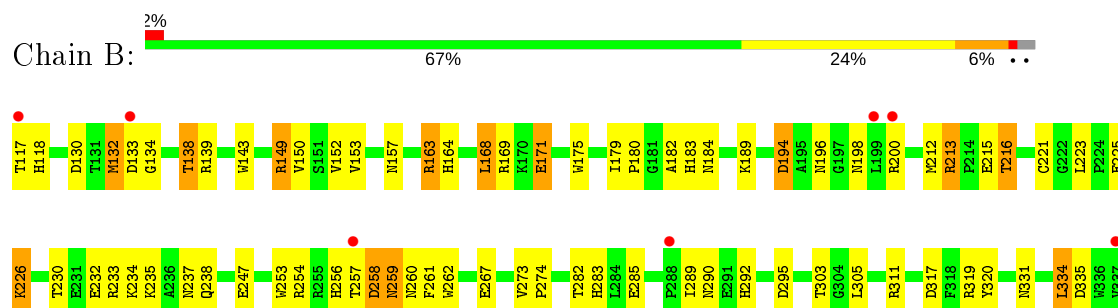
### 3 Residue-property plots

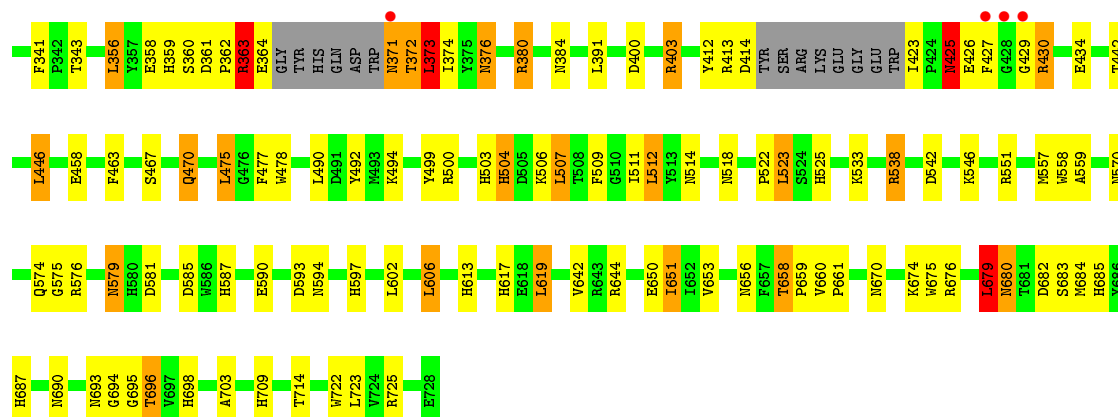
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

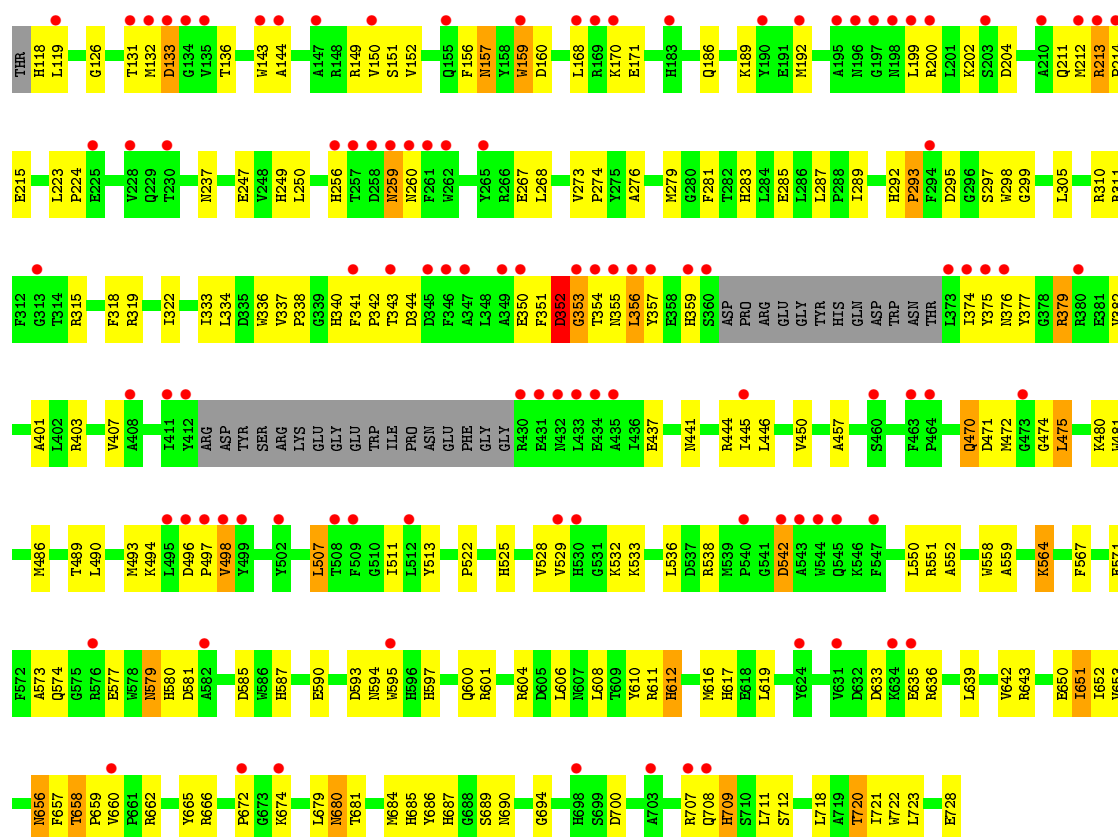


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

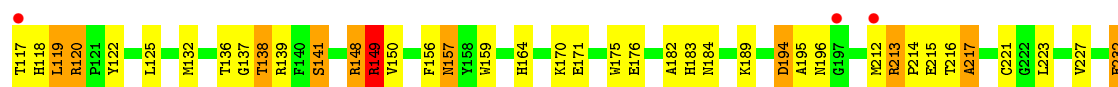


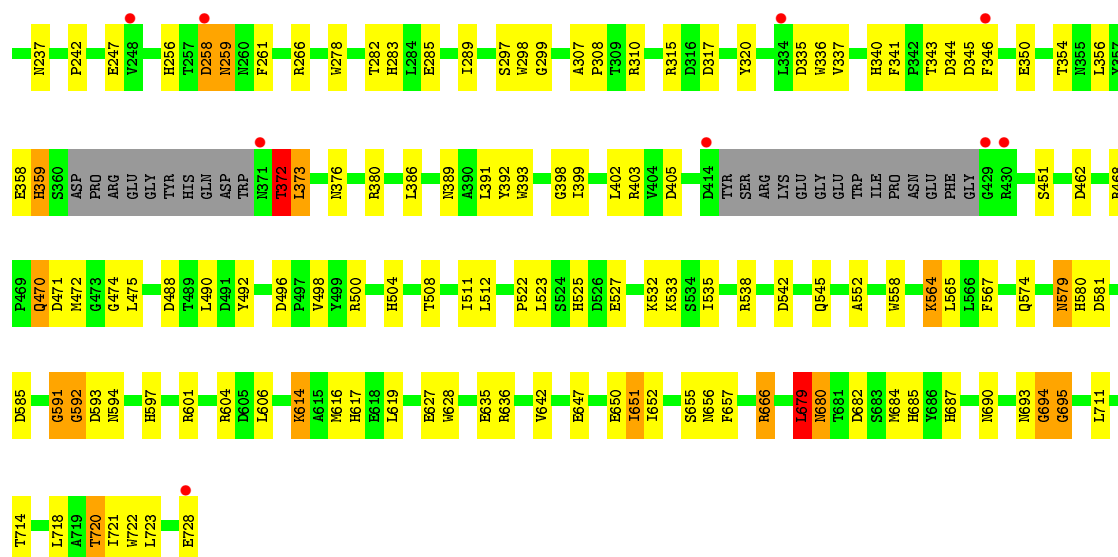


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



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





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

Chain E: 50% 50%



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

Chain F: 50% 50%



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

Chain K: 50% 50%



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

Chain M: 100%



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

Chain G: 67% 33%




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

Chain H:  100%

BGC1  
GLC2

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

Chain J:  50% 50%

BGC1  
GLC2

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

Chain N:  50% 50%

BGC1  
GLC2

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

Chain O:  100%

BGC1  
GLC2

- Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain I:  14% 86%

BGC1  
GLC2  
GLC3  
GLC4  
GLC5  
GLC6  
GLC7

- Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  75% 25%

GLC1  
GLC2  
GLC3  
GLC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.19Å 103.42Å 185.94Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 41.27 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.00-2.39) 90.4 (41.27-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.234 0.182 , 0.231	Depositor DCC
$R_{free}$ test set	6287 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, GOL, BGC

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	0.57	0/5024	0.66	5/6820 (0.1%)
1	B	0.72	1/5092 (0.0%)	0.77	5/6914 (0.1%)
1	C	0.37	0/4948	0.48	0/6719
1	D	0.56	0/5021	0.67	3/6817 (0.0%)
All	All	0.57	1/20085 (0.0%)	0.66	13/27270 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	TRP	CB-CG	5.21	1.59	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	B	373	LEU	CA-CB-CG	7.06	131.53	115.30
1	A	606	LEU	CA-CB-CG	6.50	130.26	115.30
1	B	723	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	643	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	120	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	D	679	LEU	CA-CB-CG	-5.89	101.74	115.30
1	A	606	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	403	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	723	LEU	CA-CB-CG	5.16	127.17	115.30
1	D	636	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	679	LEU	CA-CB-CG	-5.15	103.46	115.30
1	A	643	ARG	CG-CD-NE	-5.02	101.26	111.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4870	0	4590	218	0
1	B	4935	0	4647	207	0
1	C	4795	0	4527	158	0
1	D	4867	0	4586	180	0
2	E	23	0	21	2	0
2	F	23	0	21	4	0
2	K	23	0	21	0	0
2	M	23	0	21	1	0
3	G	34	0	30	6	0
4	H	23	0	21	4	0
4	J	23	0	21	7	0
4	N	23	0	21	7	0
4	O	23	0	21	0	0
5	I	78	0	66	7	0
6	L	45	0	39	1	0
7	A	18	0	24	6	0
7	B	30	0	40	12	0
7	D	18	0	24	2	0
8	B	12	0	12	0	0
9	A	220	0	0	29	0
9	B	329	0	0	49	0
9	C	72	0	0	14	0
9	D	221	0	0	17	0
All	All	20728	0	18753	768	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (768) 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:D:212[A]:MET:CE	1:D:213:ARG:HH12	1.14	1.58
1:D:212[A]:MET:CE	1:D:213:ARG:NH1	1.91	1.29
1:D:470:GLN:N	1:D:470:GLN:HE21	1.33	1.26
1:D:212[A]:MET:HG3	1:D:213:ARG:NH1	1.50	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:GLU:HG2	9:B:1114:HOH:O	1.35	1.24
1:D:470:GLN:NE2	1:D:470:GLN:H	1.33	1.22
1:B:118:HIS:HB3	9:B:1180:HOH:O	1.40	1.20
1:A:352:ASP:OD2	1:A:354:THR:HG22	1.38	1.19
1:D:212[A]:MET:HE3	1:D:213:ARG:NH1	1.51	1.16
1:D:695:GLY:HA2	9:D:1113:HOH:O	1.47	1.15
1:B:512:LEU:HD13	4:J:1:BGC:H6C1	1.17	1.13
1:A:214:PRO:HA	1:A:215:GLU:HB3	1.16	1.12
1:D:212[A]:MET:CG	1:D:213:ARG:NH1	2.12	1.11
1:A:214:PRO:CA	1:A:215:GLU:HB3	1.82	1.09
1:B:149:ARG:HG3	1:B:149:ARG:HH21	1.04	1.08
1:C:213:ARG:HB3	1:C:214:PRO:HD3	1.31	1.08
1:C:681:THR:HG22	9:C:916:HOH:O	1.51	1.07
1:B:257:THR:HA	9:B:1045:HOH:O	1.53	1.06
1:B:225:GLU:O	1:B:226:LYS:HB2	1.24	1.04
1:D:149:ARG:HH11	1:D:149:ARG:HG3	1.21	1.03
1:B:470:GLN:HE21	1:B:470:GLN:N	1.54	1.03
1:B:470:GLN:NE2	1:B:470:GLN:H	1.55	1.03
1:C:276:ALA:HA	9:C:971:HOH:O	1.60	1.02
1:A:470:GLN:HA	1:A:474:GLY:HA2	1.46	0.98
1:A:148:ARG:O	1:A:149:ARG:HG2	1.64	0.97
1:A:214:PRO:HA	1:A:215:GLU:CB	1.91	0.97
1:C:470:GLN:H	1:C:470:GLN:HE21	1.02	0.97
1:A:131:THR:HB	1:A:136:THR:HG22	1.43	0.97
1:A:233:ARG:NH1	9:A:1026:HOH:O	1.96	0.97
1:B:225:GLU:O	1:B:226:LYS:CB	2.11	0.96
1:B:364:GLU:HB2	9:B:1207:HOH:O	1.66	0.95
1:B:371:ASN:HB3	1:B:372:THR:HB	1.48	0.95
1:D:266:ARG:HD3	9:D:1017:HOH:O	1.66	0.95
1:A:358:GLU:OE2	1:A:358:GLU:N	1.99	0.95
1:C:213:ARG:CB	1:C:214:PRO:HD3	1.97	0.94
9:A:993:HOH:O	1:D:635[B]:GLU:HG2	1.66	0.94
1:B:658:THR:HG22	1:B:660:VAL:H	1.32	0.93
1:C:281:PHE:HD2	9:C:971:HOH:O	1.51	0.93
1:D:628:TRP:HE1	4:N:1:BGC:C6	1.80	0.93
1:A:259:ASN:HD22	1:A:261:PHE:H	1.14	0.91
1:B:212:MET:O	1:B:213:ARG:HB3	1.69	0.91
1:D:212[A]:MET:HG3	1:D:213:ARG:HH11	1.33	0.90
1:B:380:ARG:HD2	9:B:1203:HOH:O	1.72	0.90
1:D:212[A]:MET:HE2	1:D:213:ARG:HH22	1.35	0.89
1:D:628:TRP:HE1	4:N:1:BGC:H6C2	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:HIS:NE2	7:B:813:GOL:H32	1.86	0.89
1:D:212[A]:MET:SD	1:D:213:ARG:NH1	2.37	0.89
1:C:213:ARG:HB3	1:C:214:PRO:CD	2.02	0.88
1:C:551:ARG:HB3	1:C:681:THR:HG23	1.55	0.88
1:A:628:TRP:HE1	3:G:1:GLC:C6	1.87	0.88
1:C:213:ARG:CB	1:C:214:PRO:CD	2.52	0.88
1:A:225:GLU:O	1:A:226:LYS:HB2	1.74	0.88
1:B:683:SER:HB2	7:B:815:GOL:H2	1.53	0.88
1:B:171:GLU:HG3	9:B:1169:HOH:O	1.74	0.87
1:B:693:ASN:HD21	1:B:714:THR:H	1.23	0.87
1:B:363:ARG:HD3	1:B:364:GLU:H	1.37	0.87
1:A:209:GLU:HG2	1:A:219:LEU:HD22	1.57	0.87
1:D:693:ASN:HD21	1:D:714:THR:H	1.17	0.87
1:A:709:HIS:HD2	9:A:990:HOH:O	1.57	0.87
1:B:512:LEU:HD13	4:J:1:BGC:C6	2.04	0.86
1:C:606:LEU:HD23	1:C:679:LEU:HD11	1.55	0.86
1:A:551:ARG:HH12	7:A:807:GOL:H11	1.41	0.86
1:C:674:LYS:NZ	9:C:933:HOH:O	2.07	0.86
1:B:149:ARG:HG3	1:B:149:ARG:NH2	1.85	0.86
1:B:335:ASP:OD1	1:B:403:ARG:HD3	1.76	0.86
1:B:138:THR:HG22	1:B:182:ALA:O	1.76	0.86
1:A:209:GLU:HG2	1:A:219:LEU:CD2	2.06	0.85
1:A:151:SER:HB2	1:A:164:HIS:O	1.76	0.85
1:C:470:GLN:N	1:C:470:GLN:HE21	1.75	0.85
1:B:262:TRP:CZ3	1:B:311:ARG:HG2	2.12	0.85
1:D:148:ARG:O	1:D:149:ARG:HB2	1.74	0.85
1:B:371:ASN:CB	1:B:372:THR:HB	2.07	0.84
1:B:576:ARG:HH22	5:I:5:GLC:H62	1.41	0.84
1:D:628:TRP:NE1	4:N:1:BGC:H6C2	1.92	0.84
1:B:512:LEU:CD1	4:J:1:BGC:H6C1	2.06	0.84
1:C:199:LEU:O	1:C:200:ARG:NH1	2.11	0.84
1:A:340:HIS:HE1	1:A:405:ASP:OD2	1.60	0.83
1:A:687:HIS:O	7:A:807:GOL:H31	1.79	0.83
1:A:350:GLU:HA	1:A:354:THR:O	1.78	0.83
1:B:149:ARG:CG	1:B:149:ARG:HH21	1.92	0.82
1:D:216:THR:O	1:D:217:ALA:HB3	1.79	0.82
1:A:628:TRP:HE1	3:G:1:GLC:H61	1.45	0.82
1:A:259:ASN:ND2	1:A:261:PHE:H	1.78	0.82
1:B:694:GLY:HA3	9:B:1054:HOH:O	1.80	0.82
1:A:693:ASN:HD21	1:A:714:THR:H	1.26	0.81
1:A:594:ASN:H	1:A:597:HIS:HD2	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:O	1:A:226:LYS:CB	2.26	0.81
1:C:658:THR:H	1:C:718:LEU:HD23	1.45	0.81
1:C:684:MET:H	1:C:690:ASN:HD22	1.27	0.81
1:C:340:HIS:HD2	9:C:936:HOH:O	1.62	0.81
1:C:642:VAL:HG13	1:C:650:GLU:HB2	1.62	0.81
1:D:212[A]:MET:CE	1:D:213:ARG:CZ	2.58	0.80
1:B:163:ARG:HD2	9:B:1084:HOH:O	1.81	0.80
1:A:144:ALA:HB1	1:A:352:ASP:HB3	1.63	0.80
1:B:169:ARG:HD3	9:B:1195:HOH:O	1.81	0.80
1:D:212[A]:MET:HE3	1:D:213:ARG:HH12	1.10	0.80
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.65	0.79
1:D:212[A]:MET:HE2	1:D:213:ARG:NH2	1.96	0.79
1:D:212[A]:MET:HE3	1:D:213:ARG:CZ	2.12	0.79
1:D:216:THR:O	1:D:217:ALA:CB	2.31	0.79
1:C:359:HIS:HB2	1:C:376:ASN:HB2	1.62	0.79
1:D:372:THR:HG23	1:D:372:THR:O	1.83	0.79
1:D:693:ASN:O	1:D:694:GLY:C	2.19	0.79
1:D:594:ASN:H	1:D:597:HIS:HD2	1.30	0.79
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.18	0.79
7:B:815:GOL:H12	9:B:1035:HOH:O	1.83	0.78
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.17	0.78
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.66	0.78
1:A:551:ARG:HH12	7:A:807:GOL:C1	1.97	0.78
1:D:138:THR:HG23	1:D:182:ALA:O	1.85	0.78
1:D:212[A]:MET:HE2	1:D:213:ARG:HH12	1.44	0.77
1:B:371:ASN:HD22	1:B:371:ASN:C	1.87	0.77
1:A:628:TRP:NE1	3:G:1:GLC:H62	1.99	0.77
1:B:362:PRO:CA	1:B:363:ARG:HB2	2.15	0.77
1:B:494:LYS:HD2	1:B:538:ARG:HG2	1.65	0.77
1:B:371:ASN:CA	1:B:372:THR:HB	2.15	0.77
1:A:680:ASN:HD22	1:A:682:ASP:H	1.32	0.76
1:B:518:ASN:HD21	4:H:2:GLC:H62	1.50	0.76
1:D:213:ARG:N	1:D:214:PRO:HD2	1.99	0.76
1:B:371:ASN:O	1:B:371:ASN:ND2	2.18	0.76
1:C:657:PHE:O	1:C:658:THR:HB	1.86	0.76
1:A:132:MET:HE3	1:A:132:MET:HA	1.66	0.76
1:D:373:LEU:H	1:D:373:LEU:CD2	2.00	0.75
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.67	0.75
1:B:295:ASP:OD2	1:B:311:ARG:NH2	2.20	0.74
1:D:149:ARG:HH11	1:D:149:ARG:CG	2.00	0.74
1:C:249:HIS:HB2	1:C:287:LEU:HD22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ARG:HG3	1:D:149:ARG:NH1	2.01	0.74
1:B:414:ASP:OD1	9:B:1131:HOH:O	2.06	0.74
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.69	0.74
1:A:533:LYS:O	1:A:538:ARG:NH2	2.21	0.73
1:D:337:VAL:O	1:D:337:VAL:HG23	1.89	0.73
1:D:258:ASP:HB2	9:D:979:HOH:O	1.87	0.72
1:A:131:THR:CB	1:A:136:THR:HG22	2.20	0.72
1:D:138:THR:CG2	1:D:182:ALA:O	2.38	0.72
1:A:680:ASN:ND2	1:A:682:ASP:H	1.88	0.72
1:A:655:SER:OG	1:A:720:THR:HB	1.87	0.72
1:D:278:TRP:O	1:D:604:ARG:HD2	1.88	0.72
1:B:725:ARG:HD3	9:B:1062:HOH:O	1.90	0.71
1:A:292:HIS:O	1:A:311:ARG:NH1	2.23	0.71
1:A:590[A]:GLU:OE2	1:B:676:ARG:NH2	2.23	0.71
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.25	0.71
1:B:644:ARG:HG2	1:B:650:GLU:HG2	1.72	0.71
1:D:614:LYS:HE3	9:D:997:HOH:O	1.91	0.71
1:A:147:ALA:O	1:A:148:ARG:CB	2.37	0.71
1:A:211:GLN:HE21	1:A:215:GLU:H	1.37	0.70
1:B:117:THR:OG1	1:B:118:HIS:N	2.23	0.70
1:D:212[A]:MET:HE2	1:D:213:ARG:NH1	2.03	0.70
1:B:362:PRO:CB	1:B:363:ARG:HB2	2.21	0.70
1:C:564:LYS:HE2	1:C:610:TYR:CE1	2.26	0.70
1:A:132:MET:CE	1:A:132:MET:HA	2.22	0.70
1:B:683:SER:HB2	7:B:815:GOL:C2	2.22	0.70
1:C:351:PHE:O	1:C:352:ASP:HB3	1.92	0.70
1:A:262:TRP:CH2	1:A:311:ARG:HG2	2.27	0.70
1:D:373:LEU:H	1:D:373:LEU:HD22	1.56	0.70
1:C:118:HIS:N	9:C:935:HOH:O	2.23	0.69
1:C:496:ASP:O	1:C:498:VAL:N	2.25	0.69
1:D:237:ASN:ND2	1:D:283:HIS:HE1	1.91	0.69
1:D:373:LEU:N	1:D:373:LEU:CD2	2.56	0.69
1:D:647:GLU:OE1	9:D:938:HOH:O	2.10	0.69
5:I:5:GLC:H4	5:I:6:GLC:O2	1.90	0.69
1:A:594:ASN:H	1:A:597:HIS:CD2	2.10	0.69
1:D:212[A]:MET:CE	1:D:213:ARG:HH22	2.06	0.69
1:A:259:ASN:HD22	1:A:261:PHE:N	1.88	0.69
1:C:651:ILE:HD13	1:C:722:TRP:HB3	1.74	0.69
1:A:216:THR:O	1:A:217:ALA:C	2.31	0.69
1:B:130:ASP:OD1	1:B:139:ARG:NH1	2.18	0.69
1:D:232:GLU:H	1:D:232:GLU:CD	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.91	0.68
1:C:494:LYS:HD3	1:C:538:ARG:HG2	1.76	0.68
1:A:587:HIS:NE2	9:A:949:HOH:O	2.27	0.68
1:B:413:ARG:O	1:B:414:ASP:HB2	1.92	0.68
1:A:215:GLU:O	1:A:216:THR:HG23	1.93	0.68
1:B:594:ASN:H	1:B:597:HIS:HD2	1.42	0.68
1:D:212[A]:MET:CE	1:D:213:ARG:NH2	2.57	0.68
1:A:282:THR:OG1	1:A:283:HIS:HD2	1.76	0.68
1:B:371:ASN:N	1:B:372:THR:HB	2.07	0.68
1:D:628:TRP:HE1	4:N:1:BGC:H6C1	1.59	0.68
1:B:364:GLU:CB	9:B:1207:HOH:O	2.33	0.68
1:D:373:LEU:N	1:D:373:LEU:HD22	2.09	0.68
1:D:574:GLN:NE2	1:D:585:ASP:H	1.90	0.68
1:B:132:MET:HA	1:B:132:MET:CE	2.24	0.68
1:C:657:PHE:O	1:C:658:THR:CB	2.42	0.67
1:B:194:ASP:HB3	1:B:196:ASN:H	1.58	0.67
1:A:302:PRO:HG3	1:A:337:VAL:HG21	1.76	0.67
1:A:444:ARG:HA	9:A:1087:HOH:O	1.95	0.67
1:A:142:VAL:O	1:A:143:TRP:HB2	1.95	0.67
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.48	0.67
1:A:149:ARG:HA	1:A:175:TRP:CH2	2.30	0.66
1:A:343:THR:HG22	1:A:373:LEU:HD12	1.77	0.66
1:A:544:TRP:HB2	7:A:807:GOL:H2	1.78	0.66
1:A:642:VAL:HG13	1:A:650:GLU:HB2	1.76	0.66
1:D:237:ASN:HD22	1:D:283:HIS:HE1	1.40	0.66
1:A:214:PRO:CA	1:A:215:GLU:CB	2.60	0.66
1:A:650:GLU:OE2	1:A:670:ASN:HB2	1.96	0.66
1:B:423:ILE:N	9:B:1223:HOH:O	2.26	0.66
1:A:410:MET:HE1	1:A:439:LEU:HD21	1.78	0.66
1:B:189:LYS:NZ	1:B:216:THR:HG22	2.10	0.66
1:B:658:THR:CG2	1:B:660:VAL:H	2.07	0.66
1:D:117:THR:HG21	9:D:1077:HOH:O	1.94	0.66
1:B:376:ASN:ND2	9:B:1018:HOH:O	2.23	0.66
1:C:352:ASP:OD2	1:C:353:GLY:N	2.29	0.66
1:C:635:GLU:HB3	9:C:912:HOH:O	1.96	0.65
1:D:194:ASP:HB3	1:D:196:ASN:H	1.60	0.65
1:A:335:ASP:OD1	1:A:403:ARG:HD3	1.96	0.65
1:B:292:HIS:O	1:B:311:ARG:NH1	2.29	0.65
1:B:617:HIS:HE1	9:B:1086:HOH:O	1.78	0.65
1:C:470:GLN:HA	1:C:474:GLY:HA2	1.78	0.65
1:D:594:ASN:H	1:D:597:HIS:CD2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:ASP:OD2	1:B:687:HIS:CE1	2.49	0.65
1:C:279:MET:HB2	9:C:971:HOH:O	1.96	0.65
1:C:375:TYR:O	1:C:376:ASN:HB3	1.95	0.65
1:C:728:GLU:OE2	1:D:256:HIS:HD2	1.80	0.65
1:A:181:GLY:HA2	9:A:967:HOH:O	1.96	0.65
1:B:262:TRP:CH2	1:B:311:ARG:HG2	2.32	0.65
1:B:430:ARG:H	1:B:430:ARG:HD2	1.62	0.65
1:A:168:LEU:HD12	1:A:175:TRP:CZ2	2.31	0.65
1:A:503:HIS:HB3	1:A:506:LYS:HD2	1.79	0.65
1:B:189:LYS:CE	1:B:216:THR:HG22	2.26	0.65
1:C:708:GLN:O	1:C:709:HIS:HB2	1.97	0.65
1:B:533:LYS:O	1:B:538:ARG:NH2	2.30	0.64
1:D:593:ASP:OD2	1:D:687:HIS:CE1	2.50	0.64
1:B:593:ASP:OD2	1:B:687:HIS:HE1	1.80	0.64
1:D:693:ASN:ND2	1:D:714:THR:H	1.93	0.64
5:I:2:GLC:H61	5:I:3:GLC:H2	1.80	0.64
1:B:149:ARG:HD2	1:B:149:ARG:C	2.18	0.64
1:B:171:GLU:CG	9:B:1169:HOH:O	2.40	0.64
1:B:149:ARG:HD2	1:B:150:VAL:N	2.13	0.64
1:B:685[B]:HIS:CD2	9:B:1098:HOH:O	2.51	0.64
1:B:212:MET:O	1:B:213:ARG:CB	2.43	0.63
1:B:477:PHE:O	4:H:1:BGC:H6C2	1.98	0.63
1:A:684:MET:H	1:A:690:ASN:HD22	1.47	0.63
1:D:117:THR:N	9:D:1031:HOH:O	2.31	0.63
1:B:579:ASN:HD22	1:B:581:ASP:H	1.47	0.63
1:B:613:HIS:CE1	7:B:813:GOL:H32	2.33	0.63
1:B:644:ARG:CG	1:B:650:GLU:HG2	2.28	0.63
1:C:711:LEU:O	1:C:712:SER:HB3	1.99	0.62
1:D:616:MET:SD	1:D:651:ILE:HG12	2.39	0.62
1:A:628:TRP:NE1	3:G:1:GLC:C6	2.57	0.62
1:C:356:LEU:O	1:C:357:TYR:HB2	1.98	0.62
1:D:372:THR:CG2	1:D:372:THR:O	2.47	0.62
1:B:153:VAL:HA	1:B:157:ASN:HD22	1.65	0.62
1:C:611:ARG:O	1:C:612:HIS:CB	2.46	0.62
1:D:558:TRP:HA	1:D:564:LYS:HE3	1.80	0.62
1:B:587:HIS:O	1:B:590:GLU:HG2	2.00	0.62
1:A:148:ARG:HB3	1:A:193:ILE:O	1.99	0.62
1:A:352:ASP:OD2	1:A:354:THR:CG2	2.31	0.62
1:B:371:ASN:N	1:B:372:THR:O	2.33	0.62
1:D:728:GLU:HG2	9:D:1050:HOH:O	2.00	0.62
1:A:256:HIS:HB2	1:A:259:ASN:HD21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:THR:OG1	1:B:283:HIS:HD2	1.84	0.61
1:A:152:VAL:O	1:A:157:ASN:ND2	2.34	0.61
1:B:371:ASN:N	1:B:372:THR:CB	2.63	0.61
1:A:413:ARG:HD3	1:A:430:ARG:HH12	1.64	0.61
1:D:680:ASN:C	1:D:680:ASN:HD22	2.04	0.61
1:A:337:VAL:HG23	1:A:337:VAL:O	2.01	0.61
1:D:601:ARG:HD2	1:D:685[A]:HIS:NE2	2.16	0.60
1:D:642:VAL:HG22	1:D:650:GLU:HB3	1.82	0.60
1:A:214:PRO:CB	1:A:215:GLU:HB3	2.31	0.60
1:B:259:ASN:HB2	1:B:261:PHE:CE2	2.37	0.60
1:B:247:GLU:OE1	1:B:525:HIS:HD2	1.84	0.60
1:C:728:GLU:O	6:L:4:GLC:O4	2.19	0.60
7:B:815:GOL:C1	9:B:1035:HOH:O	2.46	0.60
1:A:216:THR:O	1:A:217:ALA:O	2.20	0.60
1:D:359:HIS:HD2	1:D:376:ASN:HA	1.67	0.60
1:A:151:SER:CB	1:A:164:HIS:O	2.48	0.60
1:A:209:GLU:HG2	1:A:219:LEU:HD23	1.84	0.60
1:B:680:ASN:HD22	1:B:680:ASN:C	2.04	0.60
1:C:131:THR:OG1	1:C:136:THR:HG22	2.02	0.60
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.85	0.60
1:B:362:PRO:HA	1:B:363:ARG:HB2	1.83	0.60
1:C:551:ARG:HB3	1:C:681:THR:CG2	2.30	0.60
1:B:551:ARG:NH2	9:B:986:HOH:O	2.35	0.59
1:C:593:ASP:OD2	1:C:687:HIS:HE1	1.84	0.59
1:C:489:THR:HG22	1:C:507:LEU:HD12	1.84	0.59
1:A:233:ARG:HG2	1:A:331:ASN:HD21	1.68	0.59
1:A:168:LEU:C	1:A:168:LEU:HD23	2.23	0.59
1:D:684:MET:H	1:D:690:ASN:ND2	2.00	0.59
1:B:504:HIS:HD2	9:B:908:HOH:O	1.86	0.59
1:C:574:GLN:NE2	1:C:585:ASP:H	2.01	0.59
1:D:679:LEU:HG	1:D:680:ASN:N	2.17	0.59
1:B:189:LYS:HE2	1:B:216:THR:HG22	1.82	0.59
1:B:658:THR:HG23	1:B:659:PRO:HD2	1.85	0.59
1:C:665:TYR:O	1:C:712:SER:HA	2.02	0.59
1:A:137:GLY:HA2	9:A:1089:HOH:O	2.01	0.59
5:I:3:GLC:H62	5:I:4:GLC:O2	2.03	0.59
1:A:551:ARG:NH1	7:A:807:GOL:H11	2.15	0.59
1:B:512:LEU:HD22	4:J:2:GLC:H62	1.84	0.59
1:C:157:ASN:C	1:C:157:ASN:HD22	2.06	0.59
7:B:812:GOL:H31	9:B:942:HOH:O	2.03	0.58
1:C:635:GLU:HG3	1:C:636:ARG:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ASN:ND2	1:B:429:GLY:H	2.01	0.58
1:B:138:THR:CG2	1:B:182:ALA:O	2.51	0.58
1:D:512:LEU:HD21	4:N:1:BGC:H5	1.84	0.58
1:D:212[A]:MET:HE2	1:D:213:ARG:CZ	2.29	0.58
1:B:683:SER:CB	7:B:815:GOL:H2	2.29	0.58
1:C:202:LYS:HD2	1:C:351:PHE:CD1	2.39	0.58
1:A:680:ASN:C	1:A:680:ASN:HD22	2.07	0.58
1:C:604:ARG:NH2	9:C:910:HOH:O	2.37	0.58
1:B:574:GLN:NE2	1:B:585:ASP:H	2.02	0.58
1:B:613:HIS:NE2	7:B:813:GOL:C3	2.64	0.58
1:B:693:ASN:ND2	1:B:714:THR:H	1.96	0.58
1:C:513:TYR:HB2	9:C:939:HOH:O	2.03	0.58
1:A:132:MET:HB2	1:A:178:PHE:CE1	2.39	0.57
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.87	0.57
1:A:129:ALA:HA	1:A:138:THR:HG22	1.86	0.57
1:D:504:HIS:HD2	9:D:960:HOH:O	1.87	0.57
1:A:147:ALA:O	1:A:148:ARG:HB2	2.04	0.57
1:B:651:ILE:CD1	1:B:722:TRP:HB3	2.34	0.57
1:A:233:ARG:HD3	1:A:326:HIS:CD2	2.39	0.57
1:A:144:ALA:HB1	1:A:352:ASP:CB	2.32	0.57
1:D:212[A]:MET:HG3	1:D:213:ARG:HB2	1.85	0.57
1:D:508:THR:O	4:N:1:BGC:O6	2.20	0.57
1:A:635[A]:GLU:N	1:A:635[A]:GLU:OE2	2.32	0.57
1:A:150:VAL:HG13	1:A:192:MET:HB3	1.87	0.57
1:B:138:THR:HG23	1:B:182:ALA:HB3	1.87	0.57
1:C:694:GLY:O	1:D:591:GLY:HA2	2.05	0.57
1:A:590[A]:GLU:OE1	1:B:695:GLY:O	2.23	0.57
1:A:636:ARG:HG2	1:A:662:ARG:CZ	2.35	0.56
1:D:468:ARG:O	1:D:474:GLY:HA3	2.05	0.56
1:C:295:ASP:OD2	1:C:311:ARG:NH2	2.38	0.56
1:A:558:TRP:HA	1:A:564:LYS:HE3	1.88	0.56
1:B:685[B]:HIS:HD2	9:B:1098:HOH:O	1.88	0.56
1:D:132:MET:SD	1:D:139:ARG:NH1	2.79	0.56
1:B:194:ASP:HB2	1:B:198:ASN:H	1.69	0.56
1:C:525:HIS:HB3	1:C:567:PHE:CE1	2.41	0.56
7:D:808:GOL:H11	9:D:933:HOH:O	2.05	0.56
1:A:693:ASN:ND2	1:A:714:THR:H	1.99	0.56
1:B:134:GLY:N	9:B:1060:HOH:O	2.37	0.56
1:A:211:GLN:NE2	1:A:215:GLU:H	2.02	0.56
1:C:150:VAL:HG22	1:C:192:MET:HG3	1.87	0.56
1:A:237:ASN:ND2	1:A:283:HIS:HE1	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:608:LEU:O	1:C:611:ARG:O	2.24	0.56
1:A:436:ILE:O	1:A:440:ARG:HG3	2.06	0.56
1:A:679:LEU:HG	1:A:680:ASN:N	2.20	0.56
1:D:680:ASN:ND2	1:D:682:ASP:H	2.04	0.55
1:C:289:ILE:HG13	1:C:334:LEU:CD1	2.35	0.55
1:D:451:SER:HB3	9:D:1092:HOH:O	2.05	0.55
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.41	0.55
1:D:642:VAL:CG2	1:D:650:GLU:HB3	2.35	0.55
1:A:709:HIS:CD2	9:A:990:HOH:O	2.42	0.55
1:C:132:MET:O	1:C:133:ASP:HB2	2.05	0.55
1:B:373:LEU:HA	9:B:1164:HOH:O	2.06	0.55
1:D:399:ILE:HD11	1:D:402:LEU:HD21	1.89	0.55
1:C:700:ASP:O	1:C:709:HIS:HA	2.07	0.55
1:B:380:ARG:HD3	1:B:384:ASN:HD21	1.71	0.55
1:C:606:LEU:HD23	1:C:679:LEU:CD1	2.32	0.55
1:C:610:TYR:O	1:C:617:HIS:HD2	1.90	0.55
1:C:149:ARG:NH1	1:C:151:SER:HB2	2.22	0.55
1:C:336:TRP:CZ3	1:C:338:PRO:HG3	2.41	0.55
1:A:468:ARG:CZ	2:F:2:GLC:H61	2.37	0.54
1:A:574:GLN:NE2	1:A:585:ASP:H	2.05	0.54
1:C:480:LYS:HD3	1:C:481:TRP:O	2.07	0.54
1:A:704:SER:OG	1:A:705:HIS:CD2	2.60	0.54
1:C:351:PHE:O	1:C:352:ASP:CB	2.55	0.54
7:B:812:GOL:C3	9:B:942:HOH:O	2.55	0.54
1:C:494:LYS:CD	1:C:538:ARG:HG2	2.35	0.54
1:A:428:GLY:HA2	9:A:1040:HOH:O	2.08	0.54
1:A:504:HIS:HD2	9:A:989:HOH:O	1.89	0.54
1:A:505:ASP:HB3	9:A:1051:HOH:O	2.06	0.54
1:C:213:ARG:HB2	1:C:214:PRO:CD	2.37	0.54
1:A:171:GLU:CD	1:A:171:GLU:H	2.10	0.54
1:B:579:ASN:ND2	1:B:581:ASP:H	2.04	0.54
1:C:342:PRO:O	1:C:344:ASP:N	2.32	0.54
1:D:685[A]:HIS:CE1	9:D:1036:HOH:O	2.60	0.54
1:A:143:TRP:CH2	1:A:356:LEU:HD22	2.42	0.54
1:B:425:ASN:HD22	1:B:427:PHE:H	1.56	0.54
1:B:680:ASN:HB3	7:B:815:GOL:O2	2.07	0.54
1:C:379:ARG:HB3	1:C:382:VAL:HG23	1.89	0.54
1:D:148:ARG:NH1	1:D:195:ALA:O	2.41	0.54
1:C:273:VAL:HB	1:C:274:PRO:HD3	1.90	0.53
1:C:536:LEU:HD22	1:C:573:ALA:HB1	1.90	0.53
1:A:142:VAL:O	1:A:143:TRP:CB	2.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ASN:H	1:B:597:HIS:CD2	2.26	0.53
1:A:157:ASN:O	1:A:158:TYR:HB2	2.07	0.53
1:C:379:ARG:NH2	9:C:921:HOH:O	2.41	0.53
1:A:643:ARG:NH2	9:A:994:HOH:O	2.40	0.53
1:B:363:ARG:HD3	1:B:364:GLU:N	2.16	0.53
1:D:594:ASN:N	1:D:597:HIS:HD2	2.01	0.53
1:A:674:LYS:HD2	1:A:696:THR:HG21	1.91	0.53
1:D:680:ASN:HD22	1:D:682:ASP:H	1.55	0.53
1:D:684:MET:H	1:D:690:ASN:HD22	1.54	0.53
1:B:442:THR:HG22	1:B:446:LEU:HD22	1.90	0.53
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.57	0.52
1:C:496:ASP:C	1:C:498:VAL:H	2.12	0.52
1:C:281:PHE:CD2	9:C:971:HOH:O	2.40	0.52
1:D:118:HIS:CD2	1:D:119:LEU:HD13	2.44	0.52
1:D:157:ASN:OD1	1:D:164:HIS:HD2	1.93	0.52
1:A:428:GLY:HA2	9:A:981:HOH:O	2.08	0.52
1:B:237:ASN:ND2	1:B:283:HIS:HE1	2.06	0.52
1:B:512:LEU:HD22	4:J:2:GLC:C6	2.39	0.52
1:D:216:THR:HG22	1:D:217:ALA:N	2.24	0.52
1:A:147:ALA:O	1:A:148:ARG:HB3	2.10	0.52
1:C:633:ASP:OD2	1:C:665:TYR:OH	2.19	0.52
1:A:459:GLU:OE1	1:A:461:THR:O	2.26	0.52
1:A:587:HIS:HA	1:A:590[B]:GLU:HG3	1.90	0.52
1:A:277:LYS:NZ	9:A:1112:HOH:O	2.43	0.52
1:A:410:MET:HE3	1:A:439:LEU:HD11	1.90	0.52
1:B:343:THR:HG22	1:B:373:LEU:HD21	1.92	0.52
1:C:247:GLU:OE1	1:C:525:HIS:CD2	2.63	0.52
1:C:529:VAL:O	1:C:532:LYS:HB2	2.10	0.52
1:C:143:TRP:CH2	1:C:356:LEU:HD21	2.45	0.52
1:C:407:VAL:HG21	1:C:457:ALA:HB1	1.92	0.52
1:C:486:MET:O	1:C:490:LEU:HB2	2.10	0.52
1:A:490:LEU:O	1:A:494:LYS:HG3	2.10	0.52
1:B:362:PRO:HA	1:B:363:ARG:CB	2.38	0.52
1:A:391:LEU:O	1:A:395:GLU:HB2	2.09	0.51
1:A:667:PHE:HA	1:A:705:HIS:CD2	2.45	0.51
1:A:552:ALA:O	1:A:720:THR:CG2	2.58	0.51
1:A:358:GLU:H	1:A:358:GLU:CD	2.03	0.51
1:D:335:ASP:OD1	1:D:403:ARG:HD3	2.10	0.51
1:C:256:HIS:HE1	1:C:267:GLU:OE1	1.93	0.51
1:A:666:ARG:HA	1:A:711:LEU:O	2.09	0.51
1:A:169:ARG:NH1	1:A:169:ARG:HB2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:NH1	2:F:2:GLC:H61	2.25	0.51
1:B:651:ILE:HD11	1:B:722:TRP:HB3	1.92	0.51
1:C:359:HIS:CB	1:C:376:ASN:HB2	2.36	0.51
1:A:602:LEU:HG	1:A:606:LEU:HD22	1.92	0.51
1:D:393:TRP:HB3	1:D:399:ILE:HG12	1.93	0.51
1:C:658:THR:HG22	1:C:660:VAL:H	1.76	0.51
1:A:707:ARG:NH1	9:A:1065:HOH:O	2.42	0.50
1:B:118:HIS:CB	9:B:1180:HOH:O	2.24	0.50
1:C:237:ASN:HD21	1:C:283:HIS:HE1	1.56	0.50
1:C:550:LEU:CD2	1:C:573:ALA:HB2	2.41	0.50
1:D:350:GLU:HA	1:D:354:THR:O	2.10	0.50
1:D:488:ASP:OD2	9:D:1015:HOH:O	2.19	0.50
1:D:728:GLU:CG	9:D:1050:HOH:O	2.58	0.50
1:A:209:GLU:HB3	1:A:221:CYS:SG	2.51	0.50
1:B:233:ARG:NH1	1:B:400:ASP:OD2	2.42	0.50
1:C:611:ARG:O	1:C:612:HIS:HB3	2.10	0.50
1:A:509:PHE:HA	3:G:2:GLC:H62	1.93	0.50
1:B:709:HIS:HD2	9:B:1000:HOH:O	1.94	0.50
1:C:474:GLY:O	1:C:475:LEU:HB2	2.12	0.50
1:C:685[A]:HIS:CE1	1:D:685[A]:HIS:HD2	2.29	0.50
1:A:684:MET:H	1:A:690:ASN:ND2	2.08	0.50
1:B:260:ASN:HA	9:B:1065:HOH:O	2.10	0.50
1:B:117:THR:HB	9:B:1069:HOH:O	2.10	0.50
1:B:477:PHE:O	4:H:1:BGC:C6	2.60	0.50
1:B:362:PRO:HB2	1:B:363:ARG:HB2	1.93	0.50
1:C:298:TRP:HE1	1:C:580:HIS:CD2	2.30	0.50
1:A:149:ARG:HA	1:A:175:TRP:CZ3	2.46	0.50
1:C:525:HIS:HB3	1:C:567:PHE:CD1	2.47	0.50
1:D:216:THR:CG2	1:D:217:ALA:N	2.74	0.50
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.95	0.50
1:A:233:ARG:HG2	1:A:331:ASN:ND2	2.26	0.50
1:B:157:ASN:OD1	1:B:164:HIS:HD2	1.95	0.50
1:B:494:LYS:CD	1:B:538:ARG:HG2	2.39	0.50
1:B:579:ASN:C	1:B:579:ASN:HD22	2.16	0.50
1:C:297:SER:C	1:C:299:GLY:H	2.15	0.50
1:C:437:GLU:HA	1:C:437:GLU:OE2	2.11	0.50
1:C:616:MET:SD	1:C:651:ILE:HG12	2.51	0.50
1:D:679:LEU:HG	1:D:680:ASN:H	1.76	0.49
1:A:704:SER:OG	1:A:705:HIS:HD2	1.95	0.49
1:B:189:LYS:HZ1	1:B:216:THR:HG22	1.77	0.49
1:C:403:ARG:NE	1:C:481:TRP:CZ2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:ILE:HB	1:D:723:LEU:HB2	1.94	0.49
1:B:117:THR:N	9:B:1057:HOH:O	2.45	0.49
1:B:523:LEU:HD22	1:B:557:MET:SD	2.53	0.49
1:C:558:TRP:HA	1:C:564:LYS:HE3	1.94	0.49
1:C:642:VAL:CG1	1:C:650:GLU:HB2	2.38	0.49
1:D:266:ARG:NH1	9:D:1017:HOH:O	2.36	0.49
1:D:242:PRO:HB3	1:D:617:HIS:CD2	2.47	0.49
1:A:684:MET:HG3	1:A:685[A]:HIS:N	2.24	0.49
1:D:221:CYS:HB2	9:D:1052:HOH:O	2.12	0.49
1:D:399:ILE:HD11	1:D:402:LEU:CD2	2.42	0.49
1:A:157:ASN:OD1	1:A:164:HIS:CD2	2.65	0.49
1:A:254[B]:ARG:HD3	1:A:263:LEU:HD11	1.94	0.49
1:A:194:ASP:OD2	1:A:198:ASN:N	2.37	0.49
1:C:159:TRP:HZ3	1:C:189:LYS:HB2	1.77	0.49
1:C:551:ARG:NH1	1:C:681:THR:O	2.46	0.49
1:C:680:ASN:HD22	1:C:680:ASN:C	2.15	0.49
1:A:148:ARG:O	1:A:149:ARG:CG	2.50	0.49
1:C:672:PRO:HB3	1:C:709:HIS:CD2	2.47	0.49
1:D:120:ARG:HG2	1:D:122:TYR:OH	2.12	0.49
1:A:684:MET:HG3	1:A:685[B]:HIS:N	2.25	0.49
1:B:132:MET:HA	1:B:132:MET:HE2	1.92	0.49
1:B:143:TRP:CZ3	1:B:356:LEU:HD22	2.48	0.49
1:C:444:ARG:NH2	1:C:445:ILE:HG13	2.27	0.49
1:D:156:PHE:CD2	1:D:157:ASN:HB2	2.48	0.49
1:A:165:PRO:O	1:A:177:LEU:HD22	2.13	0.49
1:B:512:LEU:CD1	4:J:1:BGC:C6	2.81	0.49
1:A:334:LEU:HD12	1:A:335:ASP:N	2.28	0.48
1:D:213:ARG:N	1:D:214:PRO:CD	2.57	0.48
1:B:679:LEU:HG	1:B:680:ASN:N	2.27	0.48
1:C:550:LEU:HD21	1:C:573:ALA:HB2	1.93	0.48
1:D:212[B]:MET:HG2	1:D:212[B]:MET:O	2.13	0.48
1:A:382:VAL:O	1:A:385:PHE:HB3	2.13	0.48
1:B:373:LEU:CD2	9:B:1031:HOH:O	2.61	0.48
1:B:551:ARG:HG2	1:B:602:LEU:HD23	1.95	0.48
1:C:658:THR:H	1:C:718:LEU:CD2	2.21	0.48
1:C:681:THR:CG2	9:C:916:HOH:O	2.28	0.48
1:A:302:PRO:HG3	1:A:337:VAL:CG2	2.41	0.48
1:A:494:LYS:HD3	1:A:538:ARG:HG2	1.94	0.48
1:C:643:ARG:O	1:C:650:GLU:HA	2.14	0.48
1:D:565:LEU:C	1:D:565:LEU:HD23	2.34	0.48
1:A:561:PRO:HA	1:A:643:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:THR:O	9:B:1146:HOH:O	2.20	0.48
1:C:213:ARG:HB2	1:C:214:PRO:HD3	1.93	0.48
1:D:655:SER:OG	1:D:720:THR:HB	2.14	0.48
1:B:371:ASN:HB3	1:B:372:THR:CB	2.34	0.48
1:A:245:ILE:CG2	1:A:285:GLU:HB2	2.44	0.48
1:A:120:ARG:NH2	1:A:449:GLN:OE1	2.47	0.48
1:D:317:ASP:O	1:D:320:TYR:HB3	2.13	0.48
1:D:693:ASN:O	1:D:694:GLY:O	2.31	0.48
1:B:183:HIS:HD2	1:B:184:ASN:O	1.97	0.47
1:C:571:GLU:O	1:C:600:GLN:HA	2.14	0.47
1:D:535:ILE:HA	1:D:538:ARG:HD2	1.96	0.47
1:A:142:VAL:HG22	1:A:190:TYR:CZ	2.48	0.47
1:D:261:PHE:HA	7:D:809:GOL:O2	2.14	0.47
1:A:413:ARG:HH11	1:A:430:ARG:HH12	1.60	0.47
1:B:403:ARG:NH2	9:B:1085:HOH:O	2.46	0.47
1:C:156:PHE:HB3	1:C:186:GLN:NE2	2.29	0.47
1:D:635[B]:GLU:H	1:D:635[B]:GLU:CD	2.17	0.47
1:A:132:MET:CE	1:A:132:MET:CA	2.91	0.47
1:A:169:ARG:HG3	1:A:171:GLU:OE2	2.14	0.47
1:B:467:SER:HA	1:B:477:PHE:O	2.14	0.47
1:B:658:THR:HG22	1:B:660:VAL:N	2.15	0.47
1:D:655:SER:HB3	1:D:657:PHE:CE1	2.50	0.47
1:A:230:THR:O	1:A:234:LYS:HG3	2.14	0.47
1:B:503:HIS:HB3	1:B:506:LYS:HD2	1.96	0.47
1:A:168:LEU:HD12	1:A:175:TRP:CE2	2.49	0.47
1:B:559:ALA:HB1	1:B:653:VAL:HG21	1.97	0.47
1:C:528:VAL:O	1:C:577:GLU:HB2	2.15	0.47
1:D:591:GLY:O	1:D:592:GLY:O	2.32	0.47
1:D:693:ASN:HD21	1:D:714:THR:N	1.98	0.47
1:A:494:LYS:CD	1:A:538:ARG:HG2	2.45	0.47
1:B:200:ARG:HA	9:B:1208:HOH:O	2.13	0.47
1:B:617:HIS:CE1	9:B:1086:HOH:O	2.61	0.47
1:C:552:ALA:HA	1:C:720:THR:HG22	1.96	0.47
1:D:232:GLU:N	1:D:232:GLU:CD	2.67	0.47
1:B:341:PHE:CZ	1:B:358:GLU:HB3	2.49	0.47
1:B:570:ASN:ND2	9:B:1014:HOH:O	2.48	0.47
1:B:658:THR:HG23	1:B:659:PRO:CD	2.44	0.47
1:D:189:LYS:CE	1:D:216:THR:HG22	2.45	0.47
1:A:157:ASN:OD1	1:A:164:HIS:HD2	1.98	0.47
1:A:153:VAL:HA	1:A:157:ASN:HD22	1.80	0.46
1:B:117:THR:CB	9:B:1069:HOH:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:HIS:HE1	1:B:267:GLU:OE2	1.98	0.46
1:B:285:GLU:OE1	1:B:403:ARG:HD2	2.14	0.46
1:C:666:ARG:HA	1:C:712:SER:HA	1.96	0.46
1:D:297:SER:C	1:D:299:GLY:H	2.17	0.46
1:D:532:LYS:O	1:D:533:LYS:HB2	2.15	0.46
1:A:475:LEU:HD12	1:A:475:LEU:N	2.30	0.46
1:A:644:ARG:CD	9:A:1107:HOH:O	2.62	0.46
1:B:680:ASN:HD22	1:B:682:ASP:H	1.62	0.46
1:B:680:ASN:ND2	1:B:682:ASP:H	2.13	0.46
1:D:593:ASP:HA	1:D:597:HIS:CD2	2.50	0.46
1:A:580:HIS:HD2	9:A:980:HOH:O	1.98	0.46
1:B:693:ASN:HD21	1:B:714:THR:N	2.02	0.46
1:C:680:ASN:HA	1:C:721:ILE:HG22	1.96	0.46
1:A:231:GLU:HG3	9:A:1029:HOH:O	2.15	0.46
1:A:580:HIS:CD2	9:A:980:HOH:O	2.67	0.46
1:D:525:HIS:HB3	1:D:567:PHE:CE1	2.51	0.46
1:C:152:VAL:HG12	1:C:156:PHE:HZ	1.81	0.46
1:A:258:ASP:HB3	9:A:1111:HOH:O	2.14	0.46
1:A:233:ARG:HD2	1:A:400:ASP:OD2	2.14	0.46
1:D:149:ARG:CG	1:D:149:ARG:NH1	2.65	0.46
1:A:133:ASP:N	1:A:133:ASP:OD2	2.48	0.46
1:A:428:GLY:CA	9:A:981:HOH:O	2.61	0.46
1:C:211:GLN:HB3	1:C:215:GLU:HB2	1.98	0.46
1:C:587:HIS:HA	1:C:590:GLU:HG2	1.97	0.46
1:A:570:ASN:ND2	9:A:906:HOH:O	2.48	0.46
1:B:684:MET:H	1:B:690:ASN:ND2	2.14	0.46
1:A:441:ASN:OD1	1:A:444:ARG:NH1	2.49	0.46
1:A:577:GLU:CD	9:A:1086:HOH:O	2.54	0.46
1:B:380:ARG:HD3	1:B:384:ASN:ND2	2.30	0.46
1:C:494:LYS:CG	1:C:538:ARG:HG2	2.46	0.46
1:B:238:GLN:HG2	9:B:1186:HOH:O	2.15	0.46
1:C:202:LYS:HD2	1:C:351:PHE:HD1	1.80	0.46
1:C:636:ARG:HG2	1:C:662:ARG:CZ	2.46	0.46
1:B:675:TRP:O	1:B:696:THR:HA	2.15	0.45
1:D:579:ASN:ND2	1:D:581:ASP:H	2.14	0.45
1:B:289:ILE:HD12	1:B:289:ILE:C	2.36	0.45
1:D:141:SER:HA	1:D:175:TRP:O	2.16	0.45
1:B:213:ARG:NH1	1:B:295:ASP:OD2	2.49	0.45
1:C:285:GLU:HA	1:C:333:ILE:O	2.15	0.45
1:C:341:PHE:CG	1:C:342:PRO:HD2	2.51	0.45
1:C:489:THR:O	1:C:493:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:TRP:CD1	2:M:1:GLC:H61	2.51	0.45
1:B:168:LEU:HG	1:B:175:TRP:CE2	2.52	0.45
1:B:256:HIS:CE1	1:B:267:GLU:OE2	2.70	0.45
1:B:373:LEU:CD2	1:B:373:LEU:H	2.29	0.45
1:C:686:TYR:O	1:C:687:HIS:HB2	2.17	0.45
1:D:259:ASN:HB3	1:D:261:PHE:H	1.80	0.45
1:A:449:GLN:O	9:A:1105:HOH:O	2.21	0.45
1:B:163:ARG:CD	9:B:1084:HOH:O	2.53	0.45
1:A:178:PHE:O	1:A:178:PHE:CD1	2.70	0.45
1:A:270:ASP:O	1:A:274:PRO:HG2	2.16	0.45
1:A:658:THR:HB	1:A:659:PRO:HD2	1.98	0.45
1:D:552:ALA:O	1:D:720:THR:CG2	2.65	0.45
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.40	0.45
1:A:285:GLU:HG3	1:A:333:ILE:CG2	2.47	0.45
1:B:425:ASN:HD21	1:B:429:GLY:H	1.65	0.45
1:D:627:GLU:HB3	1:D:642:VAL:HG12	1.98	0.45
1:A:247:GLU:OE1	1:A:525:HIS:CD2	2.68	0.45
1:C:707:ARG:NH1	9:C:919:HOH:O	2.50	0.45
1:A:517:GLU:HB2	1:A:519:PHE:CZ	2.51	0.45
1:B:412:TYR:CD2	1:B:430:ARG:HG2	2.52	0.45
1:A:186:GLN:O	1:A:220:ILE:HG13	2.17	0.45
1:C:259:ASN:O	1:C:260:ASN:HB3	2.17	0.45
1:B:149:ARG:CG	1:B:149:ARG:NH2	2.62	0.44
1:C:450:VAL:HG23	1:C:450:VAL:O	2.16	0.44
1:C:559:ALA:HB1	1:C:653:VAL:HG21	1.98	0.44
1:B:463:PHE:CE2	1:B:475:LEU:HD13	2.52	0.44
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.97	0.44
1:C:375:TYR:O	1:C:376:ASN:CB	2.64	0.44
1:C:564:LYS:HD2	1:C:564:LYS:N	2.32	0.44
1:D:212[A]:MET:HB2	1:D:310:ARG:HG2	1.99	0.44
5:I:2:GLC:H4	5:I:3:GLC:H2	1.66	0.44
1:A:168:LEU:HD23	1:A:169:ARG:C	2.38	0.44
1:A:237:ASN:HD22	1:A:283:HIS:HE1	1.66	0.44
1:C:636:ARG:HG2	1:C:662:ARG:NH2	2.33	0.44
1:C:658:THR:HA	1:C:659:PRO:HD3	1.77	0.44
1:A:512:LEU:CD1	3:G:1:GLC:H5	2.47	0.44
1:A:125:LEU:HA	1:A:141:SER:HB2	1.98	0.44
1:A:412:TYR:O	9:A:992:HOH:O	2.21	0.44
1:B:319:ARG:NH1	9:B:971:HOH:O	2.50	0.44
1:C:126:GLY:HA2	1:C:204:ASP:OD2	2.17	0.44
1:C:318:PHE:O	1:C:322:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:HIS:CD2	1:C:525:HIS:H	2.36	0.44
1:A:467:SER:HA	1:A:477:PHE:O	2.17	0.44
1:A:644:ARG:HD2	9:A:1107:HOH:O	2.17	0.44
1:A:643:ARG:O	1:A:650:GLU:HA	2.17	0.44
1:B:458:GLU:HG3	9:B:1085:HOH:O	2.18	0.44
1:C:639:LEU:HD13	1:C:657:PHE:HE1	1.81	0.44
7:A:807:GOL:H32	9:A:1078:HOH:O	2.17	0.44
1:B:259:ASN:ND2	1:B:259:ASN:H	2.15	0.44
1:B:619:LEU:HA	9:B:1012:HOH:O	2.17	0.44
1:D:148:ARG:O	1:D:149:ARG:CB	2.56	0.44
1:A:444:ARG:O	1:A:448:GLU:HG3	2.18	0.44
1:A:650:GLU:HG2	1:A:671:GLN:OE1	2.18	0.44
1:B:694:GLY:CA	9:B:1054:HOH:O	2.54	0.44
1:D:341:PHE:CZ	1:D:358:GLU:HB3	2.53	0.44
1:D:136:THR:HG22	1:D:137:GLY:N	2.33	0.43
1:C:375:TYR:HB2	1:C:377:TYR:CZ	2.53	0.43
1:C:594:ASN:H	1:C:597:HIS:HD2	1.66	0.43
1:D:227:VAL:HG11	1:D:398:GLY:HA3	2.00	0.43
1:B:371:ASN:N	1:B:372:THR:CA	2.81	0.43
1:A:211:GLN:HE21	1:A:216:THR:H	1.66	0.43
1:B:259:ASN:HB2	1:B:261:PHE:CD2	2.53	0.43
1:D:496:ASP:OD1	1:D:498:VAL:HG22	2.19	0.43
1:B:509:PHE:HA	4:J:2:GLC:H62	1.99	0.43
1:A:292:HIS:CG	1:A:299:GLY:HA2	2.54	0.43
1:A:492:TYR:CZ	1:A:507:LEU:HD22	2.52	0.43
1:A:563:LYS:C	1:A:564:LYS:HD3	2.39	0.43
1:D:258:ASP:O	1:D:259:ASN:HB2	2.17	0.43
1:A:644:ARG:NH2	1:A:650:GLU:OE1	2.51	0.43
1:B:230:THR:O	1:B:234:LYS:HG3	2.19	0.43
1:D:527:GLU:O	1:D:538:ARG:NH2	2.51	0.43
1:D:597:HIS:HB3	1:D:601:ARG:NH1	2.33	0.43
1:A:254[B]:ARG:HE	2:E:2:GLC:C6	2.31	0.43
1:A:485:TRP:CE2	1:A:489:THR:HG21	2.54	0.43
1:B:179:ILE:HA	1:B:180:PRO:HD2	1.92	0.43
1:B:507:LEU:HA	1:B:507:LEU:HD12	1.77	0.43
1:D:389:ASN:O	1:D:392:TYR:HB3	2.19	0.43
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.78	0.43
1:B:152:VAL:O	1:B:157:ASN:ND2	2.51	0.43
1:B:359:HIS:HE1	1:B:361:ASP:OD1	2.01	0.43
1:B:542:ASP:O	1:B:546:LYS:HG3	2.19	0.43
1:C:684:MET:HB2	1:C:690:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:MET:H	1:C:690:ASN:ND2	2.05	0.43
1:D:597:HIS:HB3	1:D:601:ARG:HH12	1.84	0.43
1:A:259:ASN:ND2	1:A:261:PHE:HB2	2.34	0.43
1:A:262:TRP:CH2	1:A:311:ARG:CG	3.01	0.43
1:A:144:ALA:CB	1:A:352:ASP:HB3	2.43	0.43
1:C:144:ALA:HB1	1:C:352:ASP:HB2	2.01	0.43
1:D:532:LYS:O	1:D:533:LYS:CB	2.67	0.43
1:D:298:TRP:HE1	1:D:580:HIS:CD2	2.36	0.43
1:D:511:ILE:HB	4:N:1:BGC:H6C1	2.00	0.43
1:A:686:TYR:O	1:A:687:HIS:HB2	2.17	0.42
1:D:336:TRP:HZ2	1:D:386:LEU:O	2.02	0.42
1:D:721:ILE:HD12	1:D:723:LEU:HD21	2.00	0.42
1:B:670:ASN:HB3	9:B:1063:HOH:O	2.19	0.42
1:D:542:ASP:OD1	1:D:545:GLN:HG3	2.19	0.42
1:A:184:ASN:HA	1:A:220:ILE:O	2.19	0.42
1:A:376:ASN:C	1:A:376:ASN:HD22	2.22	0.42
1:A:340:HIS:CE1	1:A:405:ASP:OD2	2.53	0.42
1:A:705:HIS:HE1	9:A:985:HOH:O	2.02	0.42
1:B:575:GLY:HA3	5:I:2:GLC:H5	2.02	0.42
1:A:157:ASN:HB3	1:A:160:ASP:H	1.84	0.42
1:C:437:GLU:O	1:C:441:ASN:HB2	2.20	0.42
1:D:285:GLU:OE1	1:D:403:ARG:HD2	2.19	0.42
1:D:666:ARG:HA	1:D:711:LEU:O	2.19	0.42
1:B:373:LEU:HD22	9:B:1031:HOH:O	2.20	0.42
1:D:344:ASP:O	1:D:346:PHE:N	2.53	0.42
1:B:258:ASP:HB2	9:B:1070:HOH:O	2.19	0.42
1:B:317:ASP:O	1:B:320:TYR:HB3	2.19	0.42
1:B:363:ARG:CD	1:B:364:GLU:H	2.22	0.42
1:D:343:THR:HG22	1:D:373:LEU:HD21	2.02	0.42
1:A:169:ARG:CZ	1:A:169:ARG:HB2	2.49	0.42
1:A:254[B]:ARG:HE	2:E:2:GLC:H62	1.85	0.42
1:B:463:PHE:HE2	1:B:475:LEU:HD13	1.85	0.42
1:C:341:PHE:CD2	1:C:342:PRO:HD2	2.55	0.42
1:D:183:HIS:HD2	1:D:184:ASN:O	2.02	0.42
1:D:341:PHE:O	1:D:343:THR:HG23	2.20	0.42
1:D:718:LEU:HD23	1:D:718:LEU:HA	1.83	0.42
1:D:651:ILE:HD13	1:D:722:TRP:HB3	2.01	0.42
1:B:690:ASN:ND2	7:B:815:GOL:O3	2.45	0.41
1:D:215:GLU:O	1:D:216:THR:HB	2.20	0.41
1:B:380:ARG:HE	1:B:380:ARG:HB2	1.71	0.41
1:A:625:GLY:O	1:A:643:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ASN:ND2	1:C:656:ASN:C	2.73	0.41
1:B:273:VAL:HB	1:B:274:PRO:HD3	2.01	0.41
1:B:642:VAL:HG13	1:B:650:GLU:HB3	2.02	0.41
1:B:518:ASN:ND2	4:H:2:GLC:H62	2.25	0.41
1:A:568:MET:HG3	1:A:584:LEU:HD11	2.03	0.41
1:A:559:ALA:HB1	1:A:653:VAL:HG21	2.02	0.41
1:C:149:ARG:HH12	1:C:151:SER:HB2	1.85	0.41
1:C:494:LYS:HG2	1:C:538:ARG:HG2	2.02	0.41
1:C:593:ASP:OD2	1:C:687:HIS:CE1	2.70	0.41
1:C:684:MET:HB2	1:C:690:ASN:ND2	2.35	0.41
1:D:307:ALA:HA	1:D:308:PRO:HD3	1.87	0.41
1:A:162:ARG:HB2	1:A:162:ARG:HE	1.62	0.41
1:A:705:HIS:O	9:A:1065:HOH:O	2.22	0.41
1:B:232:GLU:O	1:B:235:LYS:HB3	2.20	0.41
1:B:334:LEU:HD12	1:B:335:ASP:N	2.36	0.41
1:B:343:THR:HG22	1:B:373:LEU:CD2	2.50	0.41
1:C:249:HIS:CB	1:C:287:LEU:HD22	2.46	0.41
1:C:608:LEU:HD23	1:C:608:LEU:HA	1.87	0.41
1:C:551:ARG:C	1:C:681:THR:HG21	2.41	0.41
1:D:212[A]:MET:CG	1:D:213:ARG:HH11	2.09	0.41
1:B:157:ASN:OD1	1:B:164:HIS:CD2	2.73	0.41
1:B:602:LEU:HG	1:B:606:LEU:HD22	2.01	0.41
1:D:120:ARG:HG2	1:D:122:TYR:CZ	2.55	0.41
1:B:414:ASP:CG	9:B:1131:HOH:O	2.54	0.41
1:D:373:LEU:H	1:D:373:LEU:HD23	1.79	0.41
1:A:470:GLN:C	1:A:472:MET:H	2.23	0.41
1:A:518:ASN:HD21	2:F:2:GLC:H62	1.86	0.41
1:B:499:TYR:O	1:B:503:HIS:HD2	2.03	0.41
1:B:514:ASN:ND2	9:B:958:HOH:O	2.51	0.41
1:B:674:LYS:HG2	1:B:698:HIS:HD2	1.85	0.41
1:C:292:HIS:HA	1:C:293:PRO:HD3	1.89	0.41
1:D:289:ILE:C	1:D:289:ILE:HD12	2.42	0.41
1:A:148:ARG:O	1:A:148:ARG:HG2	2.20	0.41
1:A:214:PRO:HB3	1:A:215:GLU:HB3	2.02	0.41
1:A:468:ARG:NH1	2:F:2:GLC:C6	2.84	0.41
1:B:606:LEU:HD13	1:B:679:LEU:HD11	2.03	0.41
1:A:213:ARG:NH1	1:A:293:PRO:O	2.53	0.41
5:I:1:BGC:H6	5:I:2:GLC:C2	2.34	0.41
1:A:693:ASN:HD21	1:A:714:THR:N	2.03	0.40
1:D:564:LYS:HD2	1:D:564:LYS:N	2.36	0.40
1:B:363:ARG:HA	1:B:364:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:PRO:HB2	1:C:319:ARG:HH22	1.87	0.40
1:C:579:ASN:HD21	1:C:581:ASP:HB3	1.86	0.40
1:C:601:ARG:CZ	1:D:685[B]:HIS:HE2	2.34	0.40
1:D:125:LEU:HA	1:D:125:LEU:HD23	1.77	0.40
1:D:183:HIS:CD2	1:D:184:ASN:O	2.74	0.40
1:D:405:ASP:N	1:D:405:ASP:OD1	2.53	0.40
1:A:256:HIS:HE1	1:A:267:GLU:OE2	2.03	0.40
1:B:362:PRO:CA	1:B:363:ARG:CB	2.88	0.40
1:C:157:ASN:O	1:C:160:ASP:HB2	2.21	0.40
1:C:354:THR:O	1:C:356:LEU:N	2.54	0.40
1:D:237:ASN:ND2	1:D:283:HIS:CE1	2.81	0.40
1:C:652:ILE:O	1:C:722:TRP:HA	2.22	0.40
1:D:149:ARG:HD2	1:D:150:VAL:N	2.36	0.40
1:D:538:ARG:NH1	9:D:1079:HOH:O	2.54	0.40
1:D:721:ILE:CD1	1:D:723:LEU:HD21	2.51	0.40
1:A:375:TYR:HB2	1:A:377:TYR:CZ	2.57	0.40
1:A:463:PHE:HA	1:A:464:PRO:HD3	1.92	0.40
1:A:571:GLU:O	1:A:599:VAL:HG12	2.21	0.40
1:B:253:TRP:CE3	1:B:254[A]:ARG:HG3	2.56	0.40
1:B:660:VAL:HA	1:B:661:PRO:HD3	1.95	0.40
1:D:139:ARG:HD3	1:D:176:GLU:OE1	2.22	0.40
1:D:212[A]:MET:HA	1:D:213:ARG:HA	1.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/612 (96%)	546 (93%)	31 (5%)	9 (2%)	10	14
1	B	594/612 (97%)	566 (95%)	18 (3%)	10 (2%)	9	11
1	C	577/612 (94%)	512 (89%)	49 (8%)	16 (3%)	5	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	586/612 (96%)	545 (93%)	29 (5%)	12 (2%)	7	9
All	All	2343/2448 (96%)	2169 (93%)	127 (5%)	47 (2%)	7	9

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	TRP
1	A	148	ARG
1	A	215	GLU
1	A	226	LYS
1	B	194	ASP
1	B	213	ARG
1	B	226	LYS
1	C	213	ARG
1	C	343	THR
1	C	352	ASP
1	C	612	HIS
1	C	658	THR
1	D	149	ARG
1	D	194	ASP
1	D	213	ARG
1	D	259	ASN
1	D	694	GLY
1	A	142	VAL
1	A	216	THR
1	A	217	ALA
1	A	375	TYR
1	C	355	ASN
1	D	217	ALA
1	D	345	ASP
1	D	372	THR
1	D	522	PRO
1	D	591	GLY
1	D	592	GLY
1	A	522	PRO
1	B	363	ARG
1	C	472	MET
1	C	497	PRO
1	C	522	PRO
1	B	221	CYS
1	B	372	THR
1	B	425	ASN

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Mol	Chain	Res	Type
1	B	696	THR
1	C	293	PRO
1	C	542	ASP
1	B	703	ALA
1	C	159	TRP
1	C	533	LYS
1	C	709	HIS
1	D	695	GLY
1	B	522	PRO
1	C	374	ILE
1	C	353	GLY

### 5.3.2 Protein sidechains ⓘ

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	503/521 (96%)	465 (92%)	38 (8%)	13	20
1	B	510/521 (98%)	464 (91%)	46 (9%)	9	14
1	C	495/521 (95%)	460 (93%)	35 (7%)	14	23
1	D	503/521 (96%)	467 (93%)	36 (7%)	14	23
All	All	2011/2084 (96%)	1856 (92%)	155 (8%)	13	20

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	MET
1	A	133	ASP
1	A	169	ARG
1	A	171	GLU
1	A	199	LEU
1	A	212	MET
1	A	216	THR
1	A	223	LEU
1	A	228	VAL
1	A	257	THR

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Mol	Chain	Res	Type
1	A	259	ASN
1	A	285	GLU
1	A	311	ARG
1	A	315	ARG
1	A	331	ASN
1	A	356	LEU
1	A	358	GLU
1	A	376	ASN
1	A	380	ARG
1	A	391	LEU
1	A	413	ARG
1	A	434	GLU
1	A	472	MET
1	A	490	LEU
1	A	507	LEU
1	A	512	LEU
1	A	579	ASN
1	A	590[A]	GLU
1	A	590[B]	GLU
1	A	606	LEU
1	A	619	LEU
1	A	642	VAL
1	A	647	GLU
1	A	656	ASN
1	A	679	LEU
1	A	680	ASN
1	A	720	THR
1	A	723	LEU
1	B	132	MET
1	B	133	ASP
1	B	138	THR
1	B	149	ARG
1	B	163	ARG
1	B	168	LEU
1	B	171	GLU
1	B	215	GLU
1	B	216	THR
1	B	223	LEU
1	B	258	ASP
1	B	259	ASN
1	B	290	ASN
1	B	305	LEU

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Mol	Chain	Res	Type
1	B	331	ASN
1	B	334	LEU
1	B	356	LEU
1	B	360	SER
1	B	363	ARG
1	B	371	ASN
1	B	373	LEU
1	B	374	ILE
1	B	376	ASN
1	B	380	ARG
1	B	391	LEU
1	B	425	ASN
1	B	426	GLU
1	B	430	ARG
1	B	446	LEU
1	B	470	GLN
1	B	475	LEU
1	B	490	LEU
1	B	504	HIS
1	B	507	LEU
1	B	511	ILE
1	B	512	LEU
1	B	523	LEU
1	B	558	TRP
1	B	579	ASN
1	B	606	LEU
1	B	619	LEU
1	B	651	ILE
1	B	656	ASN
1	B	658	THR
1	B	679	LEU
1	B	680	ASN
1	C	119	LEU
1	C	133	ASP
1	C	157	ASN
1	C	168	LEU
1	C	170	LYS
1	C	171	GLU
1	C	212	MET
1	C	223	LEU
1	C	259	ASN
1	C	305	LEU

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Mol	Chain	Res	Type
1	C	310	ARG
1	C	315	ARG
1	C	337	VAL
1	C	350	GLU
1	C	352	ASP
1	C	356	LEU
1	C	379	ARG
1	C	446	LEU
1	C	470	GLN
1	C	471	ASP
1	C	475	LEU
1	C	498	VAL
1	C	507	LEU
1	C	511	ILE
1	C	542	ASP
1	C	564	LYS
1	C	579	ASN
1	C	595	TRP
1	C	619	LEU
1	C	651	ILE
1	C	656	ASN
1	C	680	ASN
1	C	689	SER
1	C	720	THR
1	C	723	LEU
1	D	119	LEU
1	D	138	THR
1	D	141	SER
1	D	148	ARG
1	D	149	ARG
1	D	157	ASN
1	D	170	LYS
1	D	171	GLU
1	D	223	LEU
1	D	232	GLU
1	D	258	ASP
1	D	315	ARG
1	D	356	LEU
1	D	359	HIS
1	D	372	THR
1	D	373	LEU
1	D	380	ARG

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Mol	Chain	Res	Type
1	D	391	LEU
1	D	462	ASP
1	D	470	GLN
1	D	471	ASP
1	D	472	MET
1	D	475	LEU
1	D	490	LEU
1	D	523	LEU
1	D	564	LYS
1	D	579	ASN
1	D	606	LEU
1	D	614	LYS
1	D	619	LEU
1	D	651	ILE
1	D	656	ASN
1	D	666	ARG
1	D	679	LEU
1	D	680	ASN
1	D	720	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	157	ASN
1	A	164	HIS
1	A	211	GLN
1	A	237	ASN
1	A	256	HIS
1	A	259	ASN
1	A	260	ASN
1	A	283	HIS
1	A	331	ASN
1	A	340	HIS
1	A	355	ASN
1	A	376	ASN
1	A	384	ASN
1	A	504	HIS
1	A	525	HIS
1	A	570	ASN
1	A	574	GLN
1	A	579	ASN

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Mol	Chain	Res	Type
1	A	597	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	690	ASN
1	A	693	ASN
1	A	705	HIS
1	A	708	GLN
1	A	709	HIS
1	B	157	ASN
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	283	HIS
1	B	331	ASN
1	B	340	HIS
1	B	359	HIS
1	B	371	ASN
1	B	376	ASN
1	B	384	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	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	693	ASN
1	B	705	HIS
1	C	157	ASN

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Mol	Chain	Res	Type
1	C	164	HIS
1	C	183	HIS
1	C	186	GLN
1	C	211	GLN
1	C	229	GLN
1	C	237	ASN
1	C	256	HIS
1	C	259	ASN
1	C	283	HIS
1	C	301	GLN
1	C	331	ASN
1	C	355	ASN
1	C	470	GLN
1	C	525	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	612	HIS
1	C	613	HIS
1	C	617	HIS
1	C	656	ASN
1	C	680	ASN
1	C	687	HIS
1	C	690	ASN
1	C	693	ASN
1	C	705	HIS
1	C	709	HIS
1	D	118	HIS
1	D	164	HIS
1	D	183	HIS
1	D	237	ASN
1	D	256	HIS
1	D	260	ASN
1	D	283	HIS
1	D	290	ASN
1	D	331	ASN
1	D	340	HIS
1	D	359	HIS
1	D	443	ASN

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Mol	Chain	Res	Type
1	D	470	GLN
1	D	525	HIS
1	D	545	GLN
1	D	570	ASN
1	D	574	GLN
1	D	579	ASN
1	D	597	HIS
1	D	617	HIS
1	D	656	ASN
1	D	680	ASN
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](#)

30 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	12,12,12	0.52	0	17,17,17	0.79	0
2	GLC	E	2	2	11,11,12	0.51	0	15,15,17	1.38	2 (13%)
2	GLC	F	1	2	12,12,12	0.70	0	17,17,17	1.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	F	2	2	11,11,12	0.49	0	15,15,17	2.13	2 (13%)
3	GLC	G	1	3	12,12,12	0.50	0	17,17,17	1.64	4 (23%)
3	GLC	G	2	3	11,11,12	0.77	0	15,15,17	0.84	0
3	GLC	G	3	3	11,11,12	0.60	0	15,15,17	1.56	4 (26%)
4	BGC	H	1	4	12,12,12	0.72	0	17,17,17	1.63	4 (23%)
4	GLC	H	2	4	11,11,12	0.42	0	15,15,17	2.30	3 (20%)
5	BGC	I	1	5	12,12,12	0.46	0	17,17,17	1.94	6 (35%)
5	GLC	I	2	5	11,11,12	0.50	0	15,15,17	1.64	3 (20%)
5	GLC	I	3	5	11,11,12	0.59	0	15,15,17	1.21	2 (13%)
5	GLC	I	4	5	11,11,12	0.58	0	15,15,17	1.41	2 (13%)
5	GLC	I	5	5	11,11,12	0.65	0	15,15,17	2.24	5 (33%)
5	GLC	I	6	5	11,11,12	0.62	0	15,15,17	1.33	2 (13%)
5	GLC	I	7	5	11,11,12	0.67	0	15,15,17	1.25	2 (13%)
4	BGC	J	1	4	12,12,12	0.59	0	17,17,17	1.18	0
4	GLC	J	2	4	11,11,12	0.79	0	15,15,17	1.13	1 (6%)
2	GLC	K	1	2	12,12,12	0.57	0	17,17,17	0.53	0
2	GLC	K	2	2	11,11,12	0.68	0	15,15,17	0.97	1 (6%)
6	GLC	L	1	6	12,12,12	0.66	0	17,17,17	1.43	3 (17%)
6	GLC	L	2	6	11,11,12	0.76	0	15,15,17	1.86	2 (13%)
6	GLC	L	3	6	11,11,12	0.59	0	15,15,17	1.16	1 (6%)
6	GLC	L	4	6	11,11,12	0.79	0	15,15,17	1.38	2 (13%)
2	GLC	M	1	2	12,12,12	0.50	0	17,17,17	0.80	0
2	GLC	M	2	2	11,11,12	0.57	0	15,15,17	1.42	3 (20%)
4	BGC	N	1	4	12,12,12	0.68	0	17,17,17	2.04	5 (29%)
4	GLC	N	2	4	11,11,12	0.59	0	15,15,17	1.78	3 (20%)
4	BGC	O	1	4	12,12,12	0.54	0	17,17,17	1.54	3 (17%)
4	GLC	O	2	4	11,11,12	0.53	0	15,15,17	1.67	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
3	GLC	G	1	3	-	2/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	G	3	3	-	2/2/19/22	0/1/1/1
4	BGC	H	1	4	-	2/2/22/22	0/1/1/1
4	GLC	H	2	4	-	2/2/19/22	0/1/1/1
5	BGC	I	1	5	-	2/2/22/22	0/1/1/1
5	GLC	I	2	5	-	2/2/19/22	0/1/1/1
5	GLC	I	3	5	-	2/2/19/22	0/1/1/1
5	GLC	I	4	5	-	2/2/19/22	0/1/1/1
5	GLC	I	5	5	-	1/2/19/22	0/1/1/1
5	GLC	I	6	5	-	2/2/19/22	0/1/1/1
5	GLC	I	7	5	-	0/2/19/22	0/1/1/1
4	BGC	J	1	4	-	2/2/22/22	0/1/1/1
4	GLC	J	2	4	-	0/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	1/2/19/22	0/1/1/1
6	GLC	L	1	6	-	0/2/22/22	0/1/1/1
6	GLC	L	2	6	-	2/2/19/22	0/1/1/1
6	GLC	L	3	6	-	2/2/19/22	0/1/1/1
6	GLC	L	4	6	-	0/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	2/2/19/22	0/1/1/1
4	BGC	N	1	4	-	2/2/22/22	0/1/1/1
4	GLC	N	2	4	-	2/2/19/22	0/1/1/1
4	BGC	O	1	4	-	2/2/22/22	0/1/1/1
4	GLC	O	2	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	GLC	C1-O5-C5	7.10	121.81	112.19
2	F	2	GLC	C1-O5-C5	6.68	121.25	112.19
4	N	2	GLC	C1-O5-C5	5.49	119.63	112.19
6	L	2	GLC	C1-C2-C3	5.47	116.39	109.67
5	I	5	GLC	C1-O5-C5	4.49	118.28	112.19
5	I	1	BGC	C4-C3-C2	-4.46	103.04	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	1	BGC	O5-C5-C4	4.39	117.67	109.69
4	H	1	BGC	O5-C1-C2	-4.35	102.52	110.28
4	O	2	GLC	C1-O5-C5	4.32	118.04	112.19
3	G	1	GLC	C1-O5-C5	4.29	121.75	113.66
5	I	2	GLC	C1-O5-C5	4.03	117.66	112.19
5	I	5	GLC	C1-C2-C3	3.91	114.47	109.67
6	L	4	GLC	C1-C2-C3	3.86	114.41	109.67
6	L	1	GLC	C4-C3-C2	3.84	117.53	110.82
5	I	6	GLC	O5-C1-C2	-3.73	105.02	110.77
6	L	2	GLC	C2-C3-C4	3.54	117.02	110.89
4	O	1	BGC	C4-C3-C2	-3.51	104.69	110.82
4	N	1	BGC	C1-C2-C3	-3.50	103.06	110.31
4	H	2	GLC	O5-C5-C6	3.47	112.65	107.20
3	G	3	GLC	O5-C1-C2	-3.46	105.43	110.77
5	I	5	GLC	C3-C4-C5	-3.42	104.14	110.24
4	N	1	BGC	O5-C1-C2	-3.37	104.28	110.28
6	L	3	GLC	C1-O5-C5	3.35	116.74	112.19
5	I	4	GLC	C1-O5-C5	3.23	116.57	112.19
5	I	1	BGC	C1-O5-C5	3.20	119.70	113.66
4	N	1	BGC	C3-C4-C5	3.16	115.87	110.24
3	G	1	GLC	O5-C5-C4	3.05	115.22	109.69
5	I	5	GLC	O5-C5-C6	2.95	111.83	107.20
5	I	2	GLC	C3-C4-C5	-2.94	105.00	110.24
5	I	7	GLC	C1-O5-C5	2.87	116.08	112.19
2	F	2	GLC	O5-C5-C4	2.83	117.71	110.83
6	L	4	GLC	C1-O5-C5	2.83	116.02	112.19
4	H	1	BGC	C1-O5-C5	-2.80	108.38	113.66
4	N	2	GLC	C3-C4-C5	2.75	115.14	110.24
2	K	2	GLC	C1-O5-C5	2.74	115.91	112.19
4	H	2	GLC	C2-C3-C4	-2.71	106.20	110.89
5	I	1	BGC	O2-C2-C1	2.65	115.31	109.16
4	O	2	GLC	C2-C3-C4	-2.64	106.32	110.89
2	F	1	GLC	C1-C2-C3	2.64	115.78	110.31
5	I	1	BGC	O4-C4-C5	2.63	115.82	109.30
5	I	5	GLC	O5-C1-C2	2.63	114.82	110.77
2	E	2	GLC	O5-C5-C6	2.61	111.29	107.20
2	M	2	GLC	C1-C2-C3	-2.60	106.47	109.67
2	E	2	GLC	C1-O5-C5	2.60	115.71	112.19
2	F	1	GLC	C4-C3-C2	2.59	115.35	110.82
6	L	1	GLC	C1-C2-C3	2.59	115.69	110.31
5	I	1	BGC	O4-C4-C3	2.53	116.19	110.35
4	N	2	GLC	O5-C5-C4	2.51	116.93	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	GLC	O4-C4-C5	2.49	115.47	109.30
5	I	3	GLC	C3-C4-C5	-2.47	105.83	110.24
5	I	3	GLC	O5-C5-C6	2.45	111.04	107.20
4	O	1	BGC	O4-C4-C3	2.38	115.84	110.35
3	G	1	GLC	C4-C3-C2	-2.37	106.69	110.82
3	G	1	GLC	O5-C1-C2	2.36	114.49	110.28
5	I	7	GLC	C2-C3-C4	-2.30	106.91	110.89
3	G	3	GLC	C1-O5-C5	2.28	115.28	112.19
3	G	3	GLC	O2-C2-C3	2.23	114.61	110.14
4	N	1	BGC	O2-C2-C1	2.21	114.28	109.16
4	O	1	BGC	O2-C2-C1	2.20	114.27	109.16
6	L	1	GLC	C3-C4-C5	2.17	114.11	110.24
5	I	1	BGC	O3-C3-C4	2.15	115.33	110.35
4	H	1	BGC	C4-C3-C2	2.14	114.56	110.82
2	M	2	GLC	C2-C3-C4	-2.14	107.20	110.89
4	H	1	BGC	O4-C4-C5	-2.13	104.00	109.30
4	O	2	GLC	O5-C5-C6	2.09	110.48	107.20
5	I	4	GLC	O5-C5-C6	2.07	110.45	107.20
3	G	3	GLC	C3-C4-C5	2.04	113.87	110.24
4	J	2	GLC	O5-C1-C2	-2.02	107.65	110.77
2	M	2	GLC	O2-C2-C3	2.02	114.19	110.14
5	I	6	GLC	O2-C2-C1	2.02	113.28	109.15

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	GLC	O5-C5-C6-O6
4	O	1	BGC	C4-C5-C6-O6
4	H	2	GLC	C4-C5-C6-O6
4	N	1	BGC	O5-C5-C6-O6
5	I	4	GLC	O5-C5-C6-O6
6	L	2	GLC	C4-C5-C6-O6
4	O	1	BGC	O5-C5-C6-O6
6	L	3	GLC	O5-C5-C6-O6
5	I	1	BGC	O5-C5-C6-O6
6	L	2	GLC	O5-C5-C6-O6
5	I	2	GLC	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
5	I	3	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
5	I	6	GLC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	I	2	GLC	C4-C5-C6-O6
5	I	1	BGC	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
4	J	1	BGC	C4-C5-C6-O6
3	G	1	GLC	C4-C5-C6-O6
2	M	2	GLC	O5-C5-C6-O6
5	I	6	GLC	O5-C5-C6-O6
5	I	3	GLC	C4-C5-C6-O6
3	G	3	GLC	O5-C5-C6-O6
4	J	1	BGC	O5-C5-C6-O6
3	G	3	GLC	C4-C5-C6-O6
5	I	4	GLC	C4-C5-C6-O6
4	H	1	BGC	C4-C5-C6-O6
4	H	1	BGC	O5-C5-C6-O6
6	L	3	GLC	C4-C5-C6-O6
4	N	2	GLC	O5-C5-C6-O6
4	N	1	BGC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
5	I	5	GLC	O5-C5-C6-O6
2	M	2	GLC	C4-C5-C6-O6
4	N	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6

There are no ring outliers.

17 monomers are involved in 39 short contacts:

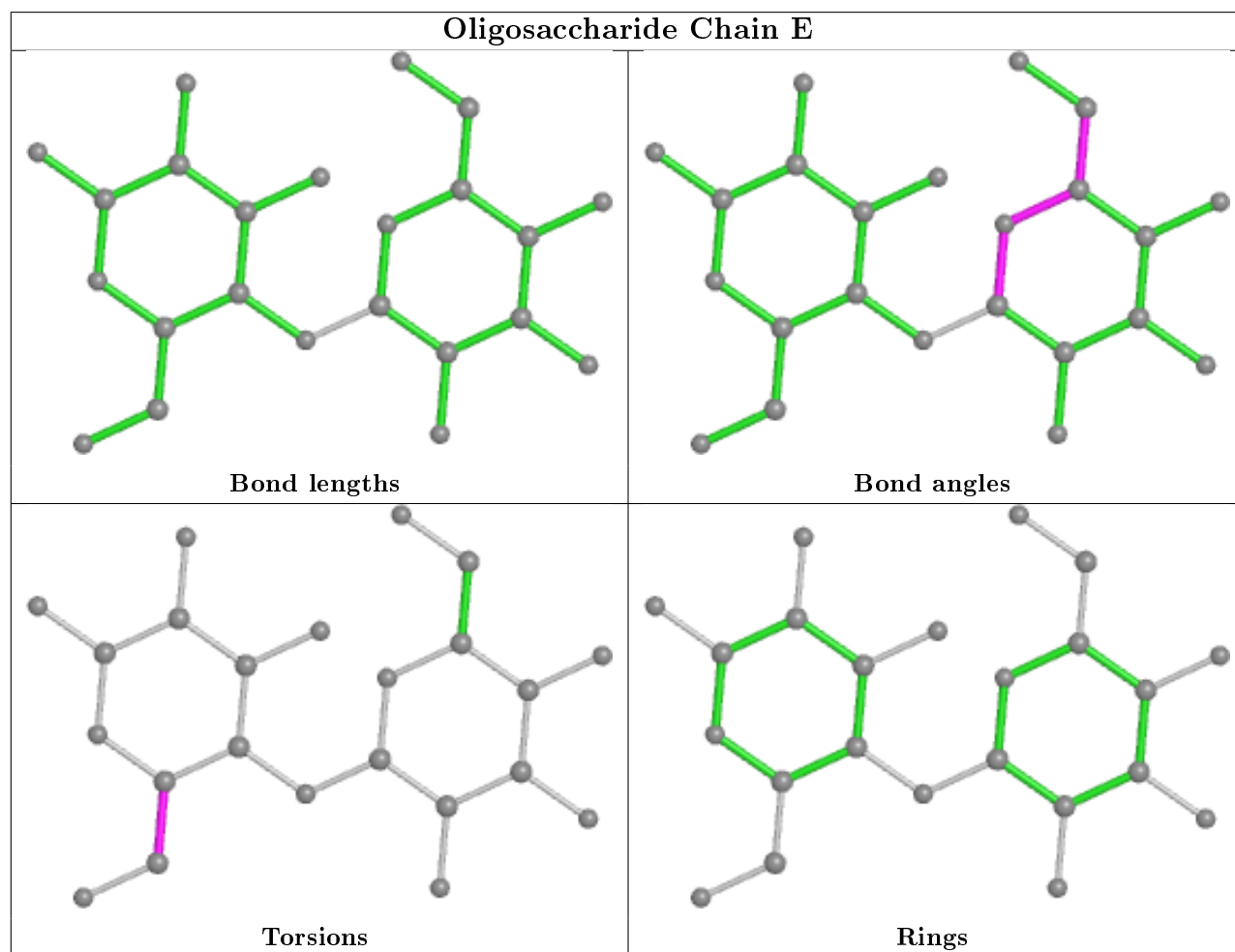
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	BGC	4	0
3	G	2	GLC	1	0
4	N	1	BGC	7	0
4	J	2	GLC	3	0
4	H	1	BGC	2	0
2	M	1	GLC	1	0
6	L	4	GLC	1	0
5	I	3	GLC	3	0
5	I	2	GLC	4	0
3	G	1	GLC	5	0
5	I	4	GLC	1	0
5	I	5	GLC	2	0
5	I	1	BGC	1	0
2	F	2	GLC	4	0

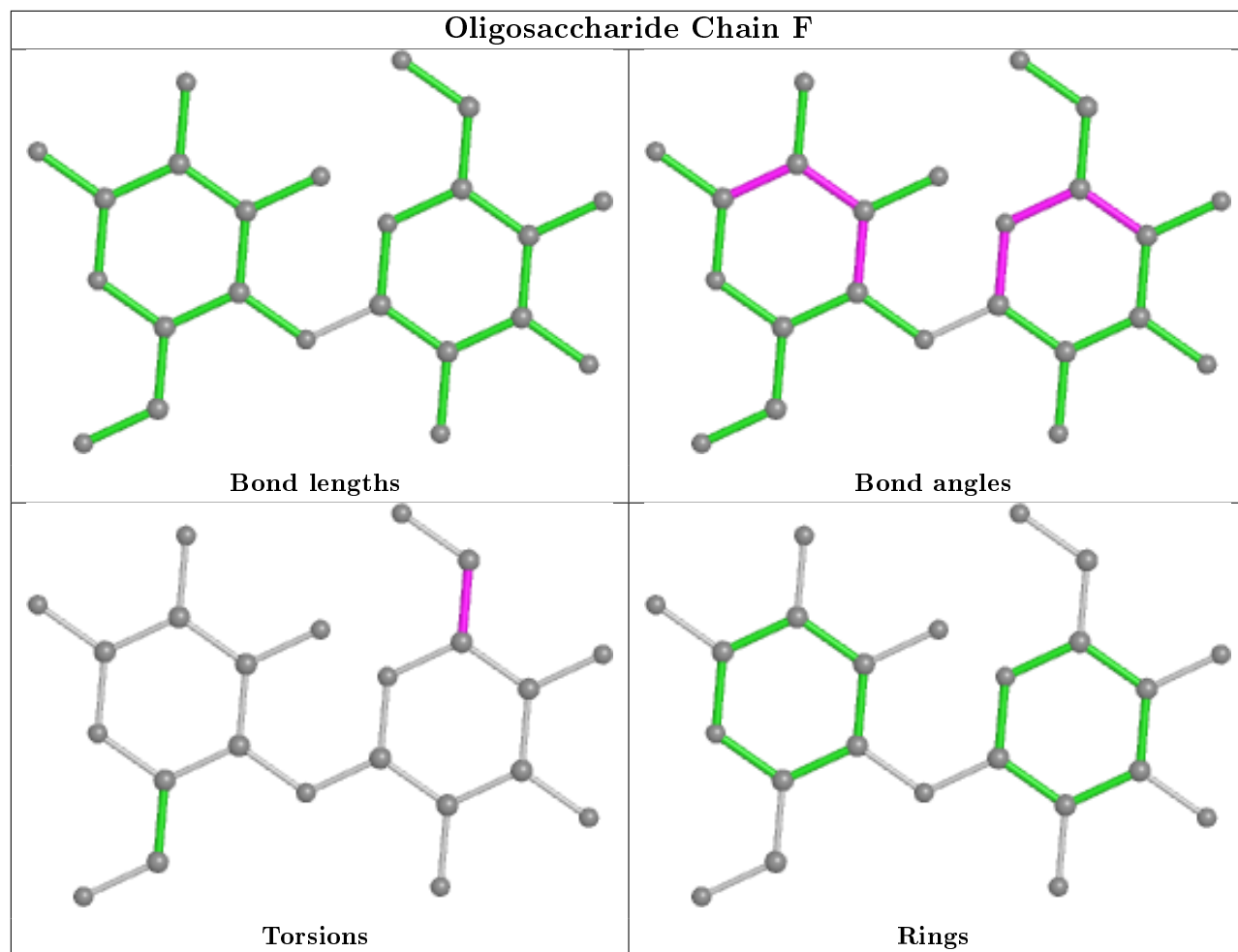
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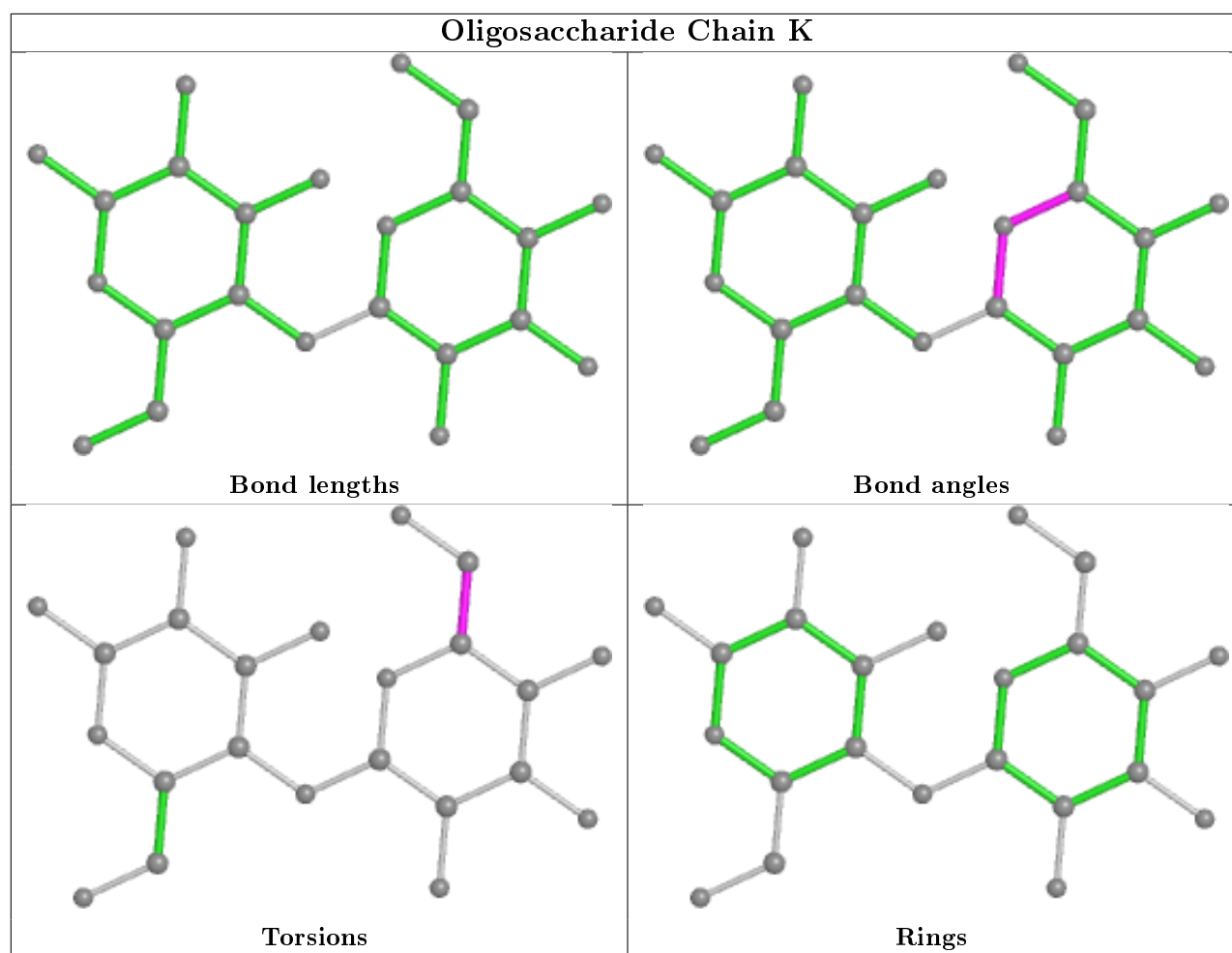
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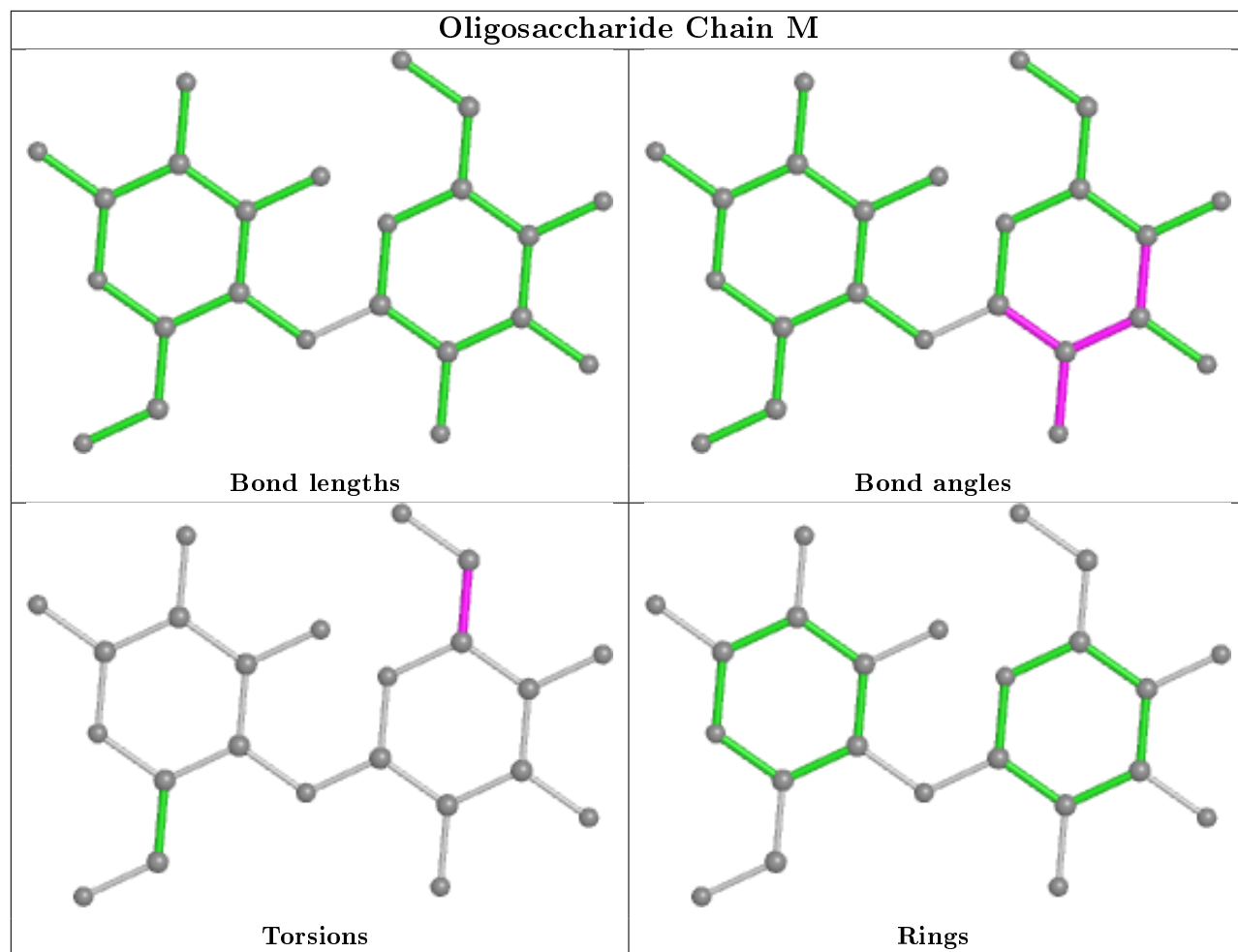
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GLC	2	0
4	H	2	GLC	2	0
5	I	6	GLC	1	0

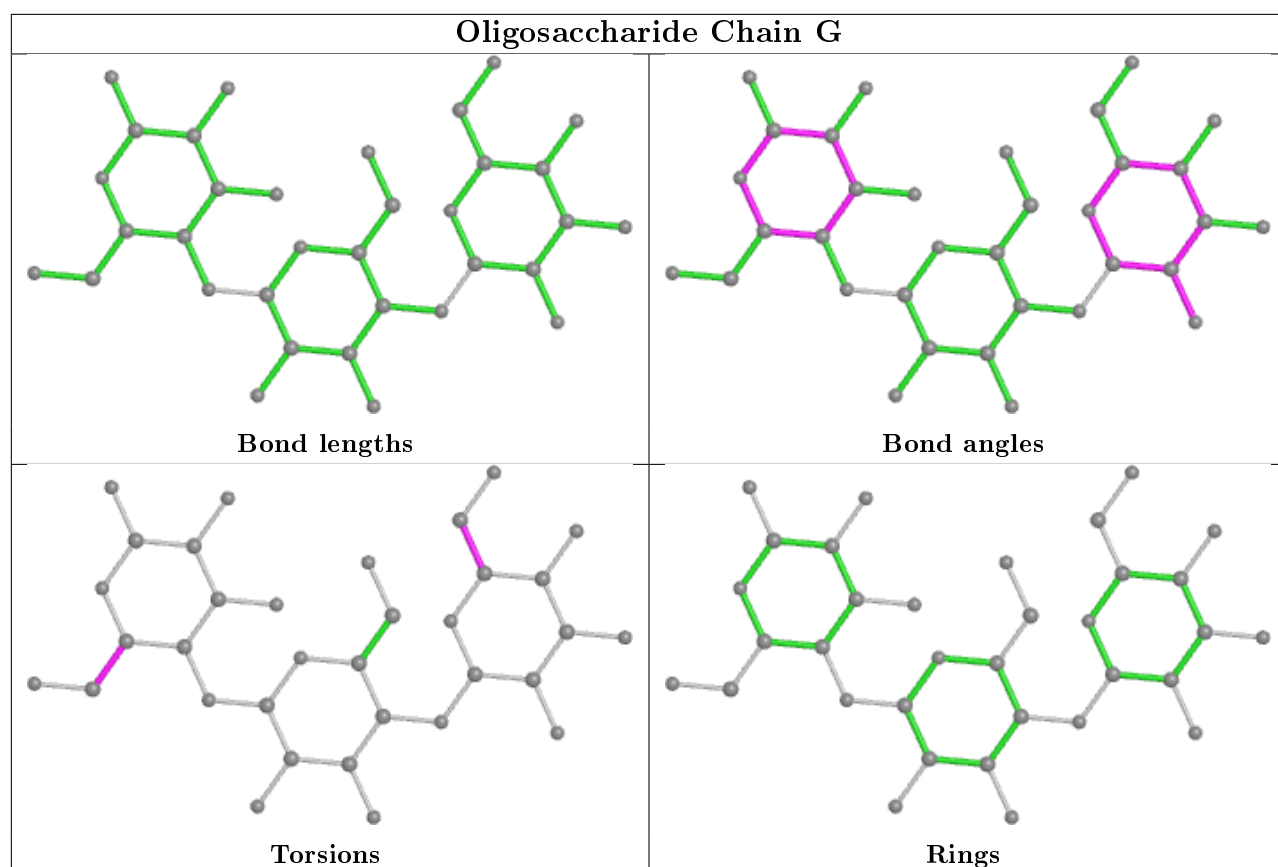
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

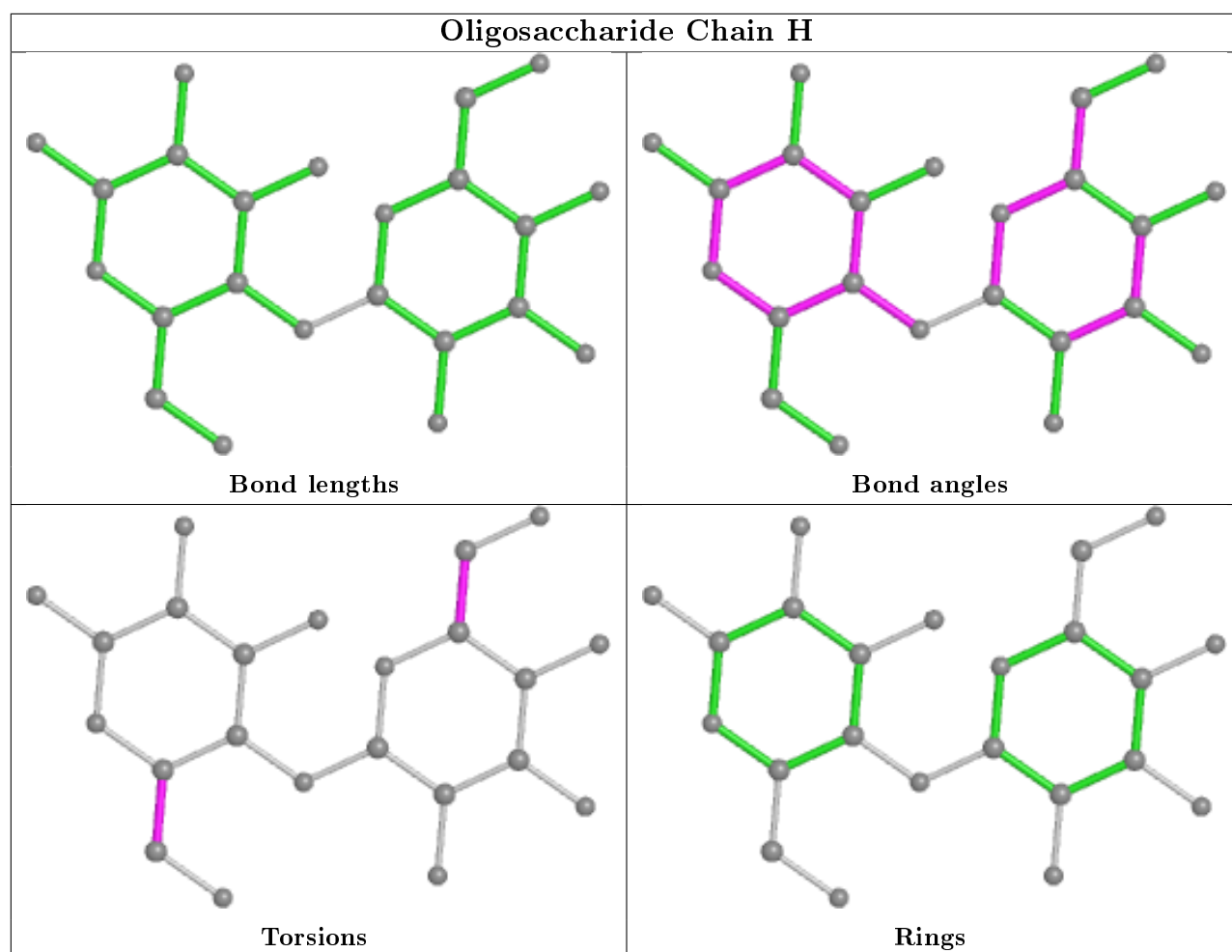


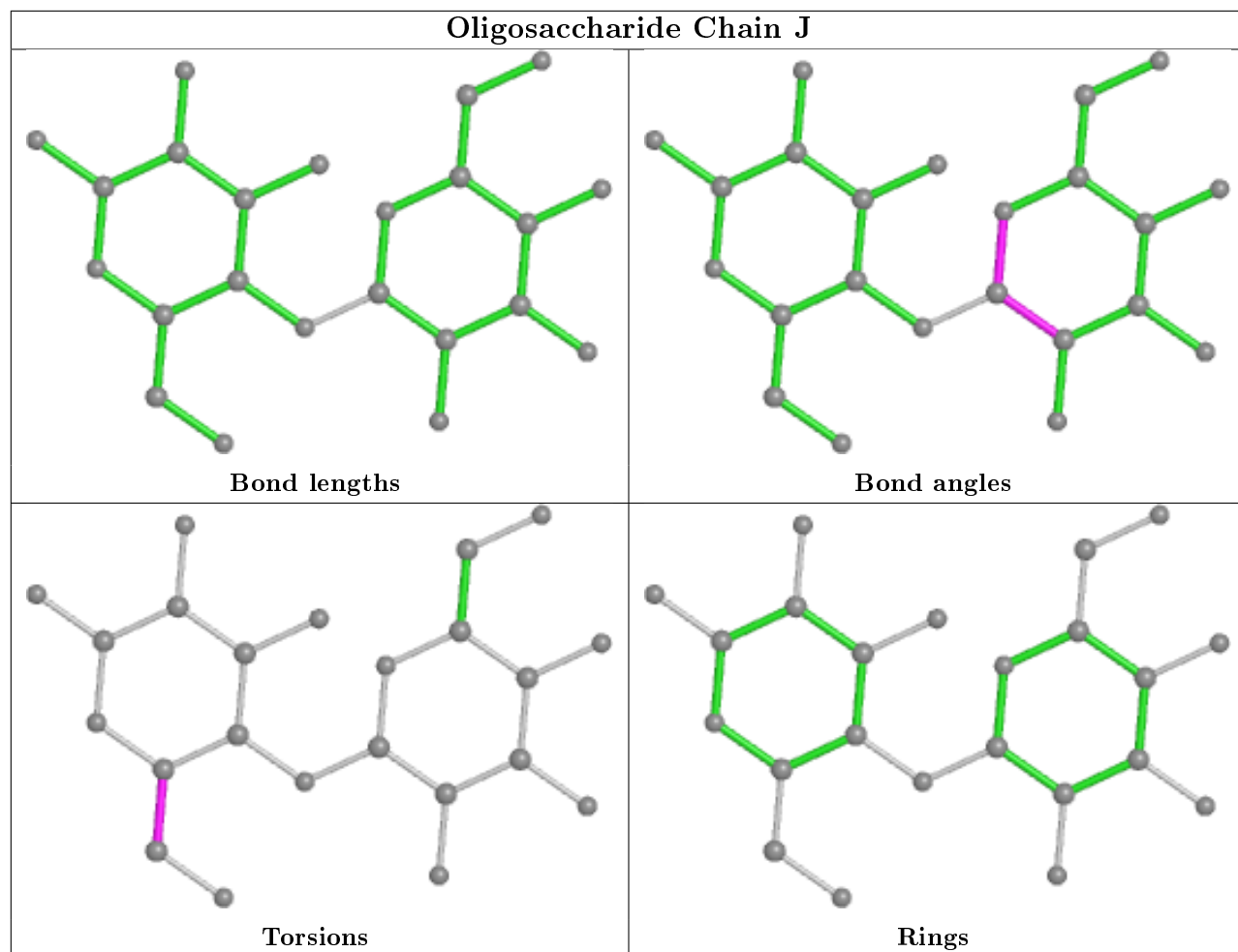


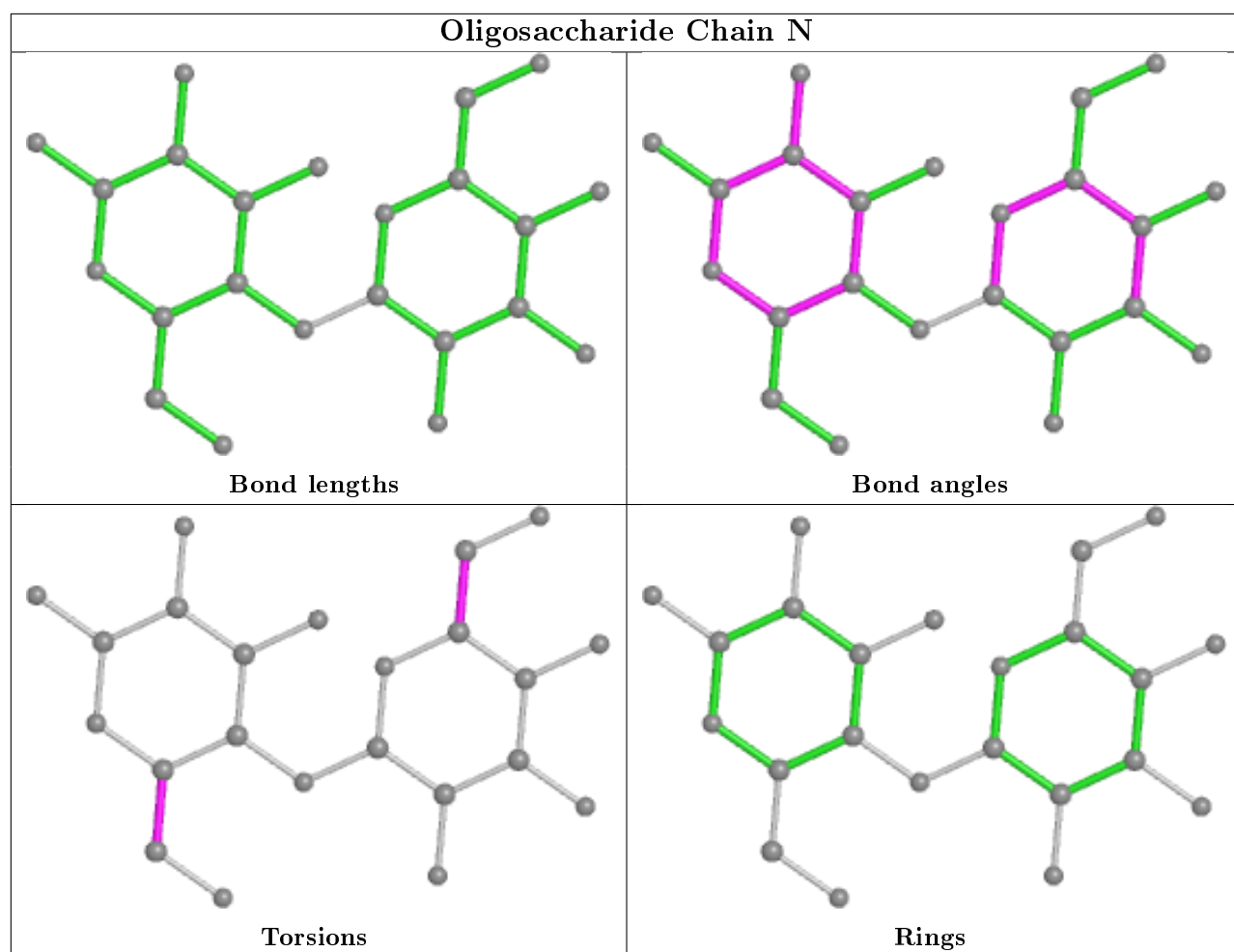


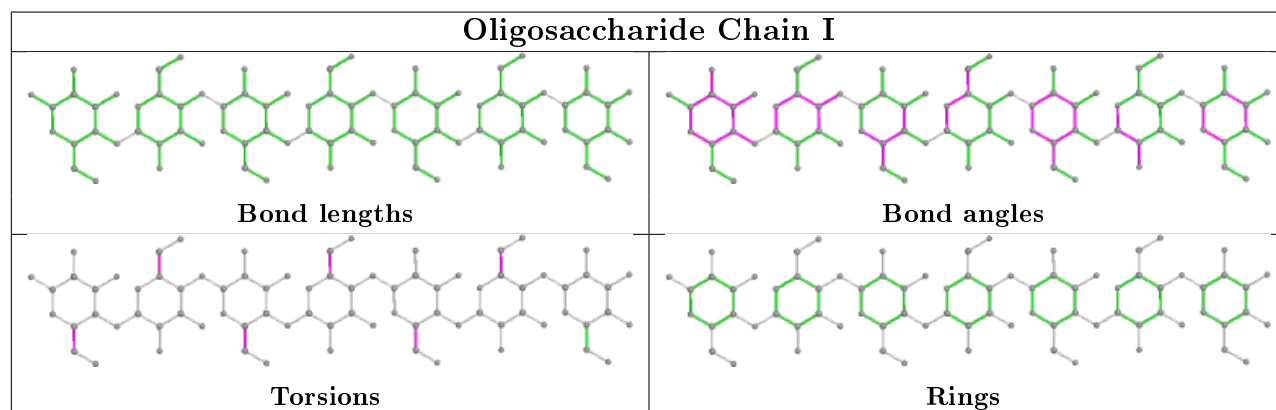
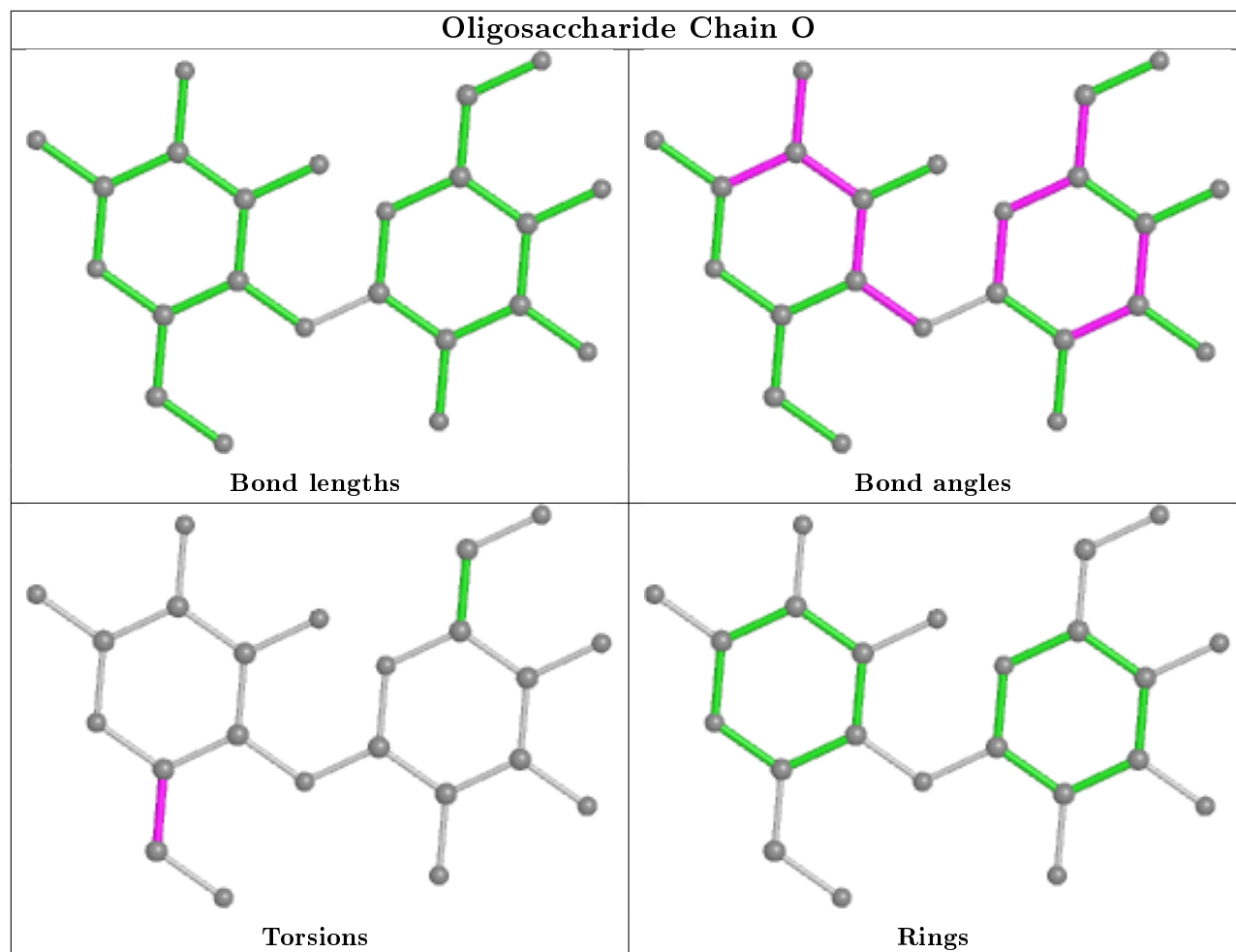


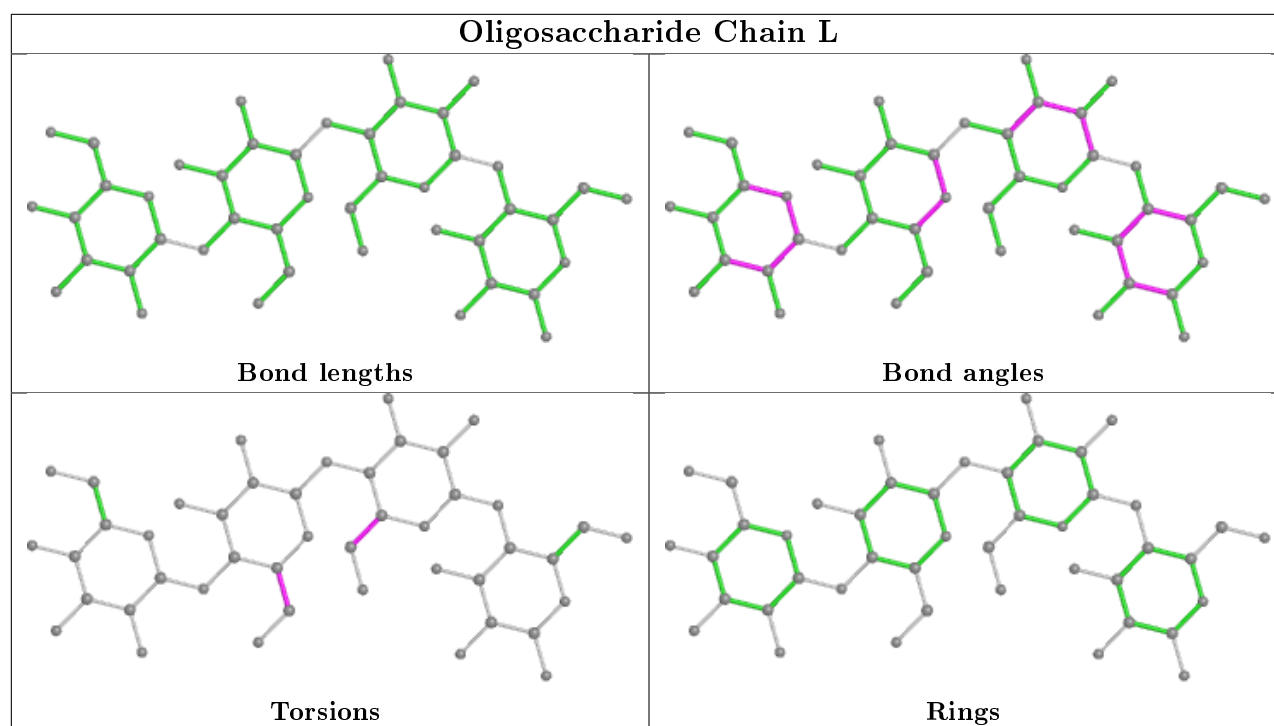












## 5.6 Ligand geometry [i](#)

12 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	$\# Z  > 2$
7	GOL	B	813	-	5,5,5	0.55	0	5,5,5	0.87	0
8	BGC	B	810	-	12,12,12	0.49	0	17,17,17	0.89	1 (5%)
7	GOL	D	808	-	5,5,5	0.34	0	5,5,5	0.42	0
7	GOL	B	812	-	5,5,5	0.43	0	5,5,5	0.67	0
7	GOL	A	807	-	5,5,5	0.43	0	5,5,5	0.85	0
7	GOL	B	811	-	5,5,5	0.46	0	5,5,5	0.24	0
7	GOL	B	815	-	5,5,5	0.44	0	5,5,5	0.49	0
7	GOL	D	809	-	5,5,5	0.35	0	5,5,5	0.43	0
7	GOL	A	806	-	5,5,5	0.27	0	5,5,5	0.46	0
7	GOL	A	805	-	5,5,5	0.48	0	5,5,5	0.31	0
7	GOL	D	807	-	5,5,5	0.34	0	5,5,5	0.33	0
7	GOL	B	814	-	5,5,5	0.38	0	5,5,5	0.38	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
7	GOL	B	813	-	-	2/4/4/4	-
8	BGC	B	810	-	-	1/2/22/22	0/1/1/1
7	GOL	D	808	-	-	4/4/4/4	-
7	GOL	B	812	-	-	4/4/4/4	-
7	GOL	A	807	-	-	0/4/4/4	-
7	GOL	B	811	-	-	0/4/4/4	-
7	GOL	B	815	-	-	4/4/4/4	-
7	GOL	D	809	-	-	2/4/4/4	-
7	GOL	A	806	-	-	0/4/4/4	-
7	GOL	A	805	-	-	4/4/4/4	-
7	GOL	D	807	-	-	2/4/4/4	-
7	GOL	B	814	-	-	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(°)
8	B	810	BGC	O4-C4-C5	2.06	114.42	109.30

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	813	GOL	O1-C1-C2-C3
7	B	812	GOL	O1-C1-C2-C3
7	B	812	GOL	C1-C2-C3-O3
7	B	815	GOL	O1-C1-C2-C3
7	A	805	GOL	O1-C1-C2-C3
7	A	805	GOL	C1-C2-C3-O3
7	D	807	GOL	O1-C1-C2-C3
7	B	814	GOL	C1-C2-C3-O3
7	B	814	GOL	O2-C2-C3-O3
7	B	812	GOL	O1-C1-C2-O2
7	D	808	GOL	O1-C1-C2-C3
7	B	815	GOL	C1-C2-C3-O3
7	D	809	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	B	813	GOL	O1-C1-C2-O2
7	B	812	GOL	O2-C2-C3-O3
7	B	815	GOL	O1-C1-C2-O2
7	D	809	GOL	O1-C1-C2-O2
7	A	805	GOL	O2-C2-C3-O3
7	D	807	GOL	O1-C1-C2-O2
7	A	805	GOL	O1-C1-C2-O2
7	D	808	GOL	O2-C2-C3-O3
7	B	815	GOL	O2-C2-C3-O3
8	B	810	BGC	O5-C5-C6-O6
7	D	808	GOL	C1-C2-C3-O3
7	D	808	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	813	GOL	3	0
7	D	808	GOL	1	0
7	B	812	GOL	2	0
7	A	807	GOL	6	0
7	B	815	GOL	7	0
7	D	809	GOL	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	587/612 (95%)	0.28	58 (9%) <b>7</b> <b>6</b>	25, 48, 124, 144	1 (0%)
1	B	598/612 (97%)	-0.11	11 (1%) 68 66	21, 38, 63, 77	5 (0%)
1	C	582/612 (95%)	0.86	106 (18%) <b>1</b> <b>1</b>	57, 88, 123, 143	2 (0%)
1	D	588/612 (96%)	0.06	12 (2%) 65 63	35, 49, 70, 86	3 (0%)
All	All	2355/2448 (96%)	0.27	187 (7%) <b>12</b> <b>11</b>	21, 51, 114, 144	11 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	SER	8.2
1	A	201	LEU	7.1
1	C	213	ARG	7.0
1	A	159	TRP	6.6
1	A	195	ALA	6.2
1	A	428	GLY	5.8
1	C	132	MET	5.7
1	C	212	MET	5.7
1	C	199	LEU	5.7
1	C	498	VAL	5.7
1	C	499	TYR	5.7
1	A	149	ARG	5.6
1	C	261	PHE	5.5
1	C	433	LEU	5.4
1	C	134	GLY	5.4
1	C	502	TYR	5.2
1	C	294	PHE	5.1
1	C	133	ASP	5.1
1	C	131	THR	5.0
1	A	147	ALA	5.0
1	A	196	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	145	PRO	4.8
1	A	170	LYS	4.7
1	C	258	ASP	4.7
1	C	512	LEU	4.6
1	A	199	LEU	4.6
1	A	193	ILE	4.6
1	C	228	VAL	4.4
1	A	175	TRP	4.4
1	C	508	THR	4.4
1	C	196	ASN	4.4
1	A	429	GLY	4.4
1	C	374	ILE	4.4
1	C	431	GLU	4.4
1	C	257	THR	4.3
1	C	359	HIS	4.2
1	A	150	VAL	4.2
1	C	430	ARG	4.1
1	A	146	ASN	4.1
1	D	117	THR	4.1
1	A	200	ARG	4.0
1	C	373	LEU	4.0
1	B	427	PHE	4.0
1	A	158	TYR	3.9
1	C	159	TRP	3.8
1	A	212	MET	3.8
1	C	543	ALA	3.8
1	A	171	GLU	3.8
1	C	168	LEU	3.7
1	C	529	VAL	3.7
1	C	214	PRO	3.7
1	A	215	GLU	3.6
1	C	260	ASN	3.6
1	C	210	ALA	3.6
1	C	135	VAL	3.6
1	C	346	PHE	3.6
1	D	371	ASN	3.6
1	C	341	PHE	3.6
1	C	530	HIS	3.6
1	A	153	VAL	3.6
1	C	412	TYR	3.6
1	C	703	ALA	3.5
1	A	191	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	473	GLY	3.5
1	A	194	ASP	3.3
1	C	411	ILE	3.3
1	D	212[A]	MET	3.3
1	D	258	ASP	3.3
1	D	429	GLY	3.2
1	C	509	PHE	3.2
1	A	346	PHE	3.2
1	D	728	GLU	3.1
1	B	371	ASN	3.1
1	C	256	HIS	3.1
1	D	430	ARG	3.1
1	C	349	ALA	3.1
1	D	346	PHE	3.1
1	C	355	ASN	3.0
1	B	199	LEU	3.0
1	C	169	ARG	3.0
1	A	118	HIS	3.0
1	C	198	ASN	3.0
1	C	259	ASN	3.0
1	A	197	GLY	3.0
1	A	117	THR	3.0
1	A	380	ARG	3.0
1	A	472	MET	2.9
1	A	148	ARG	2.9
1	C	353	GLY	2.9
1	C	707	ARG	2.9
1	C	660	VAL	2.9
1	C	624	TYR	2.9
1	A	216	THR	2.8
1	C	496	ASP	2.8
1	C	354	THR	2.8
1	C	203	SER	2.8
1	C	595	TRP	2.8
1	A	167	ARG	2.8
1	A	162	ARG	2.7
1	C	375	TYR	2.7
1	A	168	LEU	2.7
1	C	350	GLU	2.7
1	C	144	ALA	2.7
1	C	347	ALA	2.7
1	B	429	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	2.7
1	C	576	ARG	2.7
1	C	230	THR	2.7
1	C	460	SER	2.6
1	C	542	ASP	2.6
1	C	635	GLU	2.6
1	C	195	ALA	2.6
1	C	547	PHE	2.6
1	A	166	MET	2.6
1	C	143	TRP	2.6
1	C	708	GLN	2.6
1	A	160	ASP	2.6
1	C	200	ARG	2.5
1	C	343	THR	2.5
1	C	540	PRO	2.5
1	C	225	GLU	2.5
1	A	351	PHE	2.5
1	A	144	ALA	2.5
1	C	183	HIS	2.5
1	C	380	ARG	2.5
1	C	634	LYS	2.5
1	C	495	LEU	2.5
1	C	197	GLY	2.5
1	A	219	LEU	2.5
1	A	165	PRO	2.4
1	C	432	ASN	2.4
1	C	445	ILE	2.4
1	C	150	VAL	2.4
1	A	353	GLY	2.4
1	A	412	TYR	2.4
1	B	337	VAL	2.4
1	A	177	LEU	2.4
1	A	163	ARG	2.4
1	B	133	ASP	2.4
1	C	170	LYS	2.4
1	A	172	SER	2.4
1	A	192	MET	2.4
1	A	349	ALA	2.4
1	C	497	PRO	2.4
1	C	582	ALA	2.4
1	A	213	ARG	2.4
1	A	530	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	357	TYR	2.3
1	C	119	LEU	2.3
1	C	147	ALA	2.3
1	A	152	VAL	2.3
1	C	674	LYS	2.3
1	C	672	PRO	2.3
1	C	345	ASP	2.3
1	C	408	ALA	2.3
1	C	190	TYR	2.3
1	A	202	LYS	2.3
1	A	198	ASN	2.3
1	B	117	THR	2.3
1	C	356	LEU	2.3
1	C	155	GLN	2.3
1	C	545	GLN	2.3
1	A	214	PRO	2.3
1	A	187	LEU	2.2
1	C	265	TYR	2.2
1	C	698	HIS	2.2
1	C	464	PRO	2.2
1	C	435	ALA	2.2
1	A	161	GLY	2.2
1	C	262	TRP	2.2
1	B	200	ARG	2.2
1	C	313	GLY	2.2
1	C	544	TRP	2.1
1	C	631	VAL	2.1
1	D	414	ASP	2.1
1	D	334	LEU	2.1
1	D	248	VAL	2.1
1	C	434	GLU	2.1
1	B	257	THR	2.1
1	B	288	PRO	2.1
1	A	381	GLU	2.0
1	A	155	GLN	2.0
1	B	428	GLY	2.0
1	C	463	PHE	2.0
1	C	376	ASN	2.0
1	A	473	GLY	2.0
1	C	192	MET	2.0

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

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

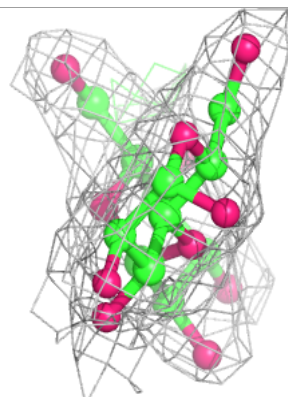
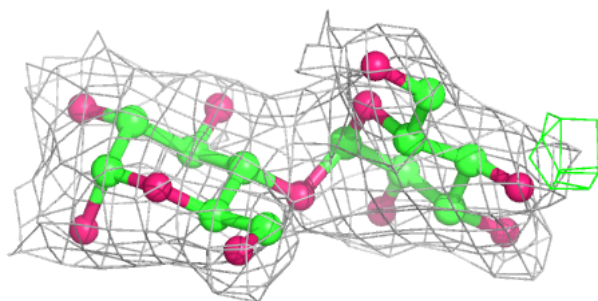
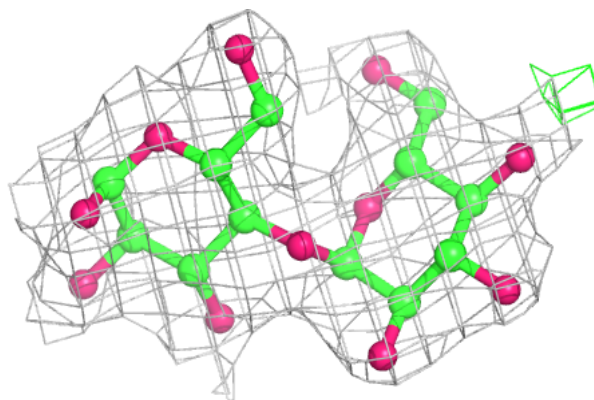
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GLC	I	3	11/12	0.22	0.68	95,96,97,97	11
5	GLC	I	4	11/12	0.55	0.57	92,94,95,95	10
4	BGC	O	1	12/12	0.64	0.31	104,106,106,106	0
5	GLC	I	5	11/12	0.64	0.34	83,87,89,89	4
4	GLC	O	2	11/12	0.68	0.40	106,107,108,109	1
4	GLC	H	2	11/12	0.72	0.31	86,87,88,89	0
6	GLC	L	1	12/12	0.80	0.43	95,98,98,99	0
3	GLC	G	3	11/12	0.82	0.30	88,90,91,92	0
2	GLC	M	2	11/12	0.83	0.30	83,84,85,86	0
2	GLC	F	1	12/12	0.83	0.20	91,92,92,93	0
4	BGC	H	1	12/12	0.84	0.23	82,84,86,89	0
2	GLC	F	2	11/12	0.84	0.23	90,90,91,92	0
5	GLC	I	2	11/12	0.84	0.34	90,91,93,93	1
4	GLC	J	2	11/12	0.85	0.32	69,71,73,74	0
5	BGC	I	1	12/12	0.85	0.20	82,86,87,88	0
4	BGC	N	1	12/12	0.86	0.27	65,69,71,73	0
3	GLC	G	2	11/12	0.86	0.23	75,78,81,85	0
4	GLC	N	2	11/12	0.86	0.32	68,70,71,73	0
6	GLC	L	2	11/12	0.87	0.35	83,91,92,93	0
2	GLC	K	2	11/12	0.89	0.28	83,84,85,85	0
5	GLC	I	7	11/12	0.89	0.16	62,69,72,72	0
3	GLC	G	1	12/12	0.89	0.21	72,76,77,79	0
4	BGC	J	1	12/12	0.90	0.22	59,69,70,71	0
5	GLC	I	6	11/12	0.90	0.24	74,76,78,79	0
2	GLC	M	1	12/12	0.91	0.14	77,79,81,81	0
2	GLC	K	1	12/12	0.91	0.28	84,85,86,86	0
6	GLC	L	4	11/12	0.92	0.16	64,70,71,73	0
6	GLC	L	3	11/12	0.94	0.17	72,74,76,78	0
2	GLC	E	2	11/12	0.95	0.21	64,69,70,71	0
2	GLC	E	1	12/12	0.96	0.21	66,68,69,70	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

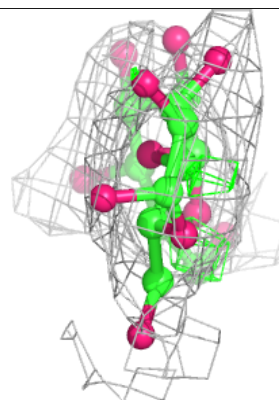
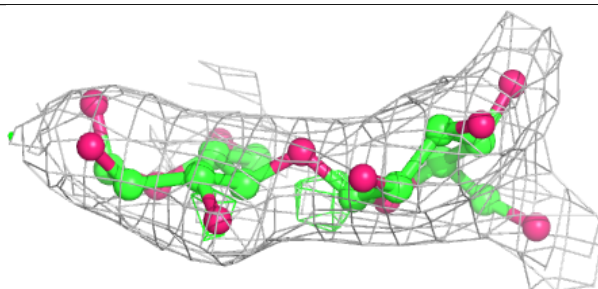
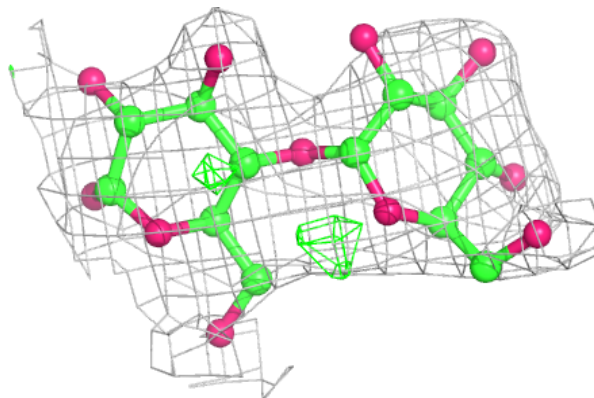
**Electron density around Chain E:**

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



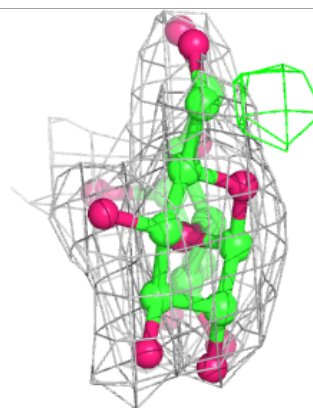
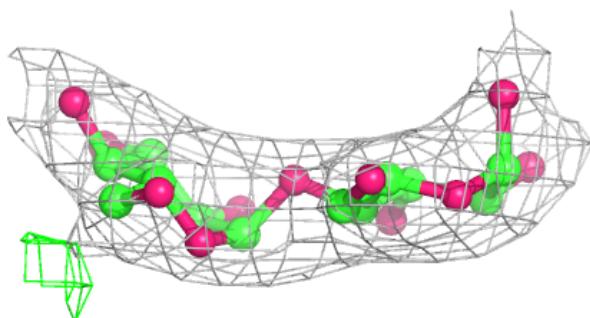
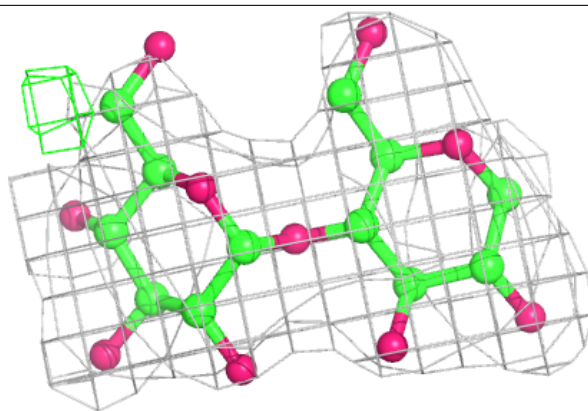
**Electron density around Chain F:**

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

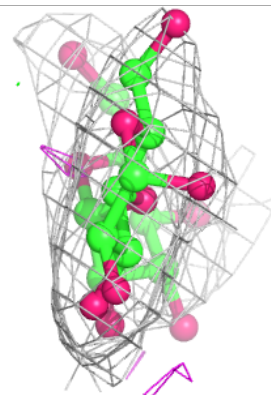
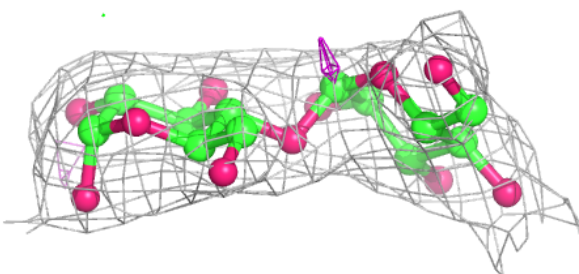
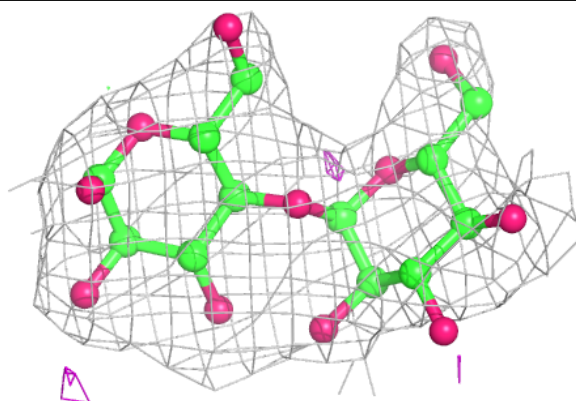


**Electron density around Chain K:**

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

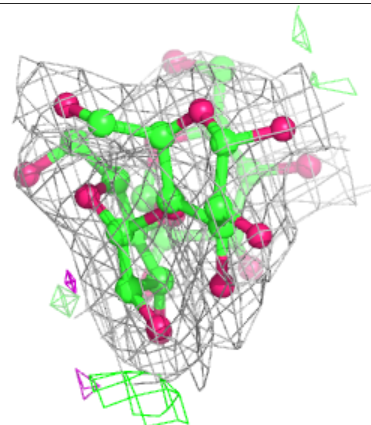
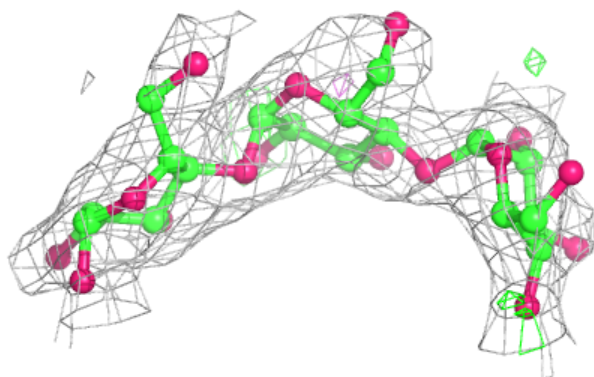
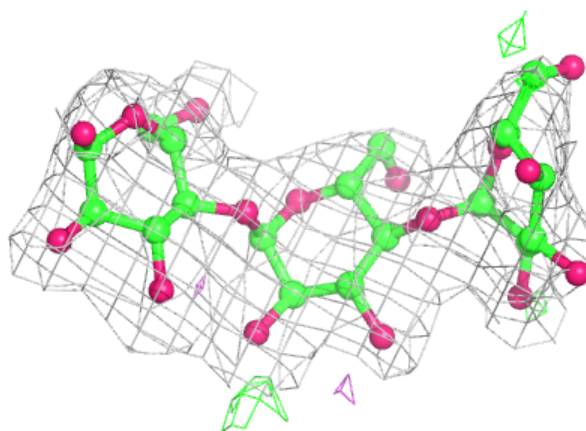
**Electron density around Chain M:**

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

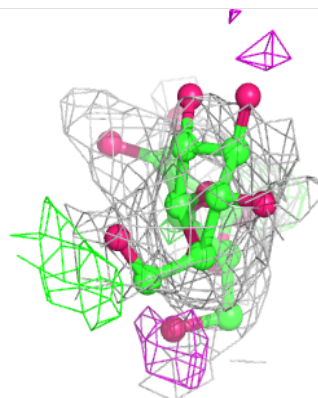
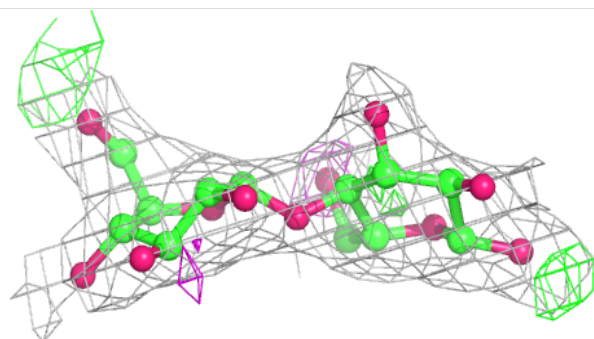
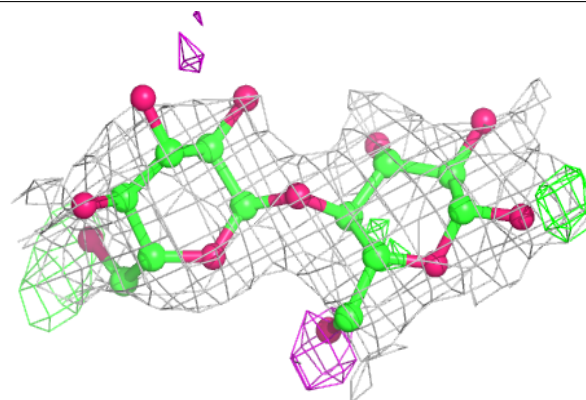


**Electron density around Chain G:**

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

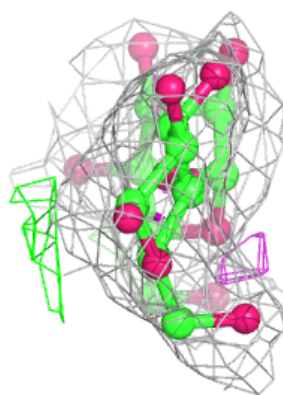
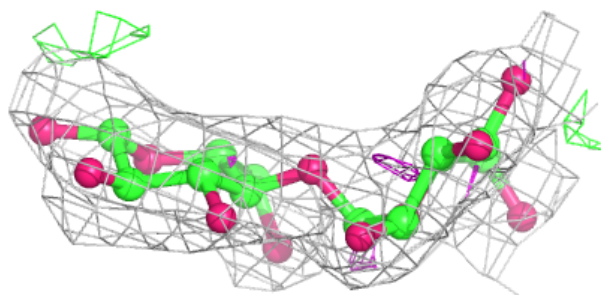
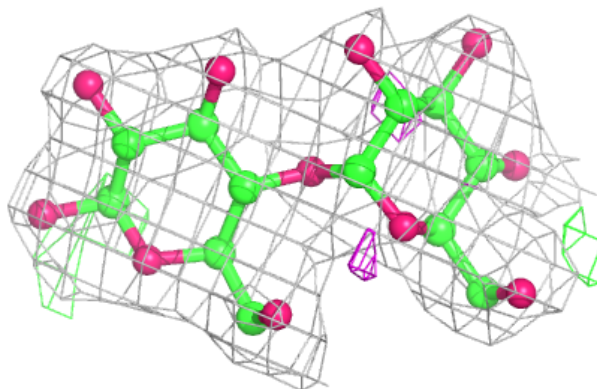
**Electron density around Chain H:**

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



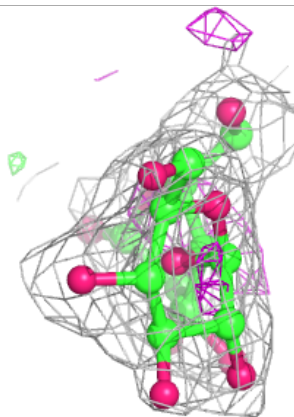
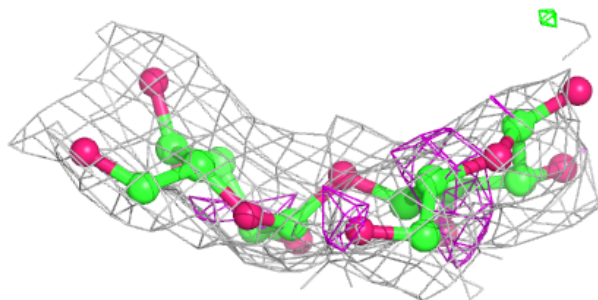
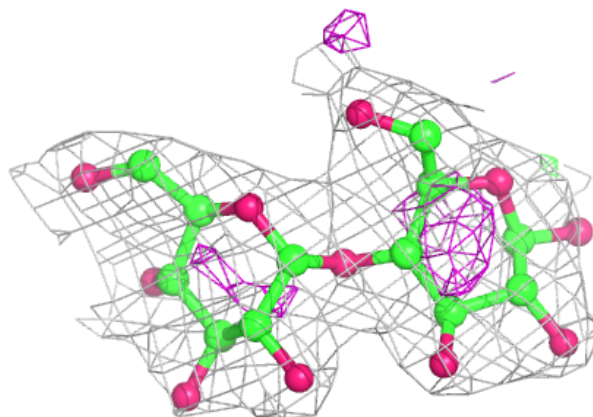
**Electron density around Chain J:**

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



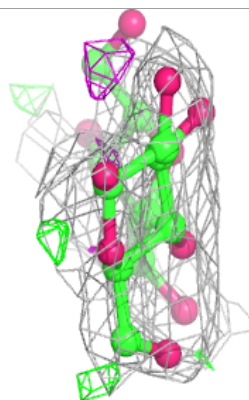
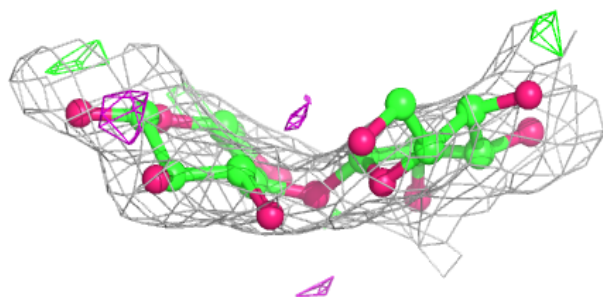
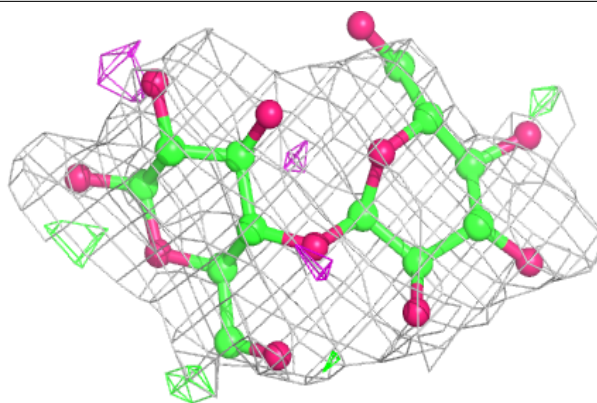
**Electron density around Chain N:**

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

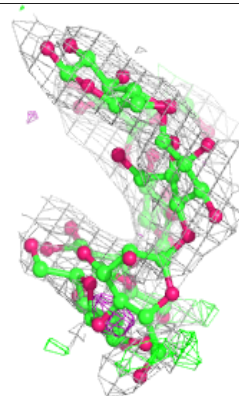
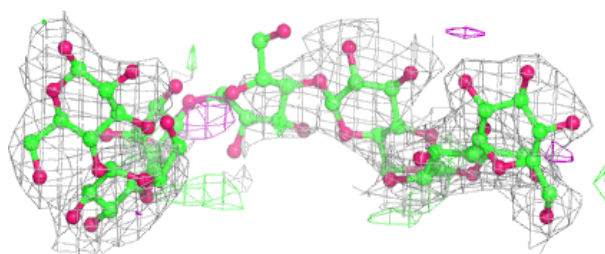
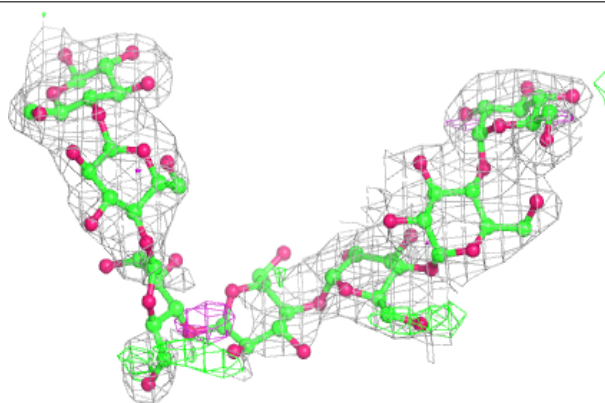


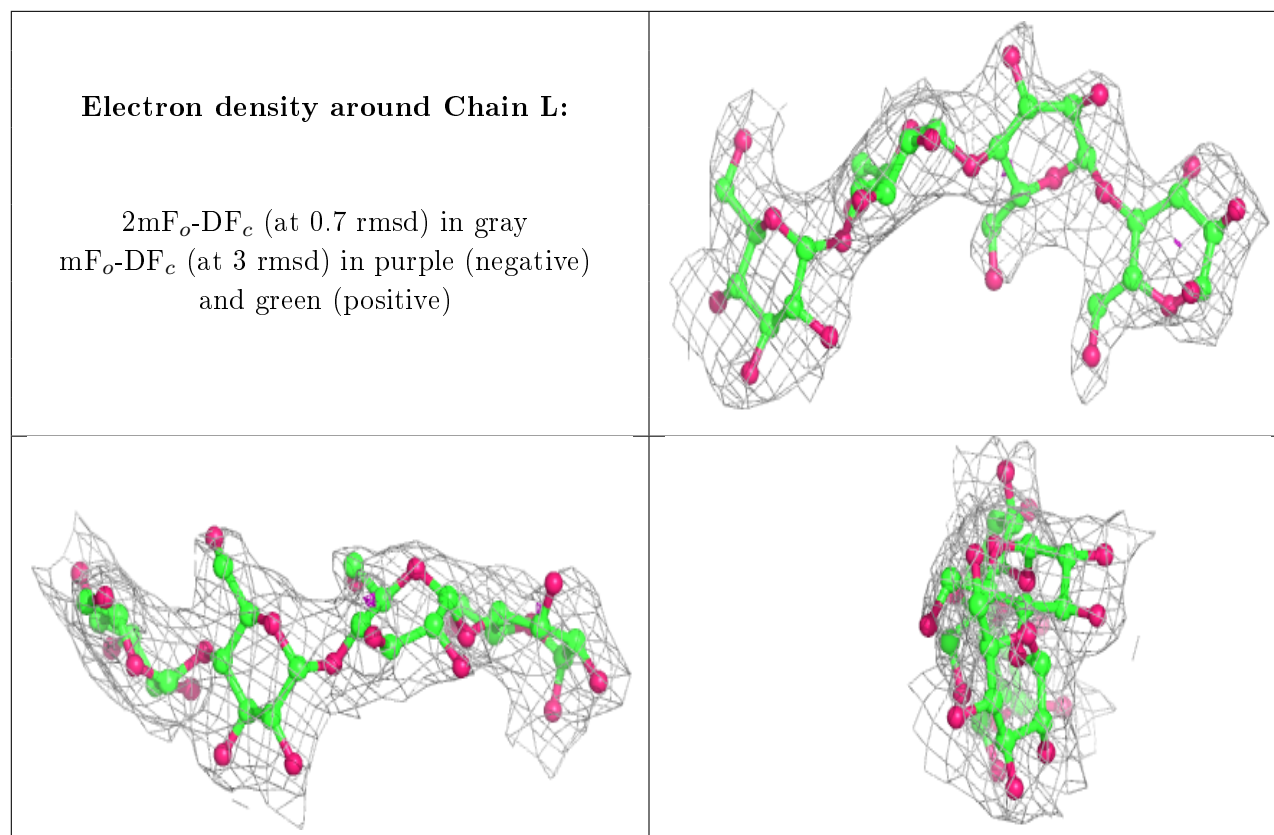
**Electron density around Chain O:**

$2mF_o-DF_c$  (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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	GOL	D	809	6/6	0.58	0.27	85,86,88,89	0
8	BGC	B	810	12/12	0.80	0.28	85,87,89,89	0
7	GOL	B	815	6/6	0.87	0.21	49,53,53,54	0
7	GOL	B	813	6/6	0.88	0.21	47,51,53,55	0
7	GOL	D	808	6/6	0.92	0.12	55,59,59,60	0
7	GOL	A	807	6/6	0.92	0.24	62,63,63,65	0
7	GOL	B	814	6/6	0.92	0.12	72,72,73,74	0
7	GOL	D	807	6/6	0.95	0.09	50,51,52,53	0
7	GOL	A	806	6/6	0.95	0.13	36,38,40,41	0
7	GOL	B	811	6/6	0.96	0.12	47,49,53,55	0
7	GOL	B	812	6/6	0.96	0.15	45,48,49,50	0
7	GOL	A	805	6/6	0.97	0.14	53,57,59,60	0

## 6.5 Other polymers

There are no such residues in this entry.