



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:00 PM UTC

PDB ID : 4LPC / pdb_00004lpc
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

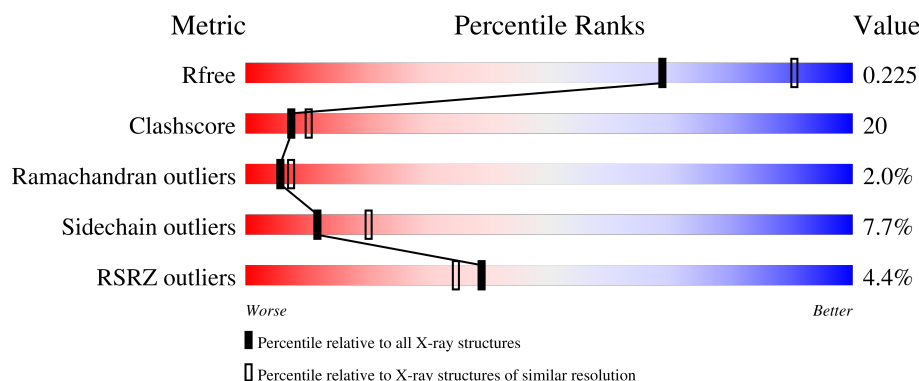
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



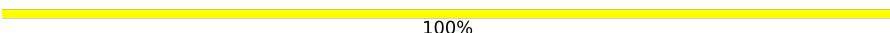
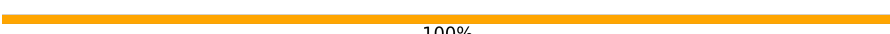
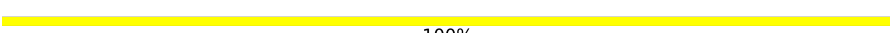
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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% 59% 32% 5%
1	B	612	% 67% 23% 7%
1	C	612	10% 61% 30% 5%
1	D	612	2% 66% 26%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	K	2	 50% 50%
2	M	2	 100%
3	G	3	 67% 33%
4	H	2	 100%
4	J	2	 100%
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	-
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.



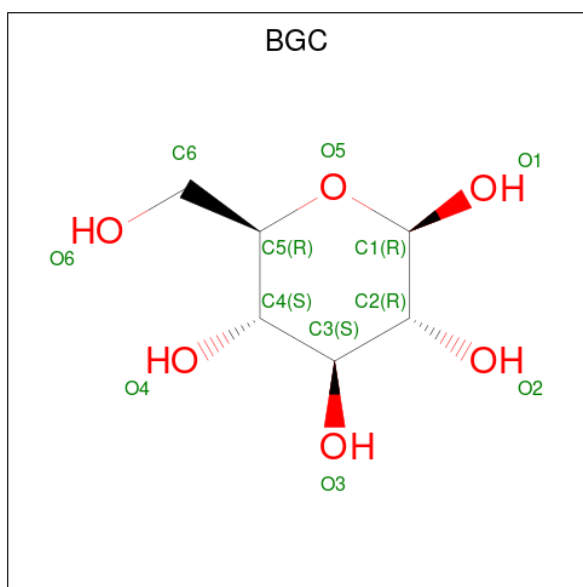
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	L	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 7 is GLYCEROL (CCD ID: 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 (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



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

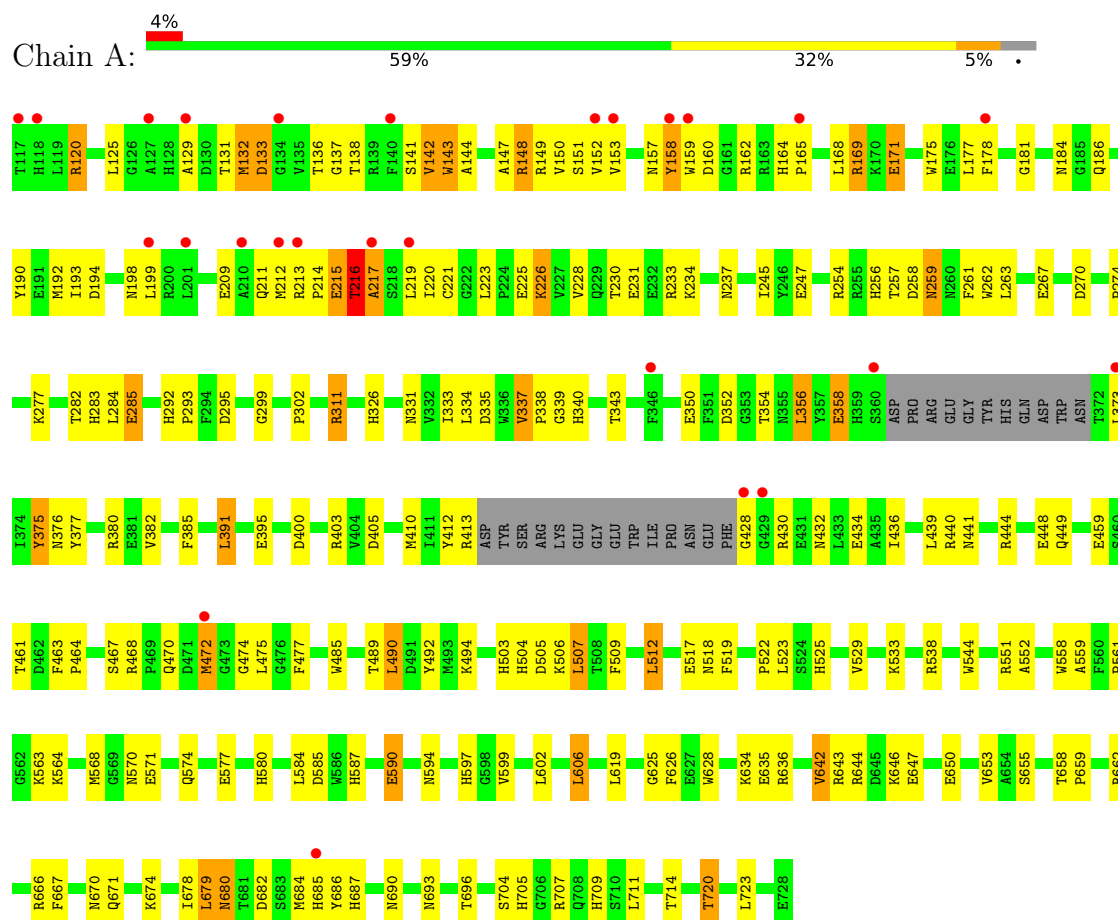
- Molecule 9 is water.

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		

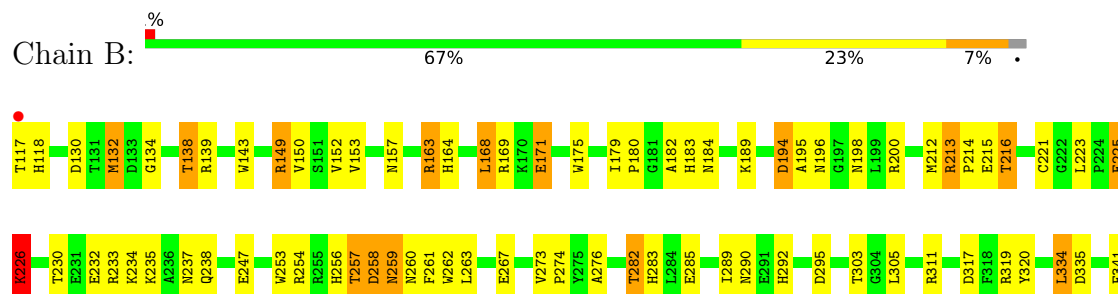
3 Residue-property plots

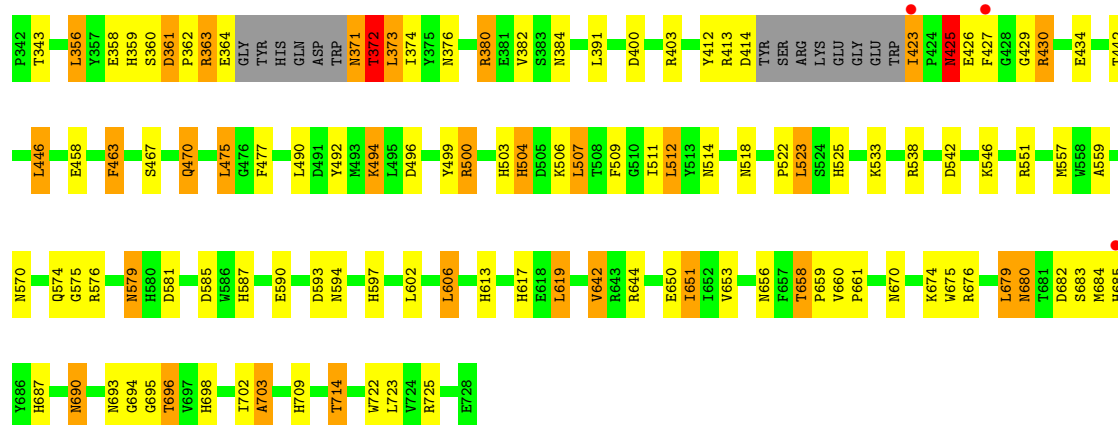
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

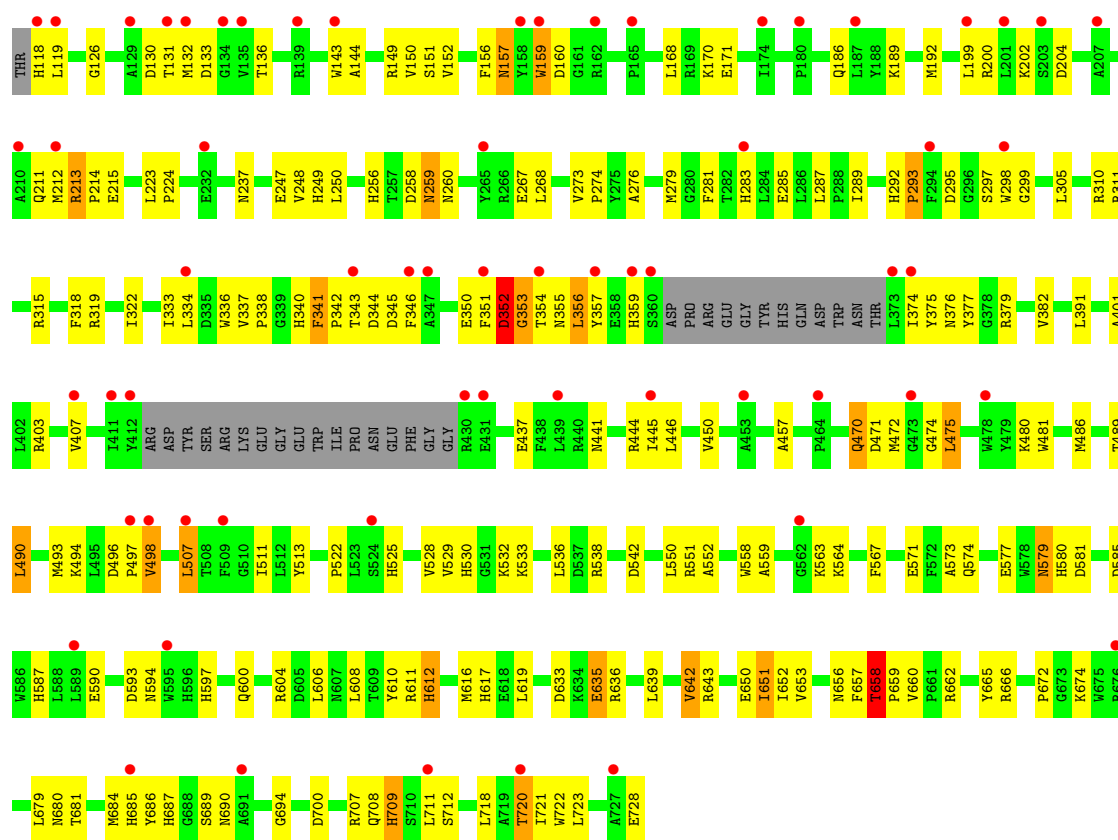


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

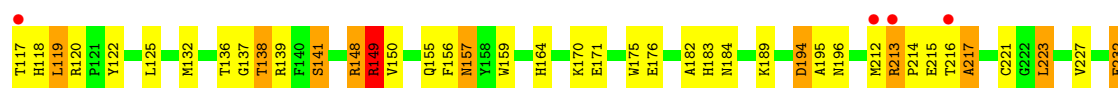


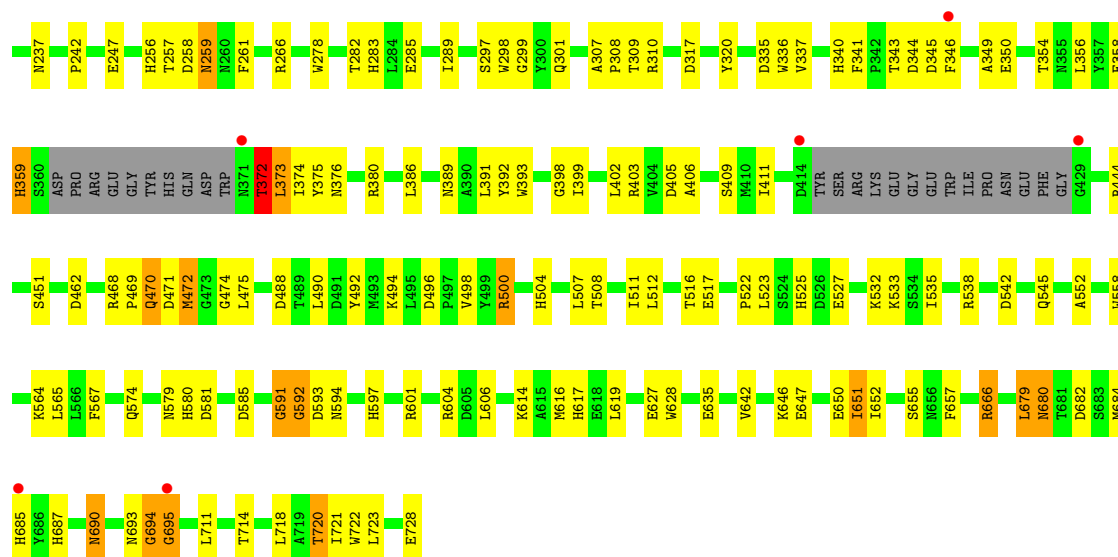


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



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





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

Chain E: 



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

Chain F: 

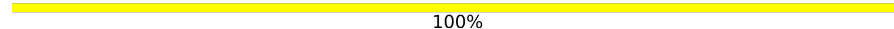


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K: 



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

Chain M: 



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

Chain G: 

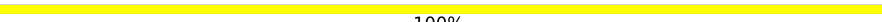


- Molecule 4: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%

BGC1
GLC2

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

Chain J:  100%

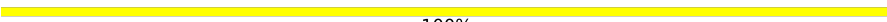
BGC1
GLC2

- 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%

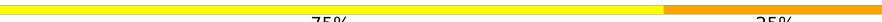
BGC1
GLC2

- 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, α , β , γ	92.19Å 103.42Å 185.94Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 50.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.00-2.39) 90.4 (50.00-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.234 (Not available) , 0.225	Depositor DCC
R_{free} test set	6306 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

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: BGC, 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	0.68	0/5024	0.90	7/6820 (0.1%)
1	B	0.86	0/5092	1.00	14/6914 (0.2%)
1	C	0.46	0/4948	0.76	2/6719 (0.0%)
1	D	0.67	0/5021	0.92	4/6817 (0.1%)
All	All	0.68	0/20085	0.90	27/27270 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	GLN	CA-C-N	8.09	128.02	119.85
1	D	301	GLN	C-N-CA	8.09	128.02	119.85
1	B	496	ASP	CA-C-N	6.02	126.19	119.32
1	B	496	ASP	C-N-CA	6.02	126.19	119.32
1	B	225	GLU	N-CA-C	5.88	117.36	111.07
1	B	361	ASP	CA-C-N	-5.83	113.93	119.76
1	B	361	ASP	C-N-CA	-5.83	113.93	119.76
1	C	341	PHE	CA-C-N	5.72	127.00	119.84
1	C	341	PHE	C-N-CA	5.72	127.00	119.84
1	B	276	ALA	N-CA-C	-5.62	105.15	112.23
1	A	678	ILE	N-CA-C	-5.58	107.84	113.47
1	B	195	ALA	N-CA-C	-5.55	106.35	113.01
1	A	158	TYR	N-CA-C	-5.33	106.35	112.86
1	A	338	PRO	N-CA-C	-5.30	109.17	114.68
1	B	463	PHE	CA-C-N	-5.30	114.27	119.99
1	B	463	PHE	C-N-CA	-5.30	114.27	119.99
1	D	223	LEU	CA-C-N	-5.25	115.17	120.21
1	D	223	LEU	C-N-CA	-5.25	115.17	120.21
1	A	337	VAL	CA-C-N	-5.21	115.51	120.83
1	A	337	VAL	C-N-CA	-5.21	115.51	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ARG	CA-C-N	5.14	125.21	119.87
1	A	120	ARG	C-N-CA	5.14	125.21	119.87
1	B	257	THR	N-CA-C	5.06	117.18	111.11
1	B	382	VAL	N-CA-C	-5.04	105.50	111.00
1	B	423	ILE	CA-C-N	5.04	124.95	119.76
1	B	423	ILE	C-N-CA	5.04	124.95	119.76
1	B	282	THR	N-CA-C	-5.02	107.54	113.97

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	227	0
1	B	4935	0	4647	214	0
1	C	4795	0	4527	167	0
1	D	4867	0	4586	171	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	8	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	30	0
9	B	329	0	0	49	0
9	C	72	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	221	0	0	17	0
All	All	20728	0	18753	785	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 (785) 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:470:GLN:HE21	1:D:470:GLN:N	1.33	1.26
1:B:434:GLU:HG2	9:B:1114:HOH:O	1.35	1.24
1:D:470:GLN:H	1:D:470:GLN:NE2	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: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:A:214:PRO:CA	1:A:215:GLU:HB3	1.82	1.09
1:B:149:ARG:HH21	1:B:149:ARG:HG3	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:HG3	1:D:149:ARG:HH11	1.21	1.03
1:B:470:GLN:HE21	1:B:470:GLN:N	1.54	1.03
1:B:470:GLN:H	1:B:470:GLN:NE2	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:B:132:MET:HE3	1:B:132:MET:HA	1.46	0.97
1:C:470:GLN:HE21	1:C:470:GLN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:380:ARG:HD2	9:B:1203:HOH:O	1.72	0.90
1:D:628:TRP:HE1	4:N:1:BGC:H6C2	1.35	0.89
1:B:613:HIS:NE2	7:B:813:GOL:H32	1.86	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:HE21	1:C:470:GLN:N	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:D:693:ASN:O	1:D:694:GLY:C	2.19	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ARG:HH21	1:B:149:ARG:CG	1.92	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:B:371:ASN:C	1:B:371:ASN:HD22	1.87	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
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: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:216:THR:O	1:D:217:ALA:HB3	1.79	0.79
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.65	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: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: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:ND2	1:B:371:ASN:O	2.18	0.76
1:C:657:PHE:O	1:C:658:THR:HB	1.86	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:A:410:MET:HE1	1:A:439:LEU:HD21	1.69	0.74
1:D:149:ARG:HH11	1:D:149:ARG:CG	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:HIS:HB2	1:C:287:LEU:HD22	1.69	0.74
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:D:232:GLU:H	1:D:232:GLU:CD	1.94	0.74
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.69	0.74
1:A:216:THR:O	1:A:217:ALA:C	2.31	0.73
1:A:533:LYS:O	1:A:538:ARG:NH2	2.21	0.73
1:D:337:VAL:HG23	1:D:337:VAL:O	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: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:CD2	1:D:373:LEU:N	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:A:259:ASN:HD22	1:A:261:PHE:N	1.88	0.69
1:B:149:ARG:C	1:B:149:ARG:HD2	2.18	0.69
1:C:651:ILE:HD13	1:C:722:TRP:HB3	1.74	0.69
1:B:130:ASP:OD1	1:B:139:ARG:NH1	2.18	0.69
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD22	1:D:373:LEU:N	2.09	0.68
1:D:574:GLN:NE2	1:D:585:ASP:H	1.90	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:132:MET:HA	1:A:132:MET:HE3	1.75	0.67
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.48	0.67
1:B:117:THR:OG1	1:B:118:HIS:N	2.23	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:A:142:VAL:O	1:A:143:TRP:HB2	1.95	0.66
1:B:423:ILE:N	9:B:1223:HOH:O	2.26	0.66
1:B:680:ASN:C	1:B:680:ASN:HD22	2.04	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:D:680:ASN:HD22	1:D:680:ASN:C	2.04	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:132:MET:HA	1:B:132:MET:CE	2.24	0.65
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:A:168:LEU:HD23	1:A:168:LEU:C	2.23	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:C:157:ASN:C	1:C:157:ASN:HD22	2.06	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:A:680:ASN:HD22	1:A:680:ASN:C	2.07	0.62
1:C:356:LEU:O	1:C:357:TYR:HB2	1.98	0.62
1:D:372:THR:O	1:D:372:THR:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:247:GLU:OE1	1:B:525:HIS:HD2	1.84	0.60
1:B:259:ASN:HB2	1:B:261:PHE:CE2	2.37	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: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: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
1:B:371:ASN:C	1:B:371:ASN:ND2	2.59	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
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: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: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:C:496:ASP:C	1:C:498:VAL:H	2.12	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:OE2	1:A:635[A]:GLU:N	2.32	0.57
1:D:469:PRO:HG2	1:D:472:MET:HE2	1.84	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:A:171:GLU:CD	1:A:171:GLU:H	2.10	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:A:358:GLU:H	1:A:358:GLU:CD	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:579:ASN:HD22	1:B:579:ASN:C	2.16	0.54
1:C:132:MET:O	1:C:133:ASP:HB2	2.05	0.54
1:C:351:PHE:O	1:C:352:ASP:CB	2.55	0.54
1:C:680:ASN:C	1:C:680:ASN:HD22	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:594:ASN:H	1:B:597:HIS:CD2	2.26	0.53
1:C:297:SER:C	1:C:299:GLY:H	2.15	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:D:565:LEU:HD23	1:D:565:LEU:C	2.34	0.53
1:A:157:ASN:O	1:A:158:TYR:HB2	2.07	0.53
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.57	0.52
1:C:130:ASP:OD2	1:C:132:MET:HE2	2.09	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:B:189:LYS:HZ3	1:B:216:THR:HG22	1.75	0.52
1:A:587:HIS:HA	1:A:590[B]:GLU:HG3	1.90	0.52
1:D:635[B]:GLU:CD	1:D:635[B]:GLU:H	2.17	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:552:ALA:O	1:A:720:THR:CG2	2.58	0.51
1:A:667:PHE:HA	1:A:705:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:A:169:ARG:NH1	2.26	0.51
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:D:297:SER:C	1:D:299:GLY:H	2.17	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:A:577:GLU:CD	9:A:1086:HOH:O	2.54	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:289:ILE:C	1:B:289:ILE:HD12	2.36	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:SER:OG	1:A:705:HIS:HD2	1.95	0.49
1:D:216:THR:CG2	1:D:217:ALA:N	2.74	0.49
1:C:403:ARG:NE	1:C:481:TRP:CZ2	2.80	0.49
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:242:PRO:HB3	1:D:617:HIS:CD2	2.47	0.49
1:D:266:ARG:NH1	9:D:1017:HOH:O	2.36	0.49
1:A:684:MET:HG3	1:A:685[A]:HIS:N	2.24	0.49
1:C:437:GLU:OE2	1:C:437:GLU:HA	2.11	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:A:148:ARG:O	1:A:149:ARG:CG	2.50	0.49
1:A:168:LEU:HD23	1:A:169:ARG:C	2.38	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: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:D:232:GLU:CD	1:D:232:GLU:N	2.67	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:O	1:D:212[B]:MET:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ASP:CG	9:B:1131:HOH:O	2.54	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:A:561:PRO:HA	1:A:643:ARG:NH2	2.29	0.48
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:A:563:LYS:C	1:A:564:LYS:HD3	2.39	0.48
1:B:371:ASN:HB3	1:B:372:THR:CB	2.34	0.48
1:A:120:ARG:NH2	1:A:449:GLN:OE1	2.47	0.48
1:A:245:ILE:CG2	1:A:285:GLU:HB2	2.44	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: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:A:376:ASN:C	1:A:376:ASN:HD22	2.22	0.47
1:B:559:ALA:HB1	1:B:653:VAL:HG21	1.97	0.47
1:B:585:ASP:OD2	5:I:6:GLC:O2	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:410:MET:HE3	1:A:439:LEU:HD11	1.97	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
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: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:233:ARG:HD2	1:A:400:ASP:OD2	2.14	0.46
1:A:258:ASP:HB3	9:A:1111:HOH:O	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:C:551:ARG:C	1:C:681:THR:HG21	2.41	0.46
1:A:441:ASN:OD1	1:A:444:ARG:NH1	2.49	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:289:ILE:C	1:D:289:ILE:HD12	2.42	0.45
1:D:579:ASN:ND2	1:D:581:ASP:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLN:C	1:A:472:MET:H	2.23	0.45
1:B:680:ASN:C	1:B:680:ASN:ND2	2.74	0.45
1:C:656:ASN:C	1:C:656:ASN:ND2	2.73	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
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:285:GLU:HG3	1:A:333:ILE:CG2	2.47	0.45
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.40	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:656:ASN:C	1:C:656:ASN:HD22	2.24	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:NH2	1:B:149:ARG:CG	2.62	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:237:ASN:HD22	1:A:283:HIS:HE1	1.66	0.44
1:A:512:LEU:CD1	3:G:1:GLC:H5	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ARG:HD2	1:C:315:ARG:C	2.42	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: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
1:C:525:HIS:CD2	1:C:525:HIS:H	2.36	0.44
1:A:432:ASN:OD1	1:A:432:ASN:C	2.61	0.44
1:A:467:SER:HA	1:A:477:PHE:O	2.17	0.44
1:A:643:ARG:O	1:A:650:GLU:HA	2.17	0.44
1:A:644:ARG:HD2	9:A:1107:HOH:O	2.17	0.44
1:B:213:ARG:HA	1:B:214:PRO:C	2.43	0.44
1:B:458:GLU:HG3	9:B:1085:HOH:O	2.18	0.44
1:C:450:VAL:HG23	1:C:450:VAL:O	2.16	0.44
1:C:639:LEU:HD13	1:C:657:PHE:HE1	1.81	0.44
1:D:516:THR:C	1:D:517:GLU:HG2	2.42	0.44
7:A:807:GOL:H32	9:A:1078:HOH:O	2.17	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:D:469:PRO:CG	1:D:472:MET:HE2	2.47	0.44
1:A:444:ARG:O	1:A:448:GLU:HG3	2.18	0.44
1:A:635[A]:GLU:H	1:A:635[A]:GLU:CD	2.17	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:C:345:ASP:O	1:C:346:PHE:C	2.61	0.43
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:B:509:PHE:HA	4:J:2:GLC:H62	1.99	0.43
1:D:496:ASP:OD1	1:D:498:VAL:HG22	2.19	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:D:258:ASP:O	1:D:259:ASN:HB2	2.17	0.43
1:A:254[B]:ARG:HE	2:E:2:GLC:C6	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:563:LYS:C	1:C:564:LYS:HD2	2.43	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: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:HD12	1:B:507:LEU:HA	1.77	0.43
1:C:684:MET:HB2	1:C:690:ASN:CG	2.44	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:A:470:GLN:C	1:A:472:MET:N	2.76	0.43
1:A:626:PHE:C	1:A:626:PHE:CD2	2.97	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:H	1:C:690:ASN:ND2	2.05	0.43
1:C:684:MET:HB2	1:C:690:ASN:HB2	2.00	0.43
1:D:406:ALA:O	1:D:409:SER:OG	2.32	0.43
1:D:597:HIS:HB3	1:D:601:ARG:HH12	1.84	0.43
1:A:144:ALA:CB	1:A:352:ASP:HB3	2.43	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:C:144:ALA:HB1	1:C:352:ASP:HB2	2.01	0.43
1:C:529:VAL:O	1:C:530:HIS:C	2.62	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:D:532:LYS:O	1:D:533:LYS:CB	2.67	0.43
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:157:ASN:C	1:A:159:TRP:N	2.76	0.42
1:A:184:ASN:HA	1:A:220:ILE:O	2.19	0.42
1:A:340:HIS:CE1	1:A:405:ASP:OD2	2.53	0.42
1:A:686:TYR:O	1:A:687:HIS:HB2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:656:ASN:C	1:B:656:ASN:HD22	2.26	0.42
1:D:542:ASP:OD1	1:D:542:ASP:C	2.63	0.42
1:D:138:THR:HG23	1:D:182:ALA:C	2.44	0.42
1:D:155:GLN:C	1:D:157:ASN:H	2.27	0.42
1:D:344:ASP:O	1:D:346:PHE:N	2.53	0.42
1:D:374:ILE:O	1:D:375:TYR:C	2.62	0.42
1:A:529:VAL:C	9:A:1086:HOH:O	2.63	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:C:496:ASP:C	1:C:498:VAL:N	2.72	0.42
1:D:343:THR:HG22	1:D:373:LEU:HD21	2.02	0.42
1:A:169:ARG:HB2	1:A:169:ARG:CZ	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:349:ALA:O	1:D:350:GLU:C	2.62	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:651:ILE:HD13	1:D:722:TRP:HB3	2.01	0.42
1:D:718:LEU:HD23	1:D:718:LEU:HA	1.83	0.42
1:A:634:LYS:O	1:A:635[B]:GLU:C	2.62	0.41
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:A:277:LYS:NZ	9:A:1112:HOH:O	2.43	0.41
1:B:259:ASN:ND2	1:B:259:ASN:H	2.15	0.41
1:B:380:ARG:HE	1:B:380:ARG:HB2	1.71	0.41
1:D:308:PRO:O	1:D:309:THR:C	2.61	0.41
1:A:625:GLY:O	1:A:643:ARG:HD2	2.20	0.41
1:B:273:VAL:HB	1:B:274:PRO:HD3	2.01	0.41
1:B:518:ASN:ND2	4:H:2:GLC:H62	2.25	0.41
1:B:642:VAL:HG13	1:B:650:GLU:HB3	2.02	0.41
1:A:559:ALA:HB1	1:A:653:VAL:HG21	2.02	0.41
1:A:568:MET:HG3	1:A:584:LEU:HD11	2.03	0.41
1:B:693:ASN:O	1:B:694:GLY:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ALA:HA	1:D:308:PRO:HD3	1.87	0.41
1:A:162:ARG:HE	1:A:162:ARG:HB2	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: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:A:337:VAL:C	1:A:339:GLY:H	2.28	0.41
1:D:373:LEU:H	1:D:373:LEU:HD23	1.79	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: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:606:LEU:HD13	1:B:679:LEU:HD11	2.03	0.41
1:B:674:LYS:HG2	1:B:698:HIS:HD2	1.85	0.41
1:C:289:ILE:C	1:C:289:ILE:HD12	2.46	0.41
1:C:292:HIS:HA	1:C:293:PRO:HD3	1.89	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:N	1:D:564:LYS:HD2	2.36	0.40
1:B:363:ARG:HA	1:B:364:GLU:OE1	2.21	0.40
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:D:125:LEU:HD23	1:D:125:LEU:HA	1.77	0.40
1:D:183:HIS:CD2	1:D:184:ASN:O	2.74	0.40
1:D:405:ASP:OD1	1:D:405:ASP:N	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:B:702:ILE:O	1:B:703:ALA:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:157:ASN:C	1:C:157:ASN:ND2	2.76	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%)	8	12
1	B	594/612 (97%)	566 (95%)	18 (3%)	10 (2%)	7	10
1	C	577/612 (94%)	512 (89%)	49 (8%)	16 (3%)	4	3
1	D	586/612 (96%)	545 (93%)	29 (5%)	12 (2%)	6	7
All	All	2343/2448 (96%)	2169 (93%)	127 (5%)	47 (2%)	6	7

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

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Mol	Chain	Res	Type
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
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%)	469 (93%)	34 (7%)	14	25
1	B	510/521 (98%)	461 (90%)	49 (10%)	8	12
1	C	495/521 (95%)	461 (93%)	34 (7%)	14	24
1	D	503/521 (96%)	465 (92%)	38 (8%)	12	21
All	All	2011/2084 (96%)	1856 (92%)	155 (8%)	12	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
1	A	259	ASN
1	A	285	GLU
1	A	311	ARG
1	A	356	LEU
1	A	358	GLU
1	A	380	ARG
1	A	391	LEU
1	A	434	GLU
1	A	472	MET
1	A	490	LEU
1	A	507	LEU
1	A	512	LEU
1	A	523	LEU
1	A	590[A]	GLU

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Mol	Chain	Res	Type
1	A	590[B]	GLU
1	A	606	LEU
1	A	619	LEU
1	A	642	VAL
1	A	646	LYS
1	A	647	GLU
1	A	679	LEU
1	A	680	ASN
1	A	720	THR
1	A	723	LEU
1	B	132	MET
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	226	LYS
1	B	258	ASP
1	B	259	ASN
1	B	263	LEU
1	B	290	ASN
1	B	305	LEU
1	B	334	LEU
1	B	356	LEU
1	B	360	SER
1	B	371	ASN
1	B	372	THR
1	B	373	LEU
1	B	374	ILE
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	494	LYS

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Mol	Chain	Res	Type
1	B	500	ARG
1	B	504	HIS
1	B	507	LEU
1	B	511	ILE
1	B	512	LEU
1	B	523	LEU
1	B	579	ASN
1	B	606	LEU
1	B	619	LEU
1	B	642	VAL
1	B	651	ILE
1	B	658	THR
1	B	679	LEU
1	B	680	ASN
1	B	690	ASN
1	B	714	THR
1	B	723	LEU
1	C	119	LEU
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	248	VAL
1	C	258	ASP
1	C	259	ASN
1	C	305	LEU
1	C	310	ARG
1	C	337	VAL
1	C	350	GLU
1	C	352	ASP
1	C	356	LEU
1	C	391	LEU
1	C	446	LEU
1	C	470	GLN
1	C	471	ASP
1	C	475	LEU
1	C	490	LEU
1	C	498	VAL
1	C	507	LEU
1	C	511	ILE

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Mol	Chain	Res	Type
1	C	579	ASN
1	C	619	LEU
1	C	635	GLU
1	C	642	VAL
1	C	651	ILE
1	C	658	THR
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	257	THR
1	D	356	LEU
1	D	359	HIS
1	D	372	THR
1	D	373	LEU
1	D	380	ARG
1	D	391	LEU
1	D	411	ILE
1	D	444	ARG
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	494	LYS
1	D	500	ARG
1	D	507	LEU
1	D	523	LEU
1	D	606	LEU
1	D	619	LEU
1	D	646	LYS
1	D	651	ILE

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Mol	Chain	Res	Type
1	D	666	ARG
1	D	679	LEU
1	D	680	ASN
1	D	690	ASN
1	D	720	THR

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	157	ASN
1	A	164	HIS
1	A	211	GLN
1	A	237	ASN
1	A	238	GLN
1	A	256	HIS
1	A	259	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	514	ASN
1	A	525	HIS
1	A	570	ASN
1	A	574	GLN
1	A	579	ASN
1	A	597	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	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	229	GLN

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Mol	Chain	Res	Type
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	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	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
1	B	693	ASN
1	B	705	HIS
1	C	157	ASN
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	283	HIS
1	C	290	ASN
1	C	301	GLN
1	C	331	ASN

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Mol	Chain	Res	Type
1	C	355	ASN
1	C	432	ASN
1	C	470	GLN
1	C	514	ASN
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	600	GLN
1	C	612	HIS
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	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	340	HIS
1	D	359	HIS
1	D	443	ASN
1	D	470	GLN
1	D	514	ASN
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

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Mol	Chain	Res	Type
1	D	656	ASN
1	D	680	ASN
1	D	687	HIS
1	D	690	ASN
1	D	693	ASN
1	D	705	HIS

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 ⓘ

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	0.51	0	17,17,17	0.78	0
2	GLC	E	2	2	11,11,12	0.49	0	15,15,17	1.28	1 (6%)
2	GLC	F	1	2	12,12,12	0.69	0	17,17,17	1.14	2 (11%)
2	GLC	F	2	2	11,11,12	0.47	0	15,15,17	2.11	2 (13%)
3	GLC	G	1	3	12,12,12	0.50	0	17,17,17	1.63	4 (23%)
3	GLC	G	2	3	11,11,12	0.75	0	15,15,17	0.81	0
3	GLC	G	3	3	11,11,12	0.58	0	15,15,17	1.35	4 (26%)
4	BGC	H	1	4	12,12,12	0.72	0	17,17,17	1.64	4 (23%)
4	GLC	H	2	4	11,11,12	0.41	0	15,15,17	2.22	3 (20%)
5	BGC	I	1	5	12,12,12	0.45	0	17,17,17	1.92	6 (35%)
5	GLC	I	2	5	11,11,12	0.49	0	15,15,17	1.62	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLC	I	3	5	11,11,12	0.57	0	15,15,17	1.11	1 (6%)
5	GLC	I	4	5	11,11,12	0.57	0	15,15,17	1.33	1 (6%)
5	GLC	I	5	5	11,11,12	0.63	0	15,15,17	2.04	4 (26%)
5	GLC	I	6	5	11,11,12	0.61	0	15,15,17	1.05	1 (6%)
5	GLC	I	7	5	11,11,12	0.65	0	15,15,17	1.21	2 (13%)
4	BGC	J	1	4	12,12,12	0.58	0	17,17,17	1.18	0
4	GLC	J	2	4	11,11,12	0.76	0	15,15,17	1.02	0
2	GLC	K	1	2	12,12,12	0.56	0	17,17,17	0.53	0
2	GLC	K	2	2	11,11,12	0.66	0	15,15,17	0.92	1 (6%)
6	GLC	L	1	6	12,12,12	0.65	0	17,17,17	1.42	3 (17%)
6	GLC	L	2	6	11,11,12	0.74	0	15,15,17	1.68	2 (13%)
6	GLC	L	3	6	11,11,12	0.57	0	15,15,17	1.10	1 (6%)
6	GLC	L	4	6	11,11,12	0.77	0	15,15,17	1.27	2 (13%)
2	GLC	M	1	2	12,12,12	0.49	0	17,17,17	0.79	0
2	GLC	M	2	2	11,11,12	0.56	0	15,15,17	1.33	2 (13%)
4	BGC	N	1	4	12,12,12	0.67	0	17,17,17	2.05	5 (29%)
4	GLC	N	2	4	11,11,12	0.58	0	15,15,17	1.78	3 (20%)
4	BGC	O	1	4	12,12,12	0.53	0	17,17,17	1.53	3 (17%)
4	GLC	O	2	4	11,11,12	0.51	0	15,15,17	1.60	2 (13%)

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
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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	GLC	C1-O5-C5	7.18	121.81	112.19
2	F	2	GLC	C1-O5-C5	6.76	121.25	112.19
4	N	2	GLC	C1-O5-C5	5.55	119.63	112.19
6	L	2	GLC	C1-C2-C3	4.64	116.39	109.64
5	I	5	GLC	C1-O5-C5	4.55	118.28	112.19
5	I	1	BGC	C4-C3-C2	-4.44	103.04	110.83
4	H	1	BGC	O5-C1-C2	-4.43	102.52	110.30
4	N	1	BGC	O5-C5-C4	4.43	117.67	109.70
4	O	2	GLC	C1-O5-C5	4.37	118.04	112.19
3	G	1	GLC	C1-O5-C5	4.19	121.75	113.65
5	I	2	GLC	C1-O5-C5	4.08	117.66	112.19
6	L	1	GLC	C4-C3-C2	3.82	117.53	110.83
4	N	1	BGC	C1-C2-C3	-3.58	103.06	110.36
6	L	2	GLC	C2-C3-C4	3.50	117.02	110.86
4	O	1	BGC	C4-C3-C2	-3.50	104.69	110.83
4	N	1	BGC	O5-C1-C2	-3.42	104.28	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	3	GLC	C1-O5-C5	3.40	116.74	112.19
5	I	5	GLC	C3-C4-C5	-3.36	104.14	110.23
5	I	5	GLC	C1-C2-C3	3.32	114.47	109.64
5	I	4	GLC	C1-O5-C5	3.27	116.57	112.19
6	L	4	GLC	C1-C2-C3	3.27	114.41	109.64
5	I	1	BGC	C1-O5-C5	3.13	119.70	113.65
4	N	1	BGC	C3-C4-C5	3.11	115.87	110.23
3	G	1	GLC	O5-C5-C4	3.07	115.22	109.70
5	I	7	GLC	C1-O5-C5	2.91	116.08	112.19
5	I	2	GLC	C3-C4-C5	-2.89	105.00	110.23
6	L	4	GLC	C1-O5-C5	2.86	116.02	112.19
2	F	2	GLC	O5-C5-C4	2.83	117.71	110.83
2	K	2	GLC	C1-O5-C5	2.77	115.91	112.19
4	H	1	BGC	C1-O5-C5	-2.72	108.38	113.65
4	N	2	GLC	C3-C4-C5	2.70	115.14	110.23
2	F	1	GLC	C1-C2-C3	2.66	115.78	110.36
4	H	2	GLC	C2-C3-C4	-2.65	106.20	110.86
5	I	1	BGC	O4-C4-C5	2.64	115.82	109.32
2	E	2	GLC	C1-O5-C5	2.63	115.71	112.19
5	I	1	BGC	O2-C2-C1	2.63	115.31	109.25
6	L	1	GLC	C1-C2-C3	2.62	115.69	110.36
4	O	2	GLC	C2-C3-C4	-2.58	106.32	110.86
2	F	1	GLC	C4-C3-C2	2.58	115.35	110.83
4	H	2	GLC	O5-C5-C6	2.56	112.65	107.66
4	N	2	GLC	O5-C5-C4	2.51	116.93	110.83
5	I	2	GLC	O4-C4-C5	2.50	115.47	109.32
5	I	1	BGC	O4-C4-C3	2.47	116.19	110.38
5	I	3	GLC	C3-C4-C5	-2.43	105.83	110.23
5	I	6	GLC	O5-C1-C2	-2.42	105.02	110.79
3	G	1	GLC	O5-C1-C2	2.38	114.49	110.30
3	G	1	GLC	C4-C3-C2	-2.36	106.69	110.83
4	O	1	BGC	O4-C4-C3	2.32	115.84	110.38
3	G	3	GLC	C1-O5-C5	2.31	115.28	112.19
5	I	7	GLC	C2-C3-C4	-2.25	106.91	110.86
3	G	3	GLC	O5-C1-C2	-2.25	105.43	110.79
2	M	2	GLC	C1-C2-C3	-2.18	106.47	109.64
4	N	1	BGC	O2-C2-C1	2.18	114.28	109.25
4	O	1	BGC	O2-C2-C1	2.18	114.27	109.25
4	H	1	BGC	O4-C4-C5	-2.16	104.00	109.32
3	G	3	GLC	O2-C2-C3	2.15	114.61	110.15
5	I	5	GLC	O5-C5-C6	2.14	111.83	107.66
6	L	1	GLC	C3-C4-C5	2.14	114.11	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	BGC	C4-C3-C2	2.13	114.56	110.83
5	I	1	BGC	O3-C3-C4	2.10	115.33	110.38
2	M	2	GLC	C2-C3-C4	-2.08	107.20	110.86
3	G	3	GLC	C3-C4-C5	2.01	113.87	110.23

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	H	2	GLC	C4-C5-C6-O6
4	N	1	BGC	O5-C5-C6-O6
4	O	1	BGC	C4-C5-C6-O6
6	L	2	GLC	C4-C5-C6-O6
4	O	1	BGC	O5-C5-C6-O6
5	I	1	BGC	O5-C5-C6-O6
5	I	4	GLC	O5-C5-C6-O6
6	L	3	GLC	O5-C5-C6-O6
5	I	2	GLC	O5-C5-C6-O6
6	L	2	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
5	I	3	GLC	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
5	I	2	GLC	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
3	G	1	GLC	C4-C5-C6-O6
5	I	6	GLC	C4-C5-C6-O6
5	I	3	GLC	C4-C5-C6-O6
5	I	6	GLC	O5-C5-C6-O6
2	M	2	GLC	O5-C5-C6-O6
4	J	1	BGC	O5-C5-C6-O6
5	I	1	BGC	C4-C5-C6-O6
3	G	3	GLC	O5-C5-C6-O6
4	J	1	BGC	C4-C5-C6-O6
3	G	3	GLC	C4-C5-C6-O6
5	I	4	GLC	C4-C5-C6-O6
4	H	1	BGC	O5-C5-C6-O6
6	L	3	GLC	C4-C5-C6-O6
4	H	1	BGC	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

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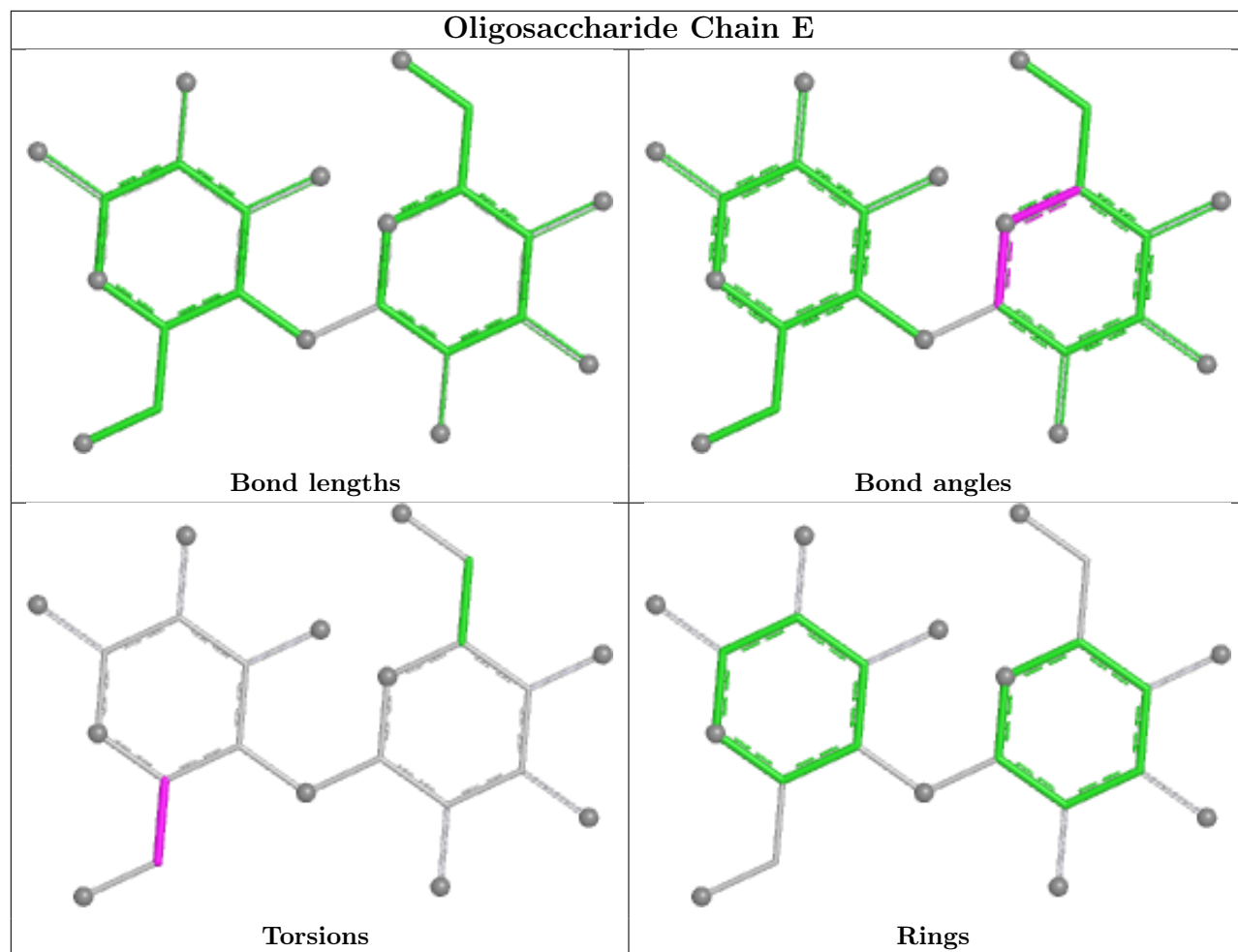
Mol	Chain	Res	Type	Atoms
5	I	5	GLC	O5-C5-C6-O6
2	M	2	GLC	C4-C5-C6-O6
4	N	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6

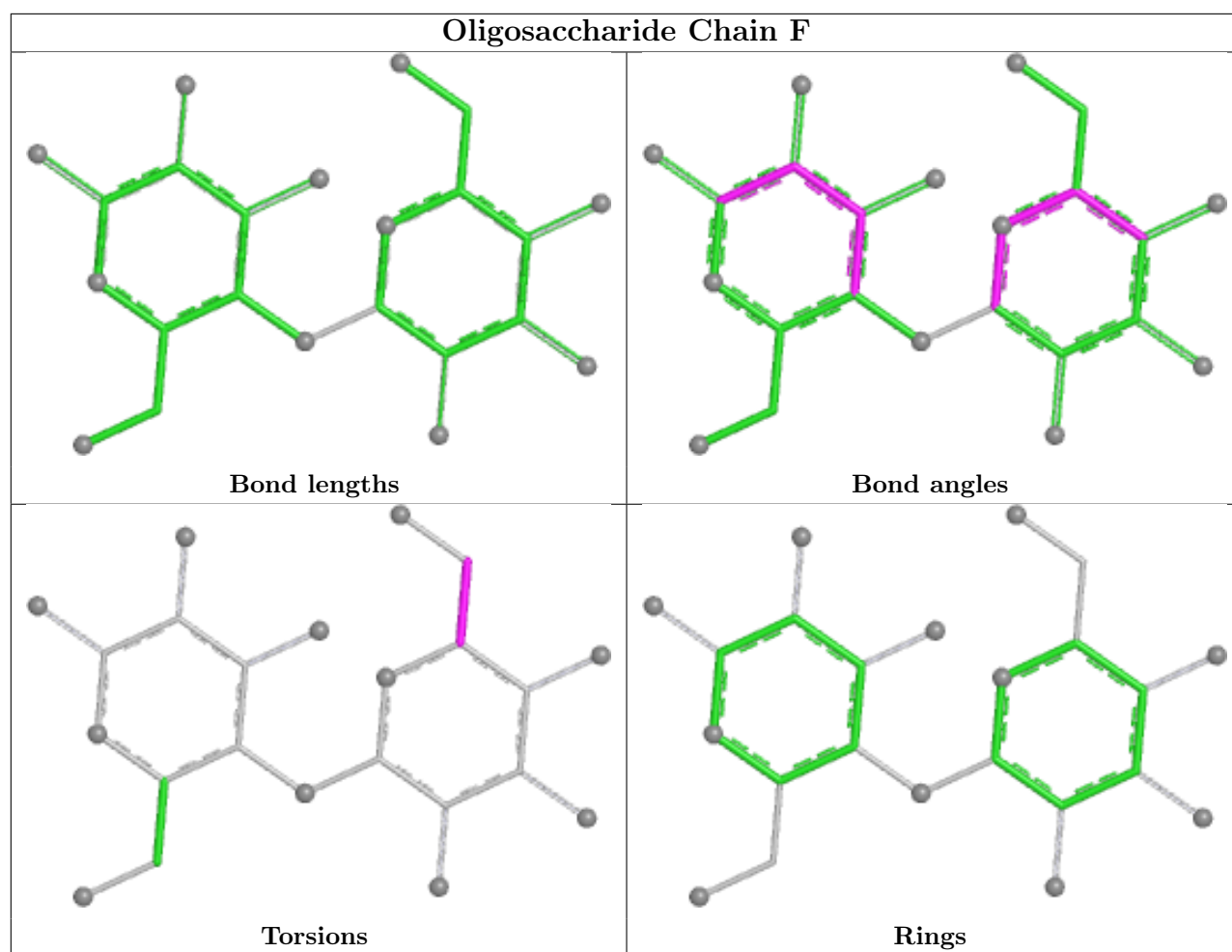
There are no ring outliers.

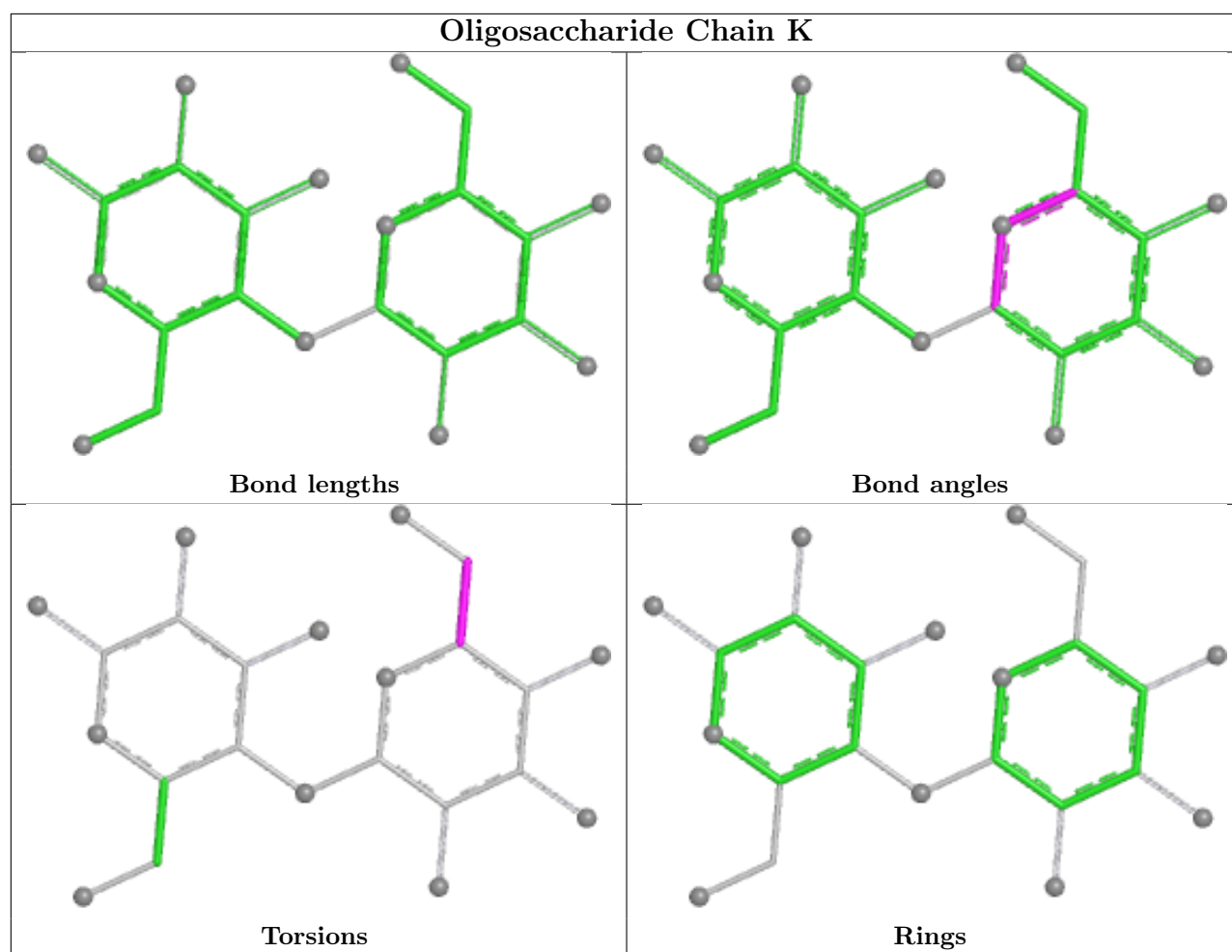
17 monomers are involved in 40 short contacts:

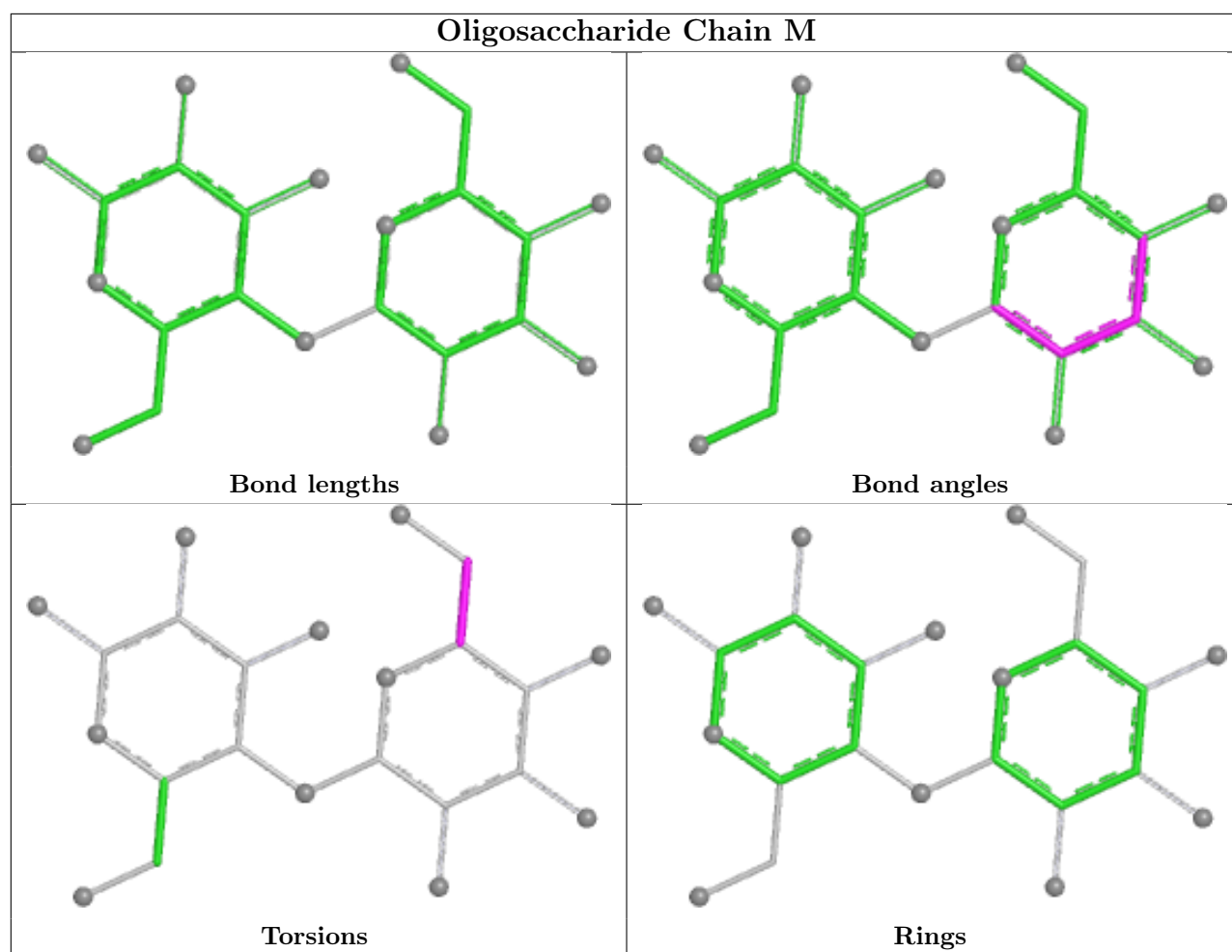
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	GLC	4	0
6	L	4	GLC	1	0
5	I	3	GLC	3	0
4	H	2	GLC	2	0
4	J	2	GLC	3	0
5	I	1	BGC	1	0
5	I	4	GLC	1	0
2	E	2	GLC	2	0
4	H	1	BGC	2	0
2	F	2	GLC	4	0
4	J	1	BGC	4	0
3	G	2	GLC	1	0
2	M	1	GLC	1	0
4	N	1	BGC	7	0
5	I	6	GLC	2	0
3	G	1	GLC	5	0
5	I	5	GLC	2	0

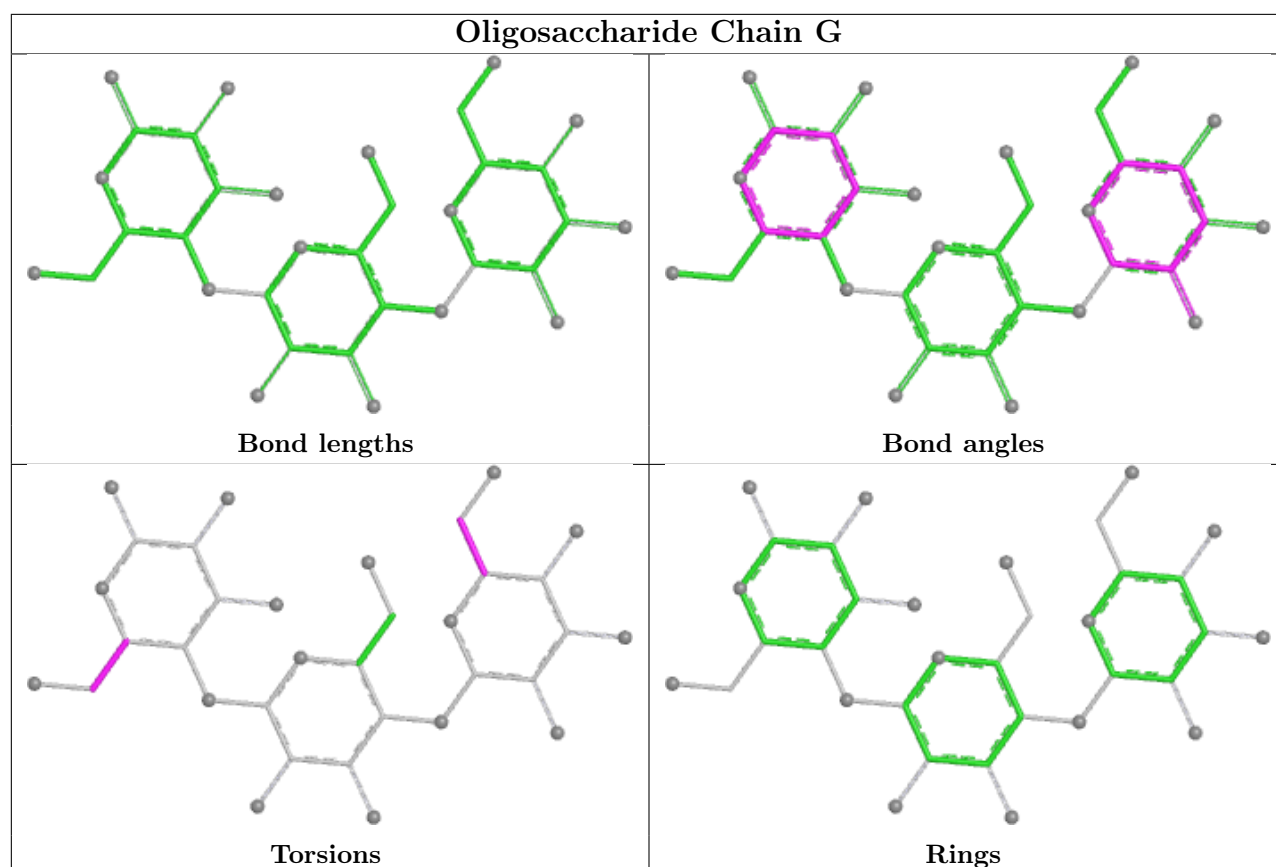
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

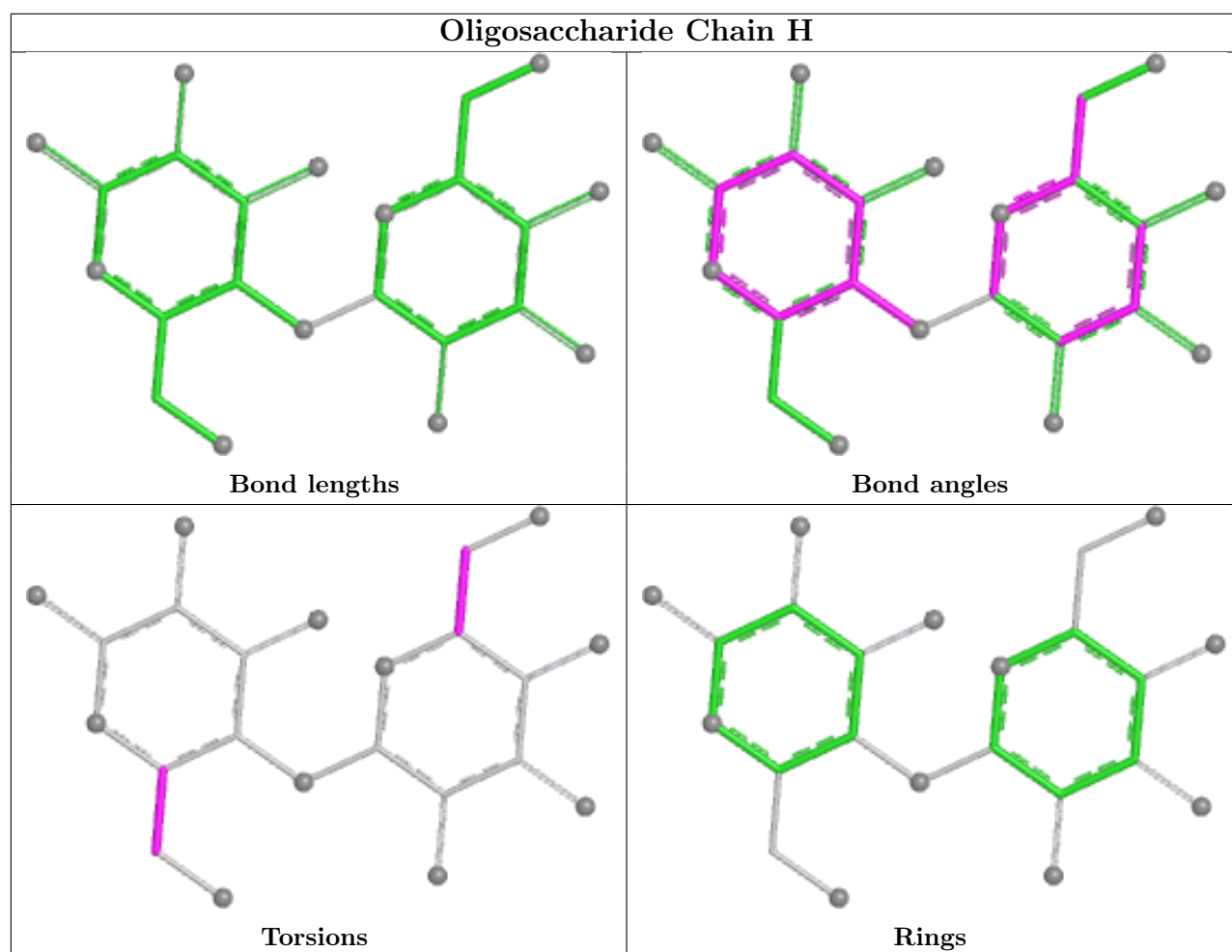


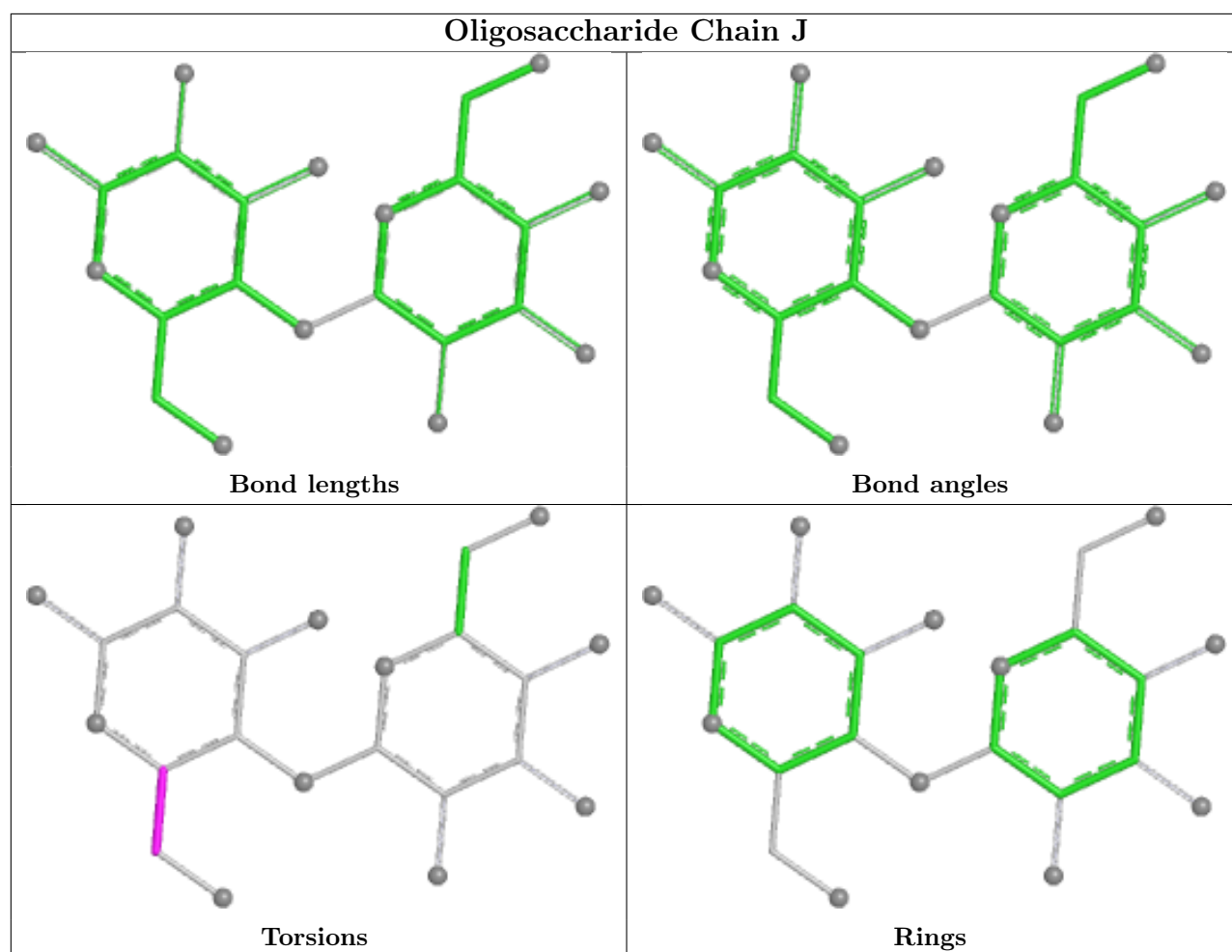


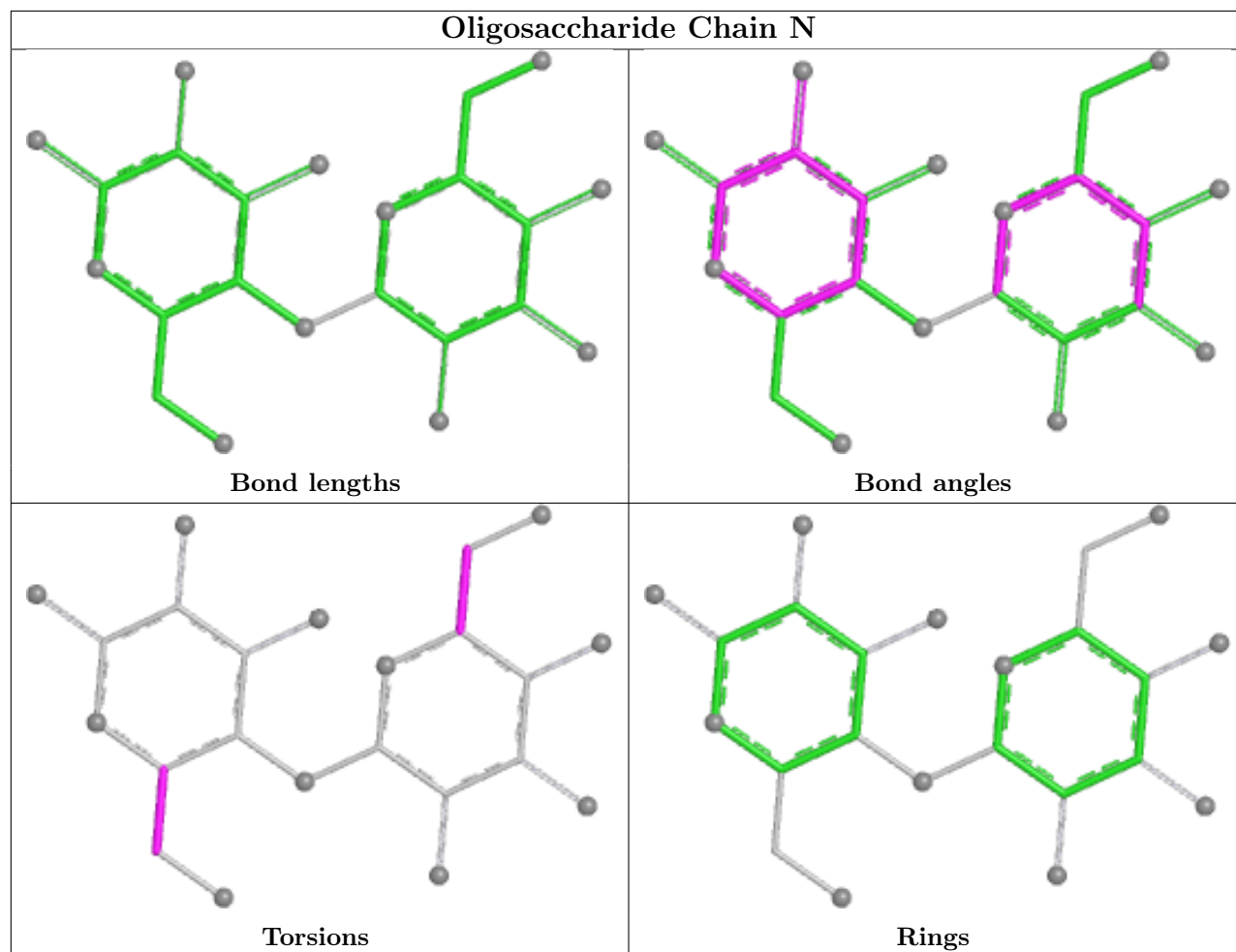


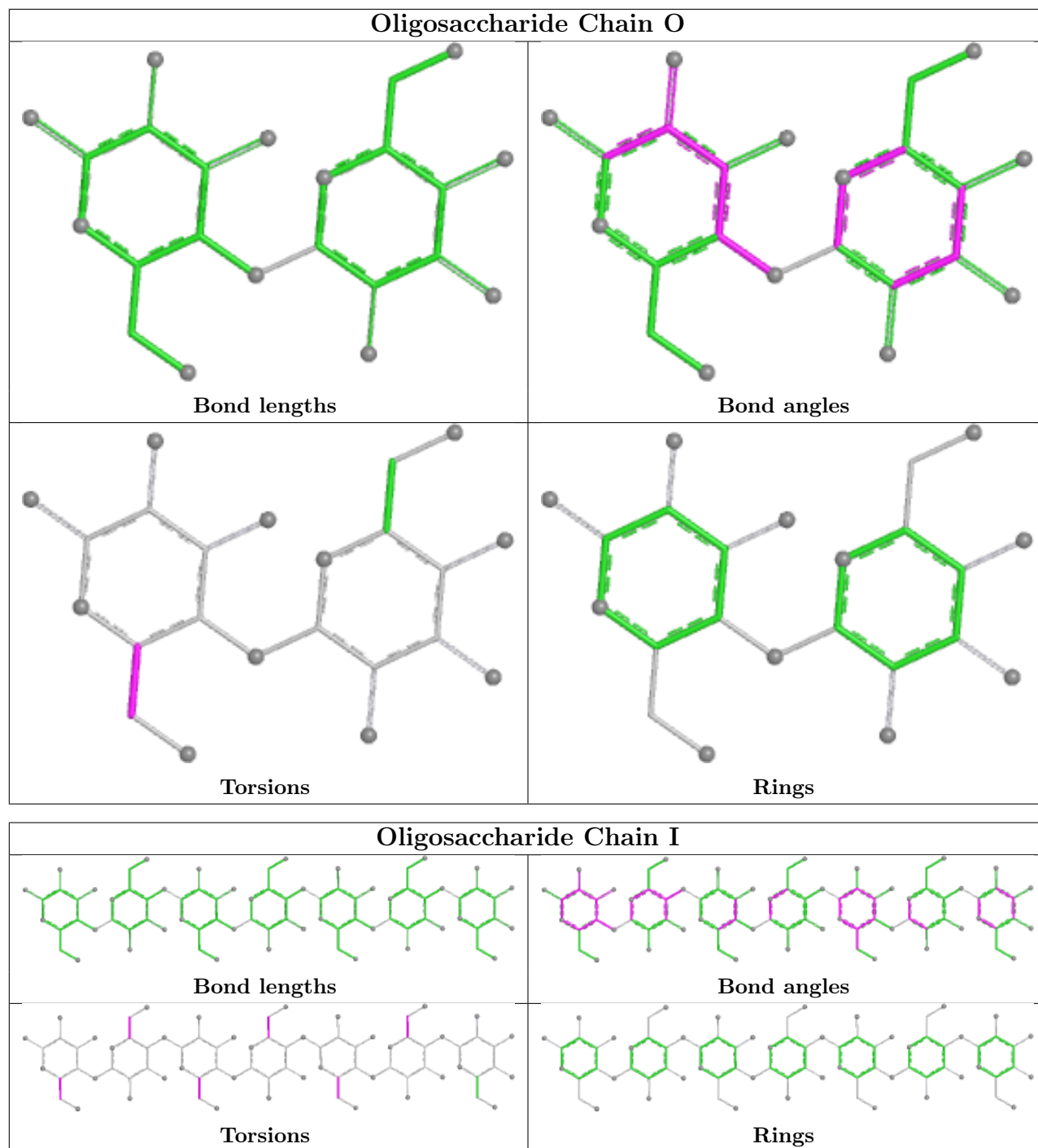


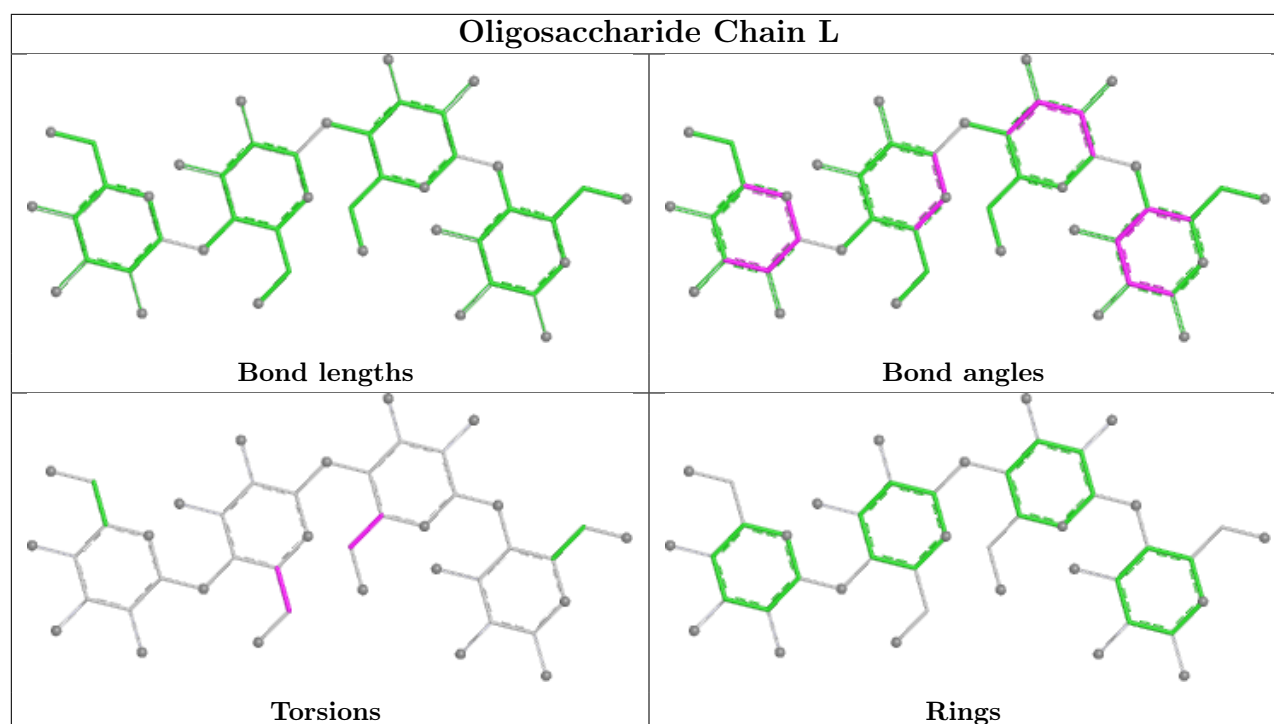












5.6 Ligand geometry [i](#)

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	A	807	-	5,5,5	0.44	0	5,5,5	0.92	0
7	GOL	B	812	-	5,5,5	0.44	0	5,5,5	0.70	0
7	GOL	D	809	-	5,5,5	0.36	0	5,5,5	0.47	0
8	BGC	B	810	-	12,12,12	0.48	0	17,17,17	0.88	1 (5%)
7	GOL	B	811	-	5,5,5	0.47	0	5,5,5	0.27	0
7	GOL	D	807	-	5,5,5	0.35	0	5,5,5	0.36	0
7	GOL	A	806	-	5,5,5	0.27	0	5,5,5	0.48	0
7	GOL	B	814	-	5,5,5	0.39	0	5,5,5	0.42	0
7	GOL	D	808	-	5,5,5	0.35	0	5,5,5	0.45	0
7	GOL	B	815	-	5,5,5	0.46	0	5,5,5	0.51	0
7	GOL	B	813	-	5,5,5	0.56	0	5,5,5	0.91	0
7	GOL	A	805	-	5,5,5	0.49	0	5,5,5	0.34	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	A	807	-	-	0/4/4/4	-
7	GOL	B	812	-	-	4/4/4/4	-
7	GOL	D	809	-	-	2/4/4/4	-
8	BGC	B	810	-	-	1/2/22/22	0/1/1/1
7	GOL	B	811	-	-	0/4/4/4	-
7	GOL	D	807	-	-	2/4/4/4	-
7	GOL	A	806	-	-	0/4/4/4	-
7	GOL	B	814	-	-	2/4/4/4	-
7	GOL	D	808	-	-	3/4/4/4	-
7	GOL	B	815	-	-	4/4/4/4	-
7	GOL	B	813	-	-	2/4/4/4	-
7	GOL	A	805	-	-	4/4/4/4	-

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	2.07	114.42	109.32

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
7	A	805	GOL	O2-C2-C3-O3
7	B	812	GOL	O2-C2-C3-O3
7	B	813	GOL	O1-C1-C2-O2
7	B	815	GOL	O1-C1-C2-O2
7	D	807	GOL	O1-C1-C2-O2
7	D	809	GOL	O1-C1-C2-O2
7	A	805	GOL	O1-C1-C2-O2
7	B	815	GOL	O2-C2-C3-O3
7	D	808	GOL	O2-C2-C3-O3
8	B	810	BGC	O5-C5-C6-O6
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	A	807	GOL	6	0
7	B	812	GOL	2	0
7	D	809	GOL	1	0
7	D	808	GOL	1	0
7	B	815	GOL	7	0
7	B	813	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	587/612 (95%)	0.18	26 (4%) 39 34	16, 48, 124, 144	6 (1%)
1	B	598/612 (97%)	-0.24	4 (0%) 84 81	17, 38, 63, 77	7 (1%)
1	C	582/612 (95%)	0.96	63 (10%) 11 8	41, 88, 123, 143	3 (0%)
1	D	588/612 (96%)	-0.05	10 (1%) 69 65	23, 49, 70, 86	7 (1%)
All	All	2355/2448 (96%)	0.21	103 (4%) 39 34	16, 51, 114, 144	23 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	373	LEU	7.0
1	D	429	GLY	4.9
1	C	374	ILE	4.8
1	A	428	GLY	4.4
1	B	685[A]	HIS	4.4
1	C	412	TYR	4.3
1	A	685[A]	HIS	4.2
1	A	159	TRP	4.0
1	A	201	LEU	3.9
1	C	354	THR	3.9
1	A	212	MET	3.8
1	C	118	HIS	3.8
1	C	430	ARG	3.7
1	C	294	PHE	3.7
1	C	199	LEU	3.6
1	B	423	ILE	3.5
1	D	212[A]	MET	3.5
1	C	346	PHE	3.4
1	C	473	GLY	3.3
1	C	497	PRO	3.3
1	C	158	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	3.1
1	C	347	ALA	2.9
1	D	117	THR	2.9
1	D	216	THR	2.9
1	C	135	VAL	2.9
1	C	360	SER	2.8
1	C	562	GLY	2.8
1	C	129	ALA	2.8
1	C	691	ALA	2.8
1	C	595	TRP	2.7
1	D	346	PHE	2.7
1	C	132	MET	2.7
1	C	162	ARG	2.6
1	D	414	ASP	2.6
1	A	134	GLY	2.6
1	C	359	HIS	2.6
1	C	201	LEU	2.6
1	B	117	THR	2.5
1	A	153	VAL	2.5
1	C	685[A]	HIS	2.5
1	C	676	ARG	2.5
1	A	129	ALA	2.5
1	D	685[A]	HIS	2.5
1	A	429	GLY	2.5
1	C	207	ALA	2.4
1	C	232	GLU	2.4
1	C	343	THR	2.4
1	C	357	TYR	2.4
1	C	464	PRO	2.4
1	A	210	ALA	2.4
1	A	360	SER	2.4
1	C	407	VAL	2.4
1	D	371	ASN	2.3
1	A	158	TYR	2.3
1	A	472	MET	2.3
1	C	131	THR	2.3
1	D	213	ARG	2.3
1	C	334	LEU	2.3
1	C	134	GLY	2.3
1	C	159	TRP	2.3
1	C	453	ALA	2.3
1	A	346	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	720	THR	2.2
1	C	119	LEU	2.2
1	C	589	LEU	2.2
1	C	212	MET	2.2
1	C	283	HIS	2.2
1	C	210	ALA	2.2
1	C	727	ALA	2.2
1	C	174	ILE	2.2
1	C	711	LEU	2.2
1	A	152	VAL	2.2
1	C	498	VAL	2.2
1	C	265	TYR	2.2
1	C	524	SER	2.2
1	B	427	PHE	2.1
1	A	118	HIS	2.1
1	D	695	GLY	2.1
1	A	217	ALA	2.1
1	C	203	SER	2.1
1	A	199	LEU	2.1
1	A	213	ARG	2.1
1	A	373	LEU	2.1
1	C	507	LEU	2.1
1	A	140	PHE	2.1
1	A	178	PHE	2.1
1	C	351	PHE	2.1
1	C	509	PHE	2.1
1	A	127	ALA	2.1
1	C	431	GLU	2.1
1	C	187	LEU	2.1
1	C	439	LEU	2.1
1	C	165	PRO	2.1
1	C	143	TRP	2.1
1	C	298	TRP	2.1
1	A	117	THR	2.0
1	C	411	ILE	2.0
1	C	445	ILE	2.0
1	A	165	PRO	2.0
1	C	478	TRP	2.0
1	C	139	ARG	2.0
1	C	180	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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

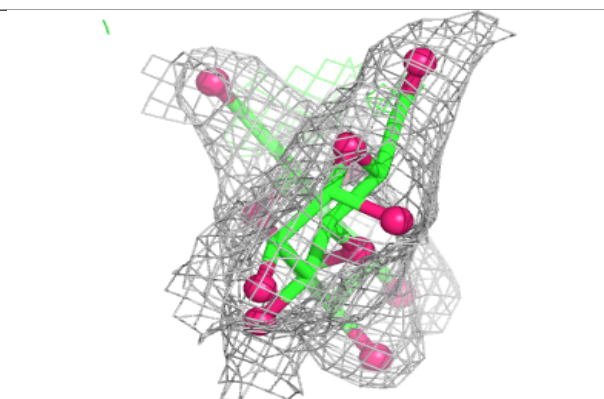
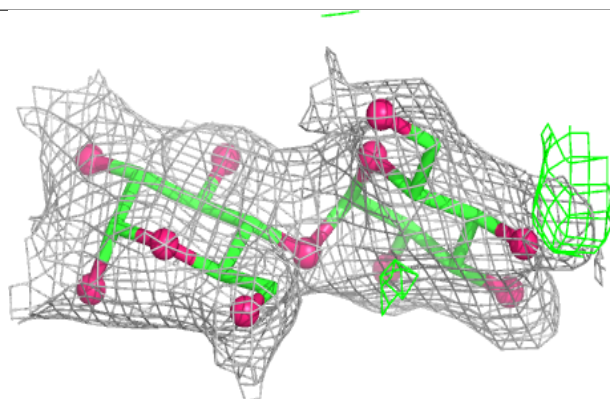
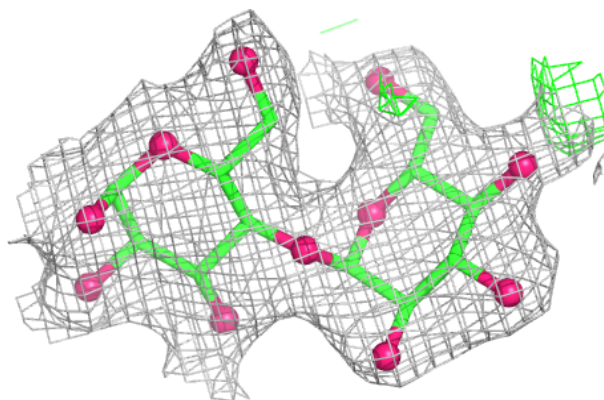
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GLC	I	3	11/12	0.40	0.26	95,96,97,97	11
5	GLC	I	4	11/12	0.56	0.24	92,94,95,95	10
5	GLC	I	5	11/12	0.59	0.20	83,87,89,89	4
3	GLC	G	3	11/12	0.62	0.17	88,90,91,92	0
6	GLC	L	1	12/12	0.67	0.13	95,98,98,99	0
4	GLC	H	2	11/12	0.75	0.18	86,87,88,89	0
4	BGC	O	1	12/12	0.77	0.21	104,106,106,106	0
2	GLC	M	2	11/12	0.78	0.14	83,84,85,86	0
4	BGC	N	1	12/12	0.80	0.12	65,69,71,73	0
6	GLC	L	2	11/12	0.81	0.13	83,91,92,93	0
4	GLC	O	2	11/12	0.82	0.19	106,107,108,109	1
2	GLC	K	2	11/12	0.82	0.10	83,84,85,85	0
4	GLC	N	2	11/12	0.83	0.11	68,70,71,73	0
2	GLC	F	1	12/12	0.83	0.14	91,92,92,93	0
4	BGC	H	1	12/12	0.85	0.17	82,84,86,89	0
3	GLC	G	2	11/12	0.85	0.12	75,78,81,85	0
4	GLC	J	2	11/12	0.85	0.13	69,71,73,74	0
3	GLC	G	1	12/12	0.86	0.10	72,76,77,79	0
4	BGC	J	1	12/12	0.86	0.11	59,69,70,71	0
5	GLC	I	2	11/12	0.87	0.14	90,91,93,93	1
2	GLC	K	1	12/12	0.87	0.09	84,85,86,86	0
2	GLC	F	2	11/12	0.87	0.10	90,90,91,92	0
5	GLC	I	7	11/12	0.89	0.13	62,69,72,72	0
2	GLC	E	2	11/12	0.89	0.09	64,69,70,71	0
2	GLC	M	1	12/12	0.89	0.10	77,79,81,81	0
5	BGC	I	1	12/12	0.90	0.12	82,86,87,88	0
5	GLC	I	6	11/12	0.92	0.10	74,76,78,79	0
2	GLC	E	1	12/12	0.92	0.08	66,68,69,70	0
6	GLC	L	4	11/12	0.93	0.09	64,70,71,73	0
6	GLC	L	3	11/12	0.94	0.09	72,74,76,78	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.

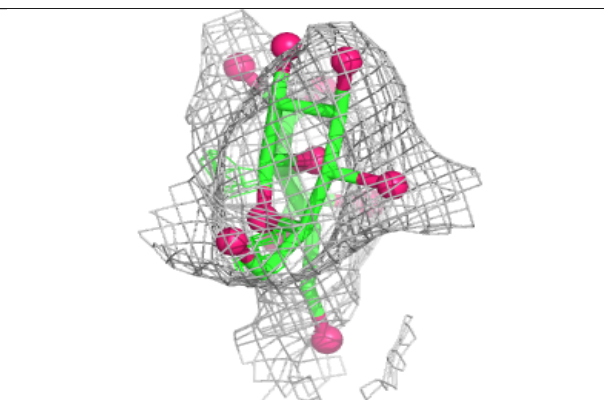
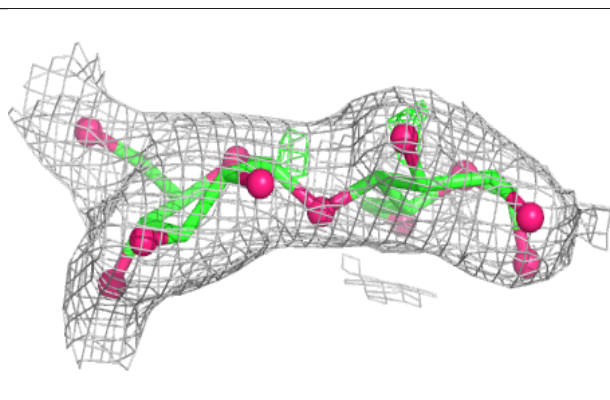
Electron density around Chain E:

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



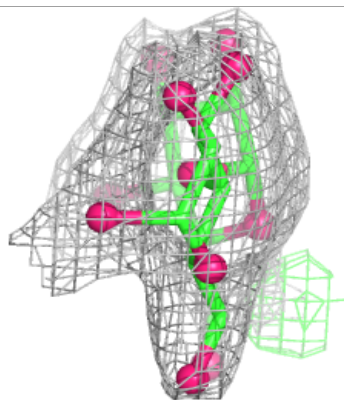
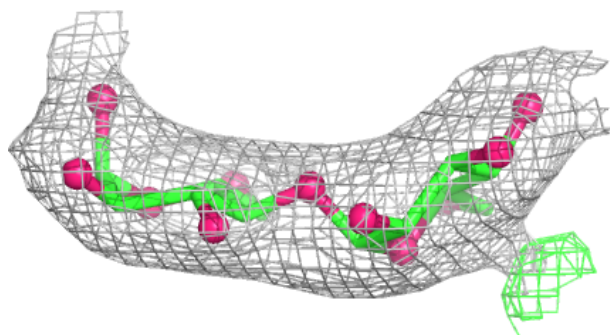
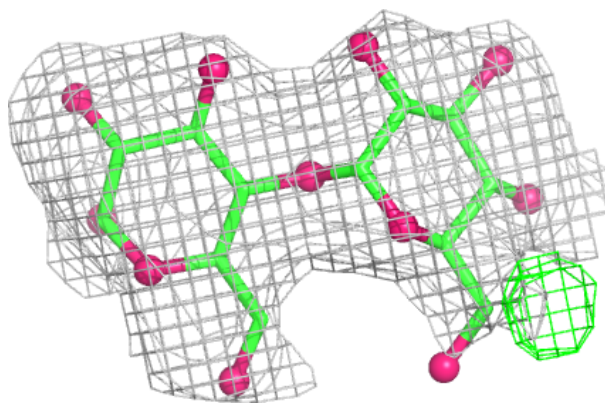
Electron density around Chain F:

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

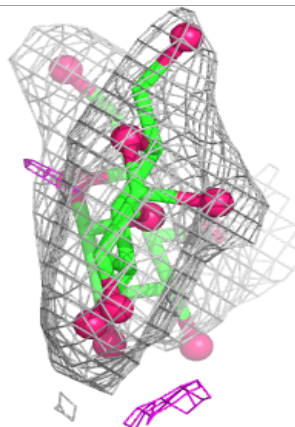
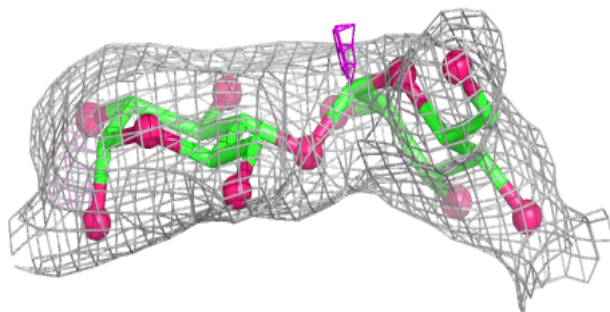
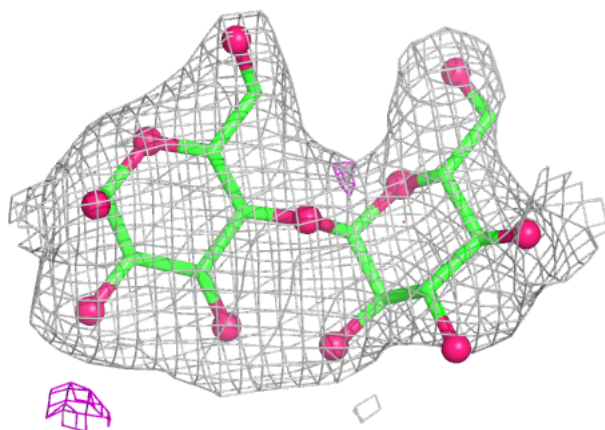


Electron density around Chain K:

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

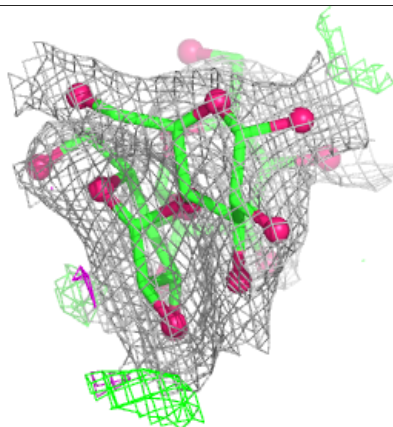
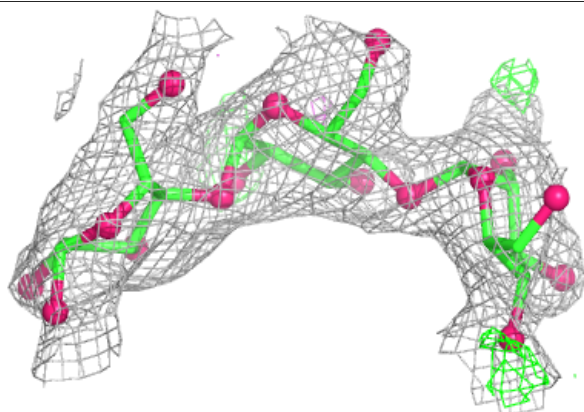
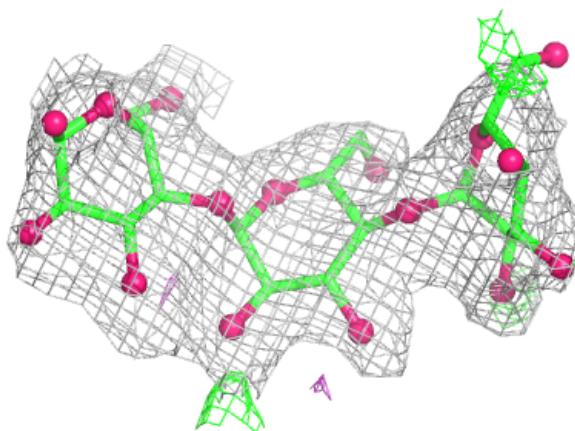
**Electron density around Chain M:**

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

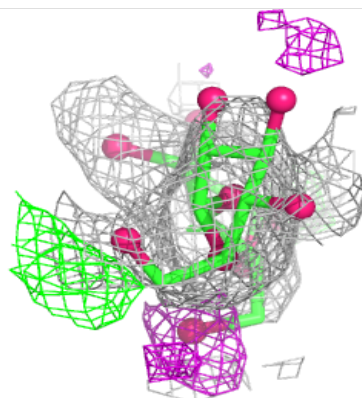
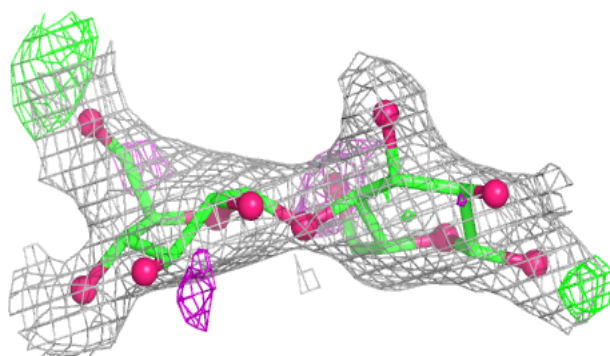
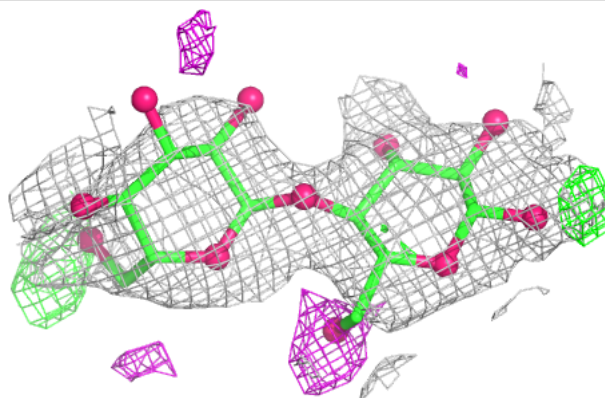


Electron density around Chain G:

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

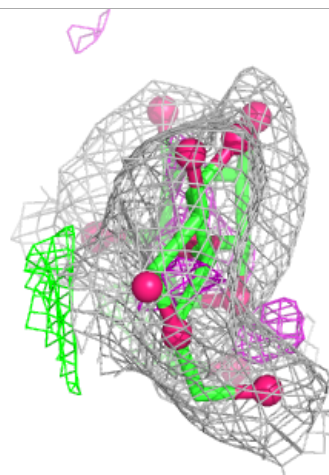
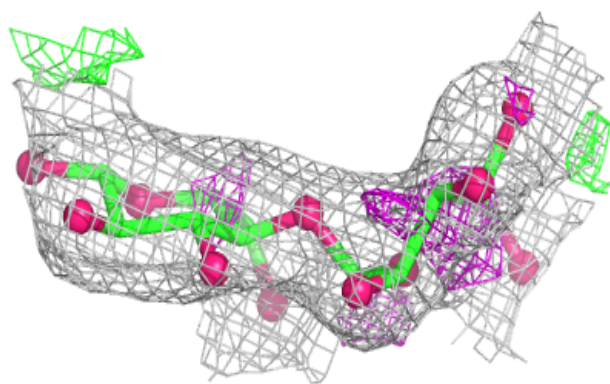
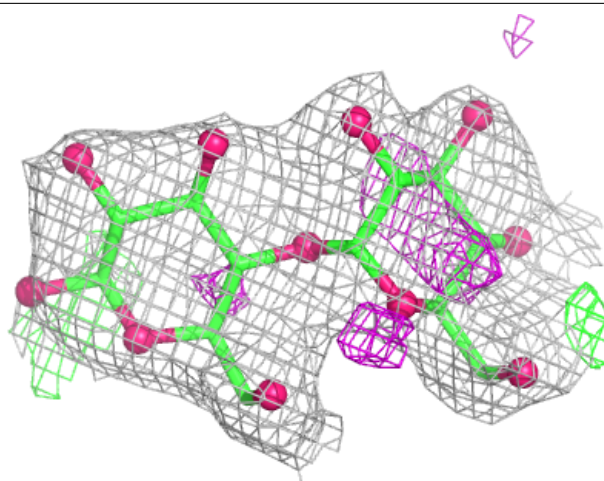
**Electron density around Chain H:**

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



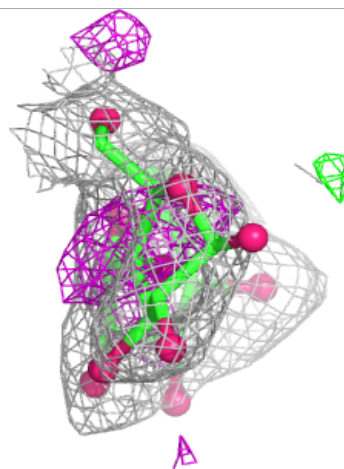
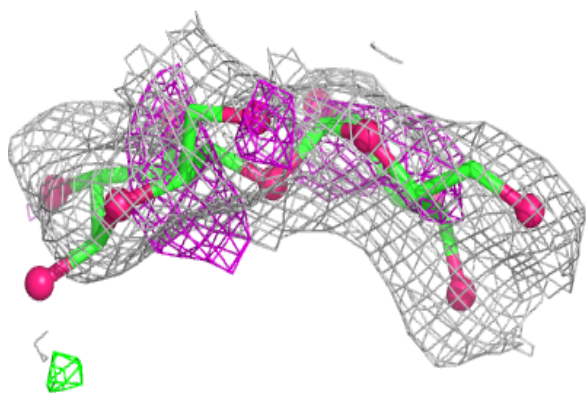
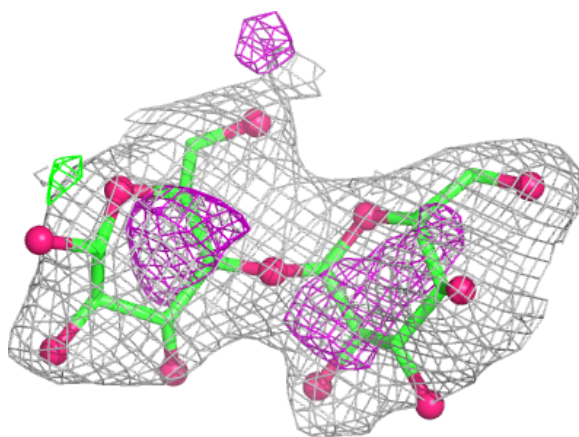
Electron density around Chain J:

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



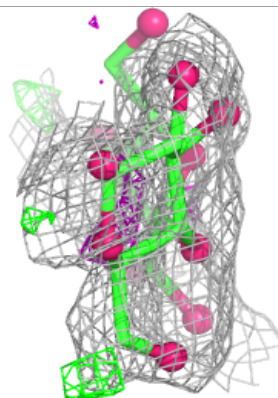
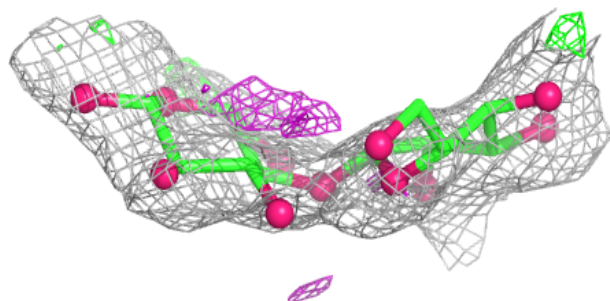
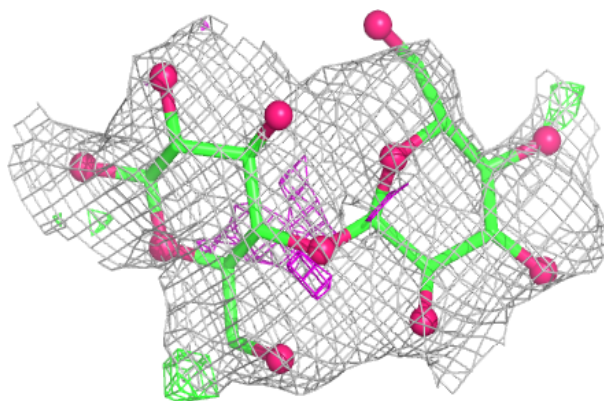
Electron density around Chain N:

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

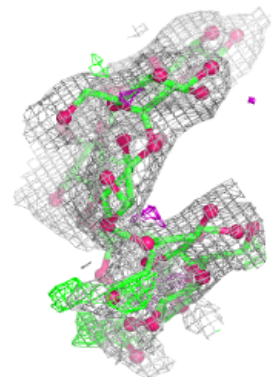
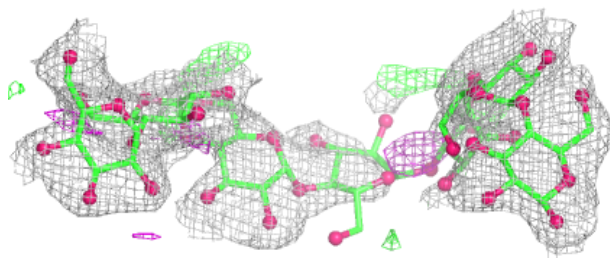
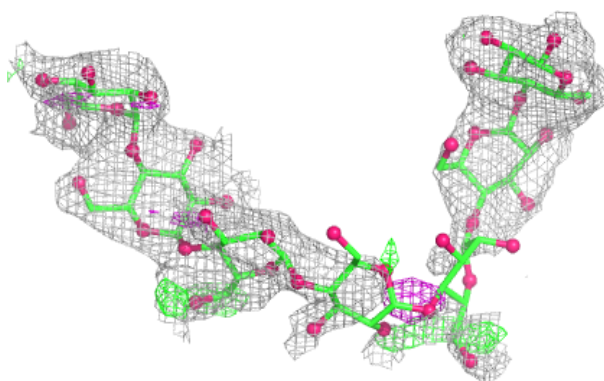


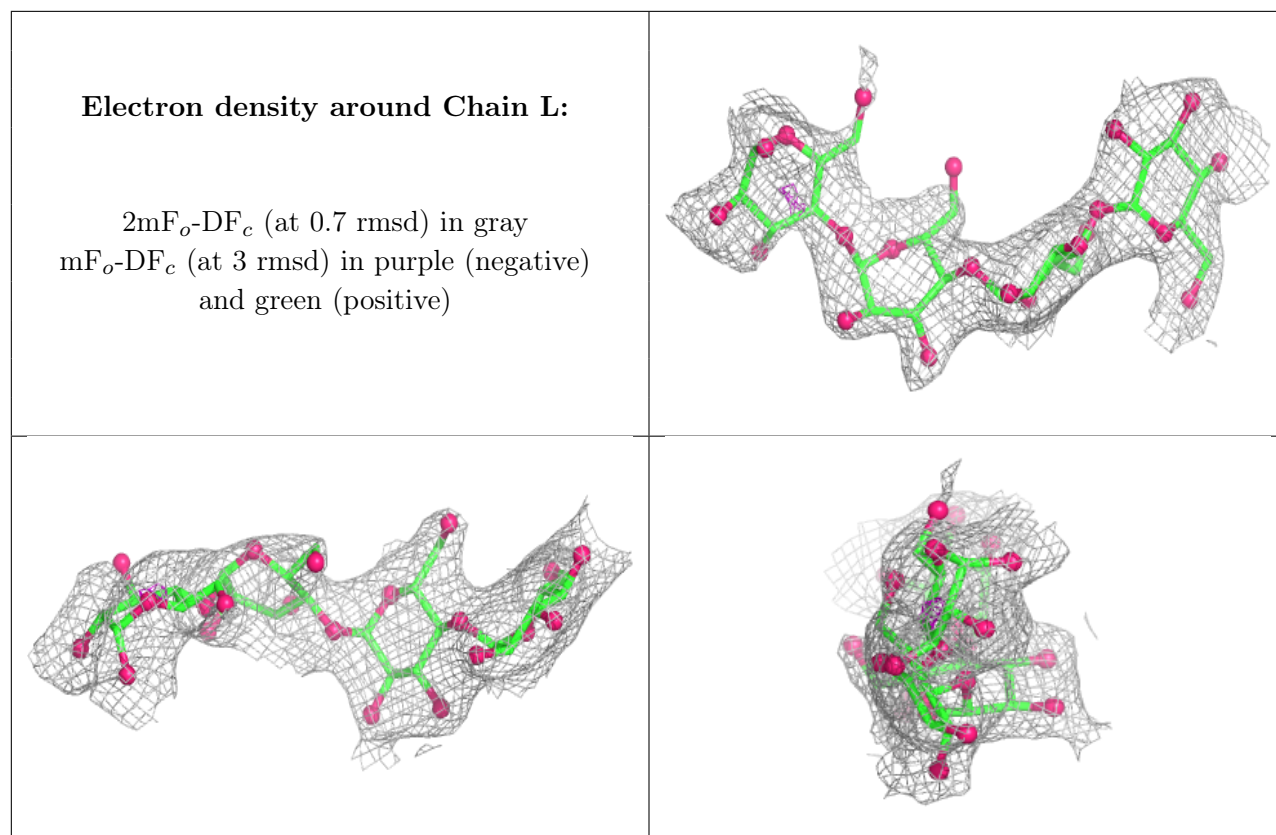
Electron density around Chain O:

$2mF_o-DF_c$ (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 [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
8	BGC	B	810	12/12	0.79	0.14	85,87,89,89	0
7	GOL	A	807	6/6	0.82	0.22	62,63,63,65	0
7	GOL	D	809	6/6	0.84	0.17	85,86,88,89	0
7	GOL	B	814	6/6	0.90	0.14	72,72,73,74	0
7	GOL	B	813	6/6	0.91	0.13	47,51,53,55	0
7	GOL	B	811	6/6	0.91	0.10	47,49,53,55	0
7	GOL	B	815	6/6	0.92	0.17	49,53,53,54	0
7	GOL	D	807	6/6	0.92	0.08	50,51,52,53	0
7	GOL	A	805	6/6	0.93	0.10	53,57,59,60	0
7	GOL	A	806	6/6	0.95	0.09	36,38,40,41	0
7	GOL	B	812	6/6	0.96	0.09	45,48,49,50	0
7	GOL	D	808	6/6	0.96	0.08	55,59,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.