Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:08 AM BST

PDB ID : 4AYJ

Title : Molecular structure of a metal-independent bacterial glycosyltransferase that catalyzes the synthesis of histo-blood group A antigen

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Deposited on : 2012-06-21

Resolution : 3.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:
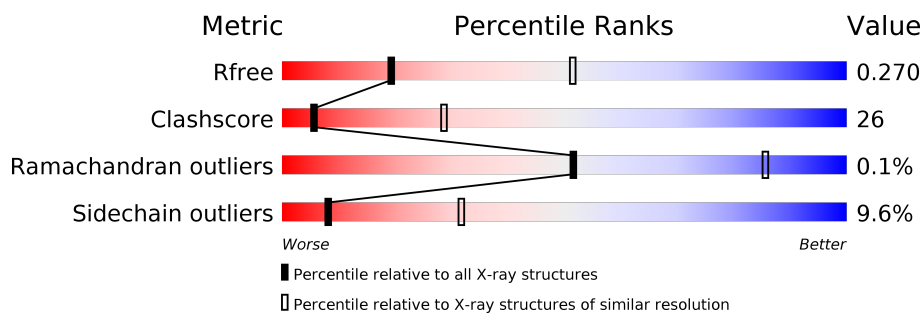
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		26
Ramachandran outliers		0.1%
Sidechain outliers		9.6%

Worse — — — — — — — — — — — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	246	52% ... 38% ... • 6%
1	B	246	46% ... 45% ... • •
1	C	246	47% ... 43% ... • 5%
1	D	246	46% ... 44% ... 6% •
2	E	3	33% ... 67%
2	F	3	67% ... 33%
2	G	3	33% ... 67%

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Mol	Chain	Length	Quality of chain
2	H	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

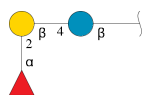| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	G	1	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7939 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 BOGT - METAL-INDEPENDENT GLYCOSYLTRANS-FERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	4	0	0
			1928	1262	311	348	7			
1	B	235	Total	C	N	O	S	0	0	0
			1961	1282	318	354	7			
1	C	233	Total	C	N	O	S	4	0	0
			1945	1272	315	351	7			
1	D	236	Total	C	N	O	S	0	0	0
			1973	1291	319	356	7			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			33	18	15			
2	F	3	Total	C	O	0	0	0
			33	18	15			
2	G	3	Total	C	O	0	0	0
			33	18	15			
2	H	3	Total	C	O	0	0	0
			33	18	15			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.
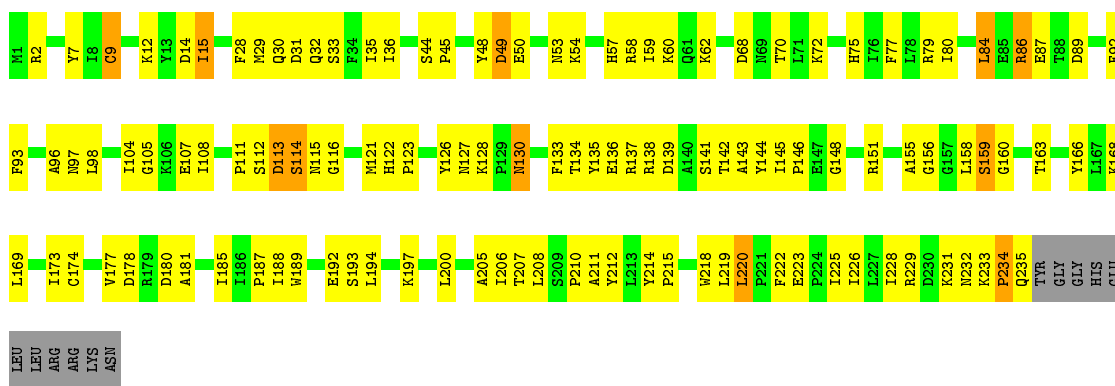
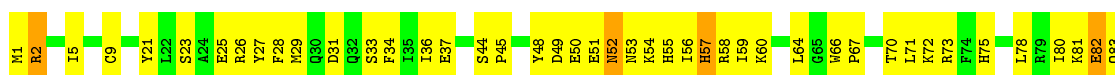- Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE

Chain A:
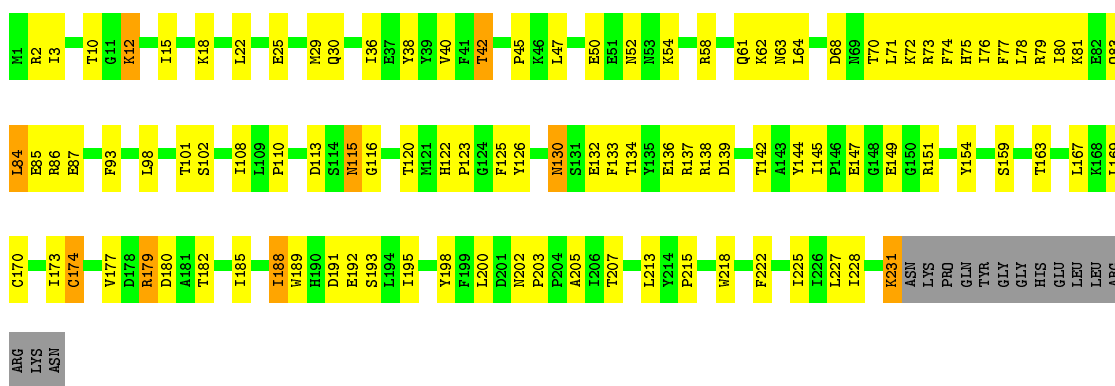
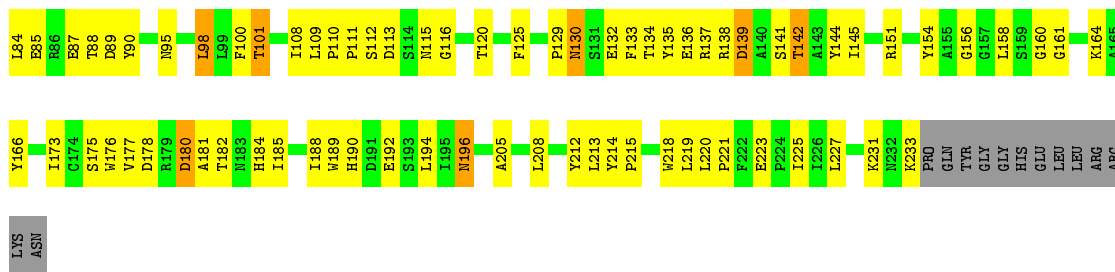- Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE

Chain B:

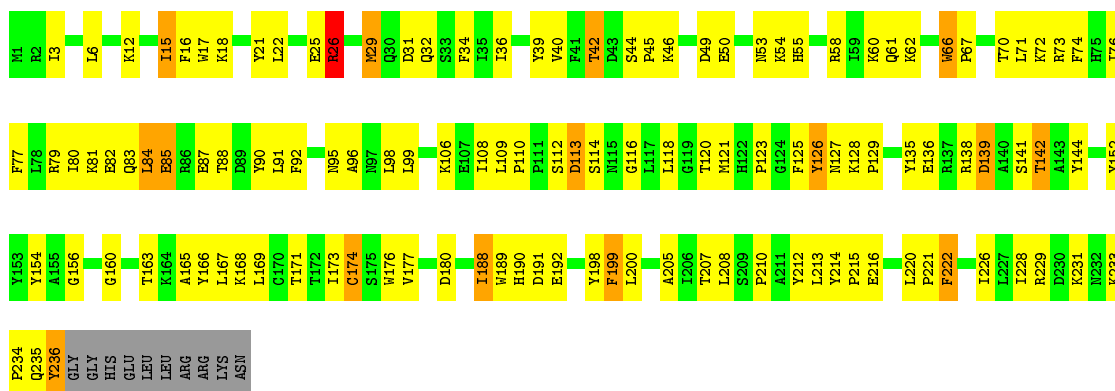- Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE

Chain C:

L84 E85 R86 E87 T88 D89 Y90 N95 L98 L99 F100 T101 I108 L109 P110 P111 S112 D113 S114 N115 G116 T120 F125 P129 N130 S131 E132 F133 T134 Y135 E136 R137 R138 D139 A140 S141 T142 A143 Y144 I145 R151 Y154 A155 G156 G157 L158 S159 G160 G161 K164 A165

Y166 I173 C174 S175 W176 V177 D178 R179 D180 A181 T182 N183 H184 I185 I188 W189 H190 D191 E192 S193 L194 I195 N196 A205 L208 Y212 L213 Y214 P215 W218 L219 L220 P221 F222 E223 P224 I225 L226 L227 K231 N232 K233 PRO GLN TYR GLY GLY HIS GLU LEU LEU ARG ARG

LYS ASN

• Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE

Chain D: 46% 44% 6% •

M1 R2 I3 L6 K12 I15 F16 W17 K18 Y21 L22 E25 R26 M29 Q30 D31 Q32 S33 F34 I35 I36 Y39 V40 F41 T42 D43 S44 P45 K46 D49 E50 N53 K54 H55 R58 I59 K60 Q61 K62 W66 P67 T70 L71 K72 R73 F74 H75 I76

F77 L78 R79 I80 K81 B82 Q83 L84 E85 R86 E87 T88 D89 Y90 L91 F92 N95 A96 N97 L98 L99 K106 E107 I108 L109 P110 P111 S112 D113 S114 N115 G116 L117 L118 G119 T120 M121 H122 P123 G124 F125 N126 N127 K128 P129 Y135 E136 R137 R138 D139 A140 S141 T142 A143 Y144 Y152

Y153 Y154 A155 G156 G160 T163 K164 A165 Y166 L167 K168 L169 C170 T171 T172 I173 C174 S175 W176 V177 D180 I188 W189 H190 D191 E192 F198 F199 L200 A205 I206 T207 L208 S209 P210 A211 Y212 L213 Y214 P215 E216 L220 P221 F222 I226 L227 I228 R229 D230 K231 N232 K233

P234 Q235 Y236 GLY HIS GLU LEU LEU ARG ARG LYS ASN

• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain E: 33% 67%

BGC1 GAL2 FUC3

• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F: 67% 33%

BGC1 GAL2 FUC3

• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain G: 33% 67%

BGC1 GAL2 FUC3

• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H:
100%

BGC1
GAL2
FUC3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.85Å 93.87Å 75.51Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	70.69 – 3.00 70.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (70.69-3.00) 93.7 (70.69-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.25 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.181 , 0.262 0.443 , 0.270	Depositor DCC
R_{free} test set	951 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.3	EDS
L-test for twinning[2]	$<|L|> = 0.29, <L^2> = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.59	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.50	0/1991	0.72	0/2704
1	B	0.47	0/2025	0.68	1/2750 (0.0%)
1	C	0.47	0/2008	0.65	0/2726
1	D	0.47	0/2038	0.67	1/2768 (0.0%)
All	All	0.48	0/8062	0.68	2/10948 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	26	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	220	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1928	0	1869	89	0
1	B	1961	0	1903	93	1
1	C	1945	0	1888	101	0
1	D	1973	0	1911	116	1
2	E	33	0	30	9	0
2	F	33	0	30	2	0
2	G	33	0	30	7	0
2	H	33	0	30	3	0
All	All	7939	0	7691	399	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (399) 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:128:LYS:NZ	2:G:1:BGC:O5	1.79	1.15
1:C:2:ARG:NH1	1:C:89:ASP:H	1.50	1.08
1:C:2:ARG:O	1:C:2:ARG:NH1	1.93	1.02
1:A:134:THR:HG21	1:A:189:TRP:HE1	1.28	0.98
1:B:229:ARG:HD3	1:C:223:GLU:OE2	1.64	0.97
1:B:128:LYS:NZ	2:E:1:BGC:O5	2.00	0.93
1:D:80:ILE:HG13	1:D:84:LEU:HD22	1.51	0.91
1:D:128:LYS:HZ1	2:G:1:BGC:C1	1.85	0.89
1:A:136:GLU:HA	1:A:188:ILE:HD11	1.56	0.88
1:B:232:ASN:OD1	1:B:233:LYS:N	2.07	0.87
1:B:208:LEU:HB3	1:B:212:TYR:HD2	1.40	0.86
1:C:2:ARG:NH2	1:C:87:GLU:O	2.09	0.85
1:B:208:LEU:HB3	1:B:212:TYR:CD2	2.12	0.85
1:C:2:ARG:CZ	1:C:88:THR:HA	2.07	0.84
1:D:50:GLU:OE2	1:D:58:ARG:NH1	2.10	0.83
1:C:51:GLU:HG2	1:C:52:ASN:OD1	1.79	0.81
1:D:165:ALA:HA	1:D:168:LYS:HE2	1.65	0.79
1:A:25:GLU:O	1:A:30:GLN:NE2	2.16	0.79
1:C:134:THR:HG21	1:C:189:TRP:CD1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:TRP:CG	1:D:67:PRO:HA	2.20	0.77
1:D:83:GLN:O	1:D:87:GLU:HG3	1.83	0.77
1:B:158:LEU:HD23	1:B:159:SER:N	2.00	0.76
1:A:80:ILE:HG13	1:A:84:LEU:HD22	1.66	0.76
1:A:134:THR:CG2	1:A:189:TRP:HE1	1.98	0.76
1:C:134:THR:HG22	1:C:134:THR:O	1.85	0.75
1:C:2:ARG:HH11	1:C:89:ASP:H	1.33	0.75
1:D:138:ARG:O	1:D:144:TYR:HB2	1.86	0.74
1:D:188:ILE:HD13	1:D:189:TRP:H	1.51	0.74
1:A:72:LYS:HD2	1:A:75:HIS:ND1	2.03	0.74
1:C:82:GLU:HA	1:C:85:GLU:HG3	1.70	0.73
1:D:121:MET:HE2	1:D:126:TYR:HB2	1.70	0.73
1:D:74:PHE:HA	1:D:77:PHE:HD2	1.52	0.73
1:D:92:PHE:CD1	1:D:160:GLY:HA3	2.23	0.73
1:C:1:MET:O	1:C:34:PHE:HA	1.90	0.72
1:A:81:LYS:O	1:A:85:GLU:HG3	1.90	0.71
1:B:86:ARG:HG2	1:B:87:GLU:HG3	1.72	0.71
1:C:84:LEU:O	1:C:88:THR:OG1	2.06	0.71
1:A:198:TYR:O	1:A:202:ASN:HB2	1.89	0.71
1:B:75:HIS:CD2	1:B:174:CYS:SG	2.84	0.71
1:C:80:ILE:HG13	1:C:84:LEU:HD11	1.72	0.70
1:D:12:LYS:O	1:D:15:ILE:HG12	1.91	0.70
1:C:134:THR:CG2	1:C:189:TRP:CD1	2.75	0.70
1:D:26:ARG:HH11	1:D:26:ARG:CB	2.05	0.70
1:A:231:LYS:HD3	1:A:231:LYS:H	1.58	0.69
1:C:2:ARG:NH1	1:C:89:ASP:N	2.34	0.69
1:C:48:TYR:CD1	1:C:49:ASP:HB2	2.29	0.68
1:D:118:LEU:HD11	1:D:208:LEU:HD11	1.75	0.68
1:D:169:LEU:O	1:D:173:ILE:HG13	1.94	0.68
1:D:31:ASP:O	1:D:32:GLN:HG2	1.94	0.68
1:A:125:PHE:HE2	2:E:2:GAL:H61	1.59	0.68
1:B:134:THR:HG21	1:B:189:TRP:HE1	1.59	0.68
1:A:62:LYS:HG2	1:A:63:ASN:N	2.09	0.67
1:A:70:THR:O	1:A:73:ARG:HG3	1.93	0.67
1:C:180:ASP:HB3	1:C:185:ILE:O	1.95	0.67
1:D:128:LYS:NZ	2:G:1:BGC:C1	2.49	0.67
2:G:1:BGC:O3	2:G:2:GAL:O5	2.04	0.66
1:B:130:ASN:HD21	1:B:148:GLY:HA2	1.61	0.66
1:D:215:PRO:HA	1:D:228:ILE:HB	1.77	0.66
1:B:29:MET:HB2	1:B:36:ILE:HD11	1.76	0.66
1:A:136:GLU:O	1:A:144:TYR:HA	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:TYR:CE1	1:C:49:ASP:HB2	2.32	0.65
1:C:50:GLU:OE2	1:C:58:ARG:NH1	2.29	0.65
1:D:6:LEU:HB3	1:D:77:PHE:HE1	1.62	0.65
1:D:233:LYS:O	1:D:236:TYR:HB2	1.97	0.64
1:A:179:ARG:O	1:A:182:THR:OG1	2.13	0.64
1:D:26:ARG:HB2	1:D:26:ARG:HH11	1.62	0.64
1:D:90:TYR:O	1:D:91:LEU:HD23	1.98	0.64
1:D:126:TYR:OH	1:D:221:PRO:HG3	1.97	0.64
1:D:50:GLU:CD	1:D:58:ARG:HH11	2.01	0.64
1:D:114:SER:HB2	1:D:205:ALA:HB2	1.80	0.64
1:D:6:LEU:HB3	1:D:77:PHE:CE1	2.33	0.64
1:D:82:GLU:HA	1:D:85:GLU:HG3	1.81	0.63
1:A:122:HIS:HE2	2:E:2:GAL:HO4	1.45	0.62
1:D:53:ASN:OD1	1:D:55:HIS:N	2.20	0.62
1:D:3:ILE:HD11	1:D:34:PHE:CE1	2.34	0.62
1:D:73:ARG:NH1	1:D:191:ASP:CG	2.52	0.62
1:C:136:GLU:HG2	1:C:141:SER:OG	2.00	0.62
1:C:139:ASP:OD1	1:C:139:ASP:N	2.28	0.62
1:A:120:THR:HG21	1:A:213:LEU:HD12	1.81	0.62
1:D:73:ARG:NH1	1:D:191:ASP:OD2	2.33	0.61
1:B:121:MET:HB2	1:B:210:PRO:HD3	1.81	0.61
1:D:126:TYR:OH	1:D:221:PRO:CG	2.49	0.61
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.66	0.61
1:A:120:THR:CG2	1:A:213:LEU:HD12	2.31	0.61
1:C:2:ARG:NH2	1:C:88:THR:HA	2.15	0.61
1:C:2:ARG:HB2	1:C:2:ARG:CZ	2.27	0.61
1:A:101:THR:OG1	1:A:225:ILE:O	2.17	0.60
1:C:2:ARG:CZ	1:C:87:GLU:O	2.49	0.60
1:B:143:ALA:HB2	1:B:194:LEU:HG	1.82	0.60
1:A:134:THR:HG21	1:A:189:TRP:NE1	2.09	0.60
1:D:73:ARG:HB3	1:D:77:PHE:HE2	1.66	0.60
1:A:145:ILE:HD13	1:A:200:LEU:HD22	1.83	0.60
1:B:92:PHE:CD1	1:B:160:GLY:HA3	2.37	0.60
1:A:180:ASP:HB3	1:A:185:ILE:O	2.02	0.60
1:C:181:ALA:O	1:C:184:HIS:N	2.26	0.59
1:C:134:THR:HG21	1:C:189:TRP:NE1	2.17	0.59
1:C:90:TYR:CZ	1:C:109:LEU:HD22	2.36	0.59
1:B:60:LYS:O	1:B:79:ARG:NH1	2.31	0.59
1:C:173:ILE:O	1:C:177:VAL:HG23	2.02	0.59
1:D:80:ILE:CG1	1:D:84:LEU:HD22	2.27	0.59
1:D:188:ILE:HD13	1:D:189:TRP:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HD22	1:B:212:TYR:CE2	2.38	0.59
1:B:128:LYS:HE2	2:E:1:BGC:O1	2.02	0.59
1:D:73:ARG:HH11	1:D:191:ASP:CG	2.06	0.59
1:D:26:ARG:HH11	1:D:26:ARG:CG	2.15	0.59
1:B:15:ILE:CD1	1:B:235:GLN:H	2.16	0.58
1:B:28:PHE:O	1:B:30:GLN:NE2	2.34	0.58
1:C:134:THR:HG22	1:C:189:TRP:HD1	1.68	0.58
1:C:115:ASN:OD1	1:C:205:ALA:HB2	2.03	0.58
1:C:142:THR:OG1	1:C:180:ASP:OD1	2.14	0.58
1:C:90:TYR:CE2	1:C:109:LEU:HD22	2.38	0.58
1:D:73:ARG:NH1	1:D:191:ASP:OD1	2.37	0.58
1:D:212:TYR:O	1:D:226:ILE:HB	2.04	0.58
1:C:214:TYR:CE2	1:C:220:LEU:HB2	2.38	0.57
1:A:215:PRO:HA	1:A:228:ILE:HB	1.87	0.57
1:B:215:PRO:HB2	1:B:218:TRP:CG	2.39	0.57
1:D:135:TYR:OH	1:D:152:TYR:O	2.21	0.57
1:A:68:ASP:HA	1:A:71:LEU:HB3	1.87	0.56
1:A:123:PRO:O	1:A:126:TYR:HD1	1.87	0.56
1:D:66:TRP:CD1	1:D:67:PRO:N	2.73	0.56
1:B:122:HIS:NE2	2:F:2:GAL:O4	2.31	0.56
1:A:138:ARG:O	1:A:144:TYR:HB2	2.05	0.56
1:C:160:GLY:HA2	1:C:166:TYR:CD2	2.41	0.56
1:D:66:TRP:CD1	1:D:67:PRO:HA	2.40	0.56
1:A:154:TYR:HE1	1:A:207:THR:HG23	1.70	0.56
1:B:233:LYS:HB2	1:B:234:PRO:HD2	1.87	0.56
1:C:134:THR:CG2	1:C:189:TRP:HD1	2.19	0.56
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.21	0.55
1:A:74:PHE:O	1:A:78:LEU:HG	2.07	0.55
1:D:67:PRO:O	1:D:70:THR:HG22	2.05	0.55
1:B:138:ARG:O	1:B:144:TYR:HB2	2.07	0.55
1:C:25:GLU:HA	1:C:25:GLU:OE1	2.06	0.55
1:D:83:GLN:HG3	1:D:87:GLU:OE2	2.07	0.55
1:B:15:ILE:HD13	1:B:235:GLN:H	1.72	0.55
1:D:73:ARG:O	1:D:76:ILE:HB	2.07	0.55
1:B:215:PRO:HB2	1:B:218:TRP:CD2	2.41	0.55
1:C:101:THR:HG23	1:C:225:ILE:O	2.07	0.55
1:A:134:THR:CG2	1:A:189:TRP:NE1	2.69	0.55
1:A:29:MET:HE2	1:A:108:ILE:HD11	1.88	0.55
1:B:48:TYR:CD1	1:B:49:ASP:HB2	2.42	0.55
1:A:83:GLN:O	1:A:87:GLU:HG3	2.06	0.54
1:B:114:SER:HB2	1:B:116:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:O	1:A:215:PRO:HD3	2.07	0.54
1:B:126:TYR:CE1	1:B:127:ASN:HB3	2.41	0.54
1:D:139:ASP:N	1:D:139:ASP:OD1	2.36	0.54
1:D:6:LEU:HD13	1:D:77:PHE:CD1	2.42	0.54
1:A:222:PHE:HA	1:D:216:GLU:HG3	1.89	0.54
1:B:59:ILE:HG21	1:B:80:ILE:HG21	1.90	0.54
1:C:51:GLU:OE1	1:C:51:GLU:N	2.34	0.54
1:A:122:HIS:NE2	2:E:2:GAL:O4	2.33	0.54
1:A:231:LYS:HD3	1:A:231:LYS:N	2.21	0.54
1:C:233:LYS:HE3	1:C:233:LYS:HA	1.90	0.54
1:C:129:PRO:HG2	1:C:132:GLU:HG2	1.88	0.54
1:C:134:THR:CG2	1:C:134:THR:O	2.55	0.54
1:C:2:ARG:NH1	1:C:88:THR:HA	2.23	0.54
1:B:197:LYS:O	1:B:200:LEU:HB3	2.07	0.53
1:B:212:TYR:O	1:B:226:ILE:HB	2.08	0.53
1:D:70:THR:HG23	1:D:71:LEU:N	2.24	0.53
1:B:135:TYR:CD1	1:B:145:ILE:HD12	2.44	0.53
1:C:142:THR:HG21	1:C:176:TRP:CD1	2.43	0.53
1:D:15:ILE:HD12	1:D:236:TYR:HA	1.91	0.53
1:C:67:PRO:HB2	1:C:190:HIS:CD2	2.44	0.53
1:D:169:LEU:HD23	1:D:173:ILE:HG13	1.90	0.52
1:A:130:ASN:HB2	1:A:133:PHE:CD2	2.44	0.52
1:A:145:ILE:HG22	1:A:149:GLU:HB3	1.91	0.52
1:B:135:TYR:CG	1:B:145:ILE:HD12	2.44	0.52
1:B:53:ASN:C	1:B:54:LYS:HE2	2.29	0.52
1:C:136:GLU:OE1	1:C:137:ARG:N	2.42	0.52
1:A:139:ASP:HA	1:A:144:TYR:CG	2.45	0.51
1:A:80:ILE:CG1	1:A:84:LEU:HD22	2.37	0.51
1:B:156:GLY:N	1:B:192:GLU:HG3	2.25	0.51
1:C:26:ARG:HG2	1:C:27:TYR:CE2	2.45	0.51
1:C:80:ILE:HG13	1:C:84:LEU:CD1	2.40	0.51
1:B:173:ILE:O	1:B:177:VAL:HG23	2.11	0.51
1:D:61:GLN:HG3	1:D:62:LYS:O	2.11	0.51
1:C:78:LEU:HD22	1:C:81:LYS:HD2	1.93	0.51
1:D:136:GLU:HG2	1:D:141:SER:OG	2.11	0.51
1:B:206:ILE:CG2	1:B:207:THR:N	2.74	0.51
1:C:156:GLY:N	1:C:192:GLU:HG3	2.26	0.51
1:D:166:TYR:O	1:D:169:LEU:HB3	2.11	0.51
1:D:66:TRP:CD1	1:D:67:PRO:CA	2.94	0.51
1:A:115:ASN:OD1	1:A:205:ALA:HB2	2.11	0.50
1:C:130:ASN:HB2	1:C:133:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ASP:N	1:D:113:ASP:OD1	2.42	0.50
1:D:163:THR:HG22	1:D:167:LEU:HD12	1.92	0.50
1:B:211:ALA:HB2	1:B:222:PHE:HB3	1.94	0.50
1:C:75:HIS:HE1	1:C:177:VAL:HG11	1.77	0.50
1:B:104:ILE:HG21	1:B:108:ILE:HD13	1.92	0.50
1:D:106:LYS:O	1:D:109:LEU:HD12	2.12	0.50
1:C:83:GLN:O	1:C:87:GLU:HG3	2.12	0.50
1:D:66:TRP:CD1	1:D:66:TRP:C	2.85	0.50
1:A:61:GLN:OE1	1:A:64:LEU:HD11	2.10	0.50
1:D:213:LEU:O	1:D:215:PRO:HD3	2.12	0.50
1:D:95:ASN:CB	1:D:98:LEU:HD13	2.41	0.50
1:B:134:THR:HG21	1:B:189:TRP:NE1	2.23	0.50
1:A:145:ILE:CG2	1:A:149:GLU:HB3	2.42	0.49
1:C:57:HIS:N	1:C:57:HIS:CD2	2.80	0.49
1:B:104:ILE:CG2	1:B:108:ILE:HD13	2.42	0.49
1:C:70:THR:O	1:C:73:ARG:HG3	2.12	0.49
1:D:91:LEU:O	1:D:160:GLY:HA2	2.13	0.49
1:A:80:ILE:HG13	1:A:84:LEU:CD2	2.40	0.49
1:B:128:LYS:NZ	2:E:1:BGC:C1	2.75	0.49
1:C:158:LEU:HB2	1:C:213:LEU:HD21	1.95	0.49
1:A:136:GLU:OE1	1:A:137:ARG:N	2.45	0.49
1:D:142:THR:HG21	1:D:176:TRP:CG	2.48	0.49
1:B:128:LYS:HZ3	2:E:1:BGC:C1	2.20	0.48
1:D:110:PRO:HB2	1:D:116:GLY:HA2	1.95	0.48
1:C:135:TYR:CG	1:C:145:ILE:HD12	2.49	0.48
1:C:2:ARG:NH1	1:C:2:ARG:C	2.66	0.48
1:B:115:ASN:OD1	1:B:205:ALA:HB2	2.13	0.48
1:D:40:VAL:HG12	1:D:42:THR:HG22	1.95	0.48
1:A:163:THR:O	1:A:167:LEU:HD12	2.13	0.48
1:C:178:ASP:O	1:C:182:THR:HG23	2.13	0.48
1:C:72:LYS:HD2	1:C:75:HIS:ND1	2.29	0.48
1:A:50:GLU:HG2	1:A:50:GLU:O	2.12	0.48
1:B:97:ASN:ND2	1:B:228:ILE:CG2	2.77	0.48
1:A:40:VAL:O	1:A:42:THR:HG22	2.14	0.48
1:C:26:ARG:HG2	1:C:27:TYR:CD2	2.49	0.48
1:D:81:LYS:O	1:D:84:LEU:HB2	2.13	0.48
1:A:29:MET:HE2	1:A:108:ILE:CD1	2.44	0.48
1:A:70:THR:OG1	1:A:191:ASP:OD2	2.31	0.48
1:C:164:LYS:HB3	1:C:164:LYS:HE2	1.68	0.48
1:C:215:PRO:HB2	1:C:218:TRP:CG	2.49	0.48
1:D:95:ASN:HB3	1:D:98:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PRO:HG2	1:B:194:LEU:HD11	1.96	0.47
1:C:208:LEU:HB3	1:C:212:TYR:CD2	2.49	0.47
1:B:225:ILE:HG22	1:B:226:ILE:HG13	1.95	0.47
1:A:192:GLU:HA	1:A:195:ILE:HG22	1.97	0.47
1:D:12:LYS:O	1:D:15:ILE:CG1	2.62	0.47
1:A:173:ILE:O	1:A:177:VAL:HG23	2.15	0.47
1:D:156:GLY:N	1:D:192:GLU:HG3	2.30	0.47
1:B:159:SER:HB2	1:B:166:TYR:HE1	1.79	0.47
1:B:72:LYS:HD3	1:B:75:HIS:ND1	2.30	0.47
1:C:36:ILE:N	1:C:36:ILE:HD12	2.30	0.47
1:D:99:LEU:HD22	1:D:229:ARG:HD3	1.97	0.47
1:B:141:SER:HB2	1:B:185:ILE:HG21	1.97	0.47
1:C:138:ARG:O	1:C:144:TYR:HB2	2.14	0.47
1:A:125:PHE:CE2	2:E:2:GAL:H61	2.46	0.47
1:C:120:THR:HG23	1:C:208:LEU:HB2	1.97	0.46
1:D:173:ILE:O	1:D:177:VAL:HG23	2.15	0.46
1:C:52:ASN:N	1:C:52:ASN:OD1	2.47	0.46
1:D:114:SER:HB2	1:D:205:ALA:CB	2.46	0.46
1:D:234:PRO:HA	1:D:235:GLN:HA	1.42	0.46
1:B:7:TYR:CE1	1:B:96:ALA:HA	2.51	0.46
1:A:189:TRP:HB2	1:A:193:SER:OG	2.15	0.46
1:B:36:ILE:N	1:B:36:ILE:HD12	2.30	0.46
1:D:26:ARG:HB2	1:D:26:ARG:NH1	2.30	0.46
1:A:36:ILE:HG22	1:A:38:TYR:CE1	2.51	0.46
1:D:39:TYR:N	1:D:39:TYR:CD1	2.83	0.46
1:C:31:ASP:OD2	1:C:33:SER:OG	2.27	0.46
1:A:18:LYS:O	1:A:22:LEU:HG	2.16	0.45
1:B:72:LYS:CD	1:B:75:HIS:ND1	2.79	0.45
1:C:215:PRO:HB2	1:C:218:TRP:CD2	2.51	0.45
1:A:202:ASN:O	1:A:203:PRO:C	2.53	0.45
1:B:158:LEU:HD23	1:B:158:LEU:C	2.35	0.45
1:C:44:SER:HA	1:C:45:PRO:HD3	1.70	0.45
1:A:98:LEU:N	1:A:98:LEU:CD1	2.79	0.45
1:C:54:LYS:O	1:C:54:LYS:HG2	2.16	0.45
1:D:198:TYR:CD1	1:D:198:TYR:O	2.70	0.45
1:A:123:PRO:O	1:A:126:TYR:CD1	2.69	0.45
1:B:134:THR:O	1:B:134:THR:HG22	2.17	0.45
1:A:77:PHE:HZ	1:A:93:PHE:CD1	2.35	0.45
1:C:21:TYR:CE1	1:C:56:ILE:HD11	2.51	0.45
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.16	0.45
1:C:71:LEU:HD13	1:C:190:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:HD1	1:B:160:GLY:HA3	1.80	0.45
1:D:36:ILE:N	1:D:36:ILE:HD12	2.32	0.45
1:D:66:TRP:CZ2	1:D:190:HIS:CE1	3.05	0.45
1:D:72:LYS:O	1:D:73:ARG:C	2.55	0.45
1:D:29:MET:HE1	1:D:108:ILE:HG12	1.97	0.45
1:A:47:LEU:HB2	1:A:50:GLU:HB2	2.00	0.44
1:C:176:TRP:HE3	1:C:194:LEU:HD22	1.82	0.44
1:C:23:SER:HB2	1:C:100:PHE:HB2	1.99	0.44
1:C:5:ILE:HD11	1:C:28:PHE:CE2	2.52	0.44
1:D:74:PHE:HA	1:D:77:PHE:CD2	2.42	0.44
1:B:178:ASP:O	1:B:181:ALA:HB3	2.16	0.44
2:H:1:BGC:O6	2:H:3:FUC:H3	2.17	0.44
1:B:50:GLU:OE2	1:B:58:ARG:NH1	2.50	0.44
1:A:12:LYS:O	1:A:15:ILE:HG12	2.18	0.44
1:C:136:GLU:O	1:C:144:TYR:HA	2.18	0.44
1:D:154:TYR:OH	1:D:207:THR:OG1	2.21	0.44
1:B:130:ASN:HA	1:B:133:PHE:CE2	2.52	0.44
1:B:75:HIS:HD2	1:B:174:CYS:SG	2.38	0.44
1:B:189:TRP:HB2	1:B:193:SER:OG	2.17	0.44
1:B:32:GLN:HG2	1:B:32:GLN:H	1.66	0.44
1:C:59:ILE:O	1:C:60:LYS:C	2.55	0.44
1:C:2:ARG:HH22	1:C:88:THR:HG22	1.82	0.44
1:B:122:HIS:HA	1:B:155:ALA:HB2	1.99	0.44
1:B:128:LYS:CE	2:E:1:BGC:O1	2.64	0.44
1:B:113:ASP:OD1	1:B:113:ASP:N	2.50	0.44
1:D:189:TRP:NE1	2:H:2:GAL:H62	2.33	0.44
1:B:121:MET:HE1	1:B:126:TYR:HB2	1.99	0.44
1:D:214:TYR:HE2	1:D:222:PHE:O	2.00	0.44
1:D:84:LEU:O	1:D:88:THR:OG1	2.29	0.44
1:A:72:LYS:O	1:A:75:HIS:HB2	2.18	0.44
1:B:122:HIS:ND1	1:B:123:PRO:HD2	2.33	0.43
1:B:2:ARG:HG2	1:B:35:ILE:HD12	2.00	0.43
1:D:66:TRP:HA	1:D:67:PRO:C	2.38	0.43
1:C:116:GLY:O	1:C:161:GLY:HA3	2.18	0.43
1:C:28:PHE:CE1	1:C:29:MET:HG2	2.54	0.43
1:A:45:PRO:O	1:A:58:ARG:CZ	2.67	0.43
1:B:206:ILE:HG22	1:B:207:THR:N	2.32	0.43
1:B:77:PHE:HZ	1:B:93:PHE:CD2	2.36	0.43
1:A:75:HIS:CD2	1:A:174:CYS:SG	3.11	0.43
1:C:139:ASP:HA	1:C:144:TYR:CG	2.53	0.43
1:D:73:ARG:HB3	1:D:77:PHE:CE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HD2	1:A:75:HIS:CE1	2.54	0.43
1:A:98:LEU:N	1:A:98:LEU:HD12	2.32	0.43
1:D:17:TRP:CZ2	1:D:21:TYR:HB2	2.53	0.43
1:D:53:ASN:OD1	1:D:54:LYS:N	2.52	0.43
1:A:169:LEU:HD23	1:A:169:LEU:C	2.39	0.43
1:C:219:LEU:HD23	1:C:219:LEU:HA	1.81	0.43
1:D:125:PHE:HZ	2:H:2:GAL:HO6	1.63	0.43
1:A:189:TRP:HA	1:A:189:TRP:CE3	2.54	0.43
1:B:84:LEU:HA	1:B:84:LEU:HD12	1.89	0.43
1:B:80:ILE:HG13	1:B:84:LEU:HD22	1.99	0.43
1:B:229:ARG:CD	1:C:223:GLU:OE2	2.52	0.43
1:B:168:LYS:O	1:B:168:LYS:HD2	2.19	0.43
1:B:231:LYS:H	1:B:231:LYS:HG3	1.58	0.43
1:D:189:TRP:HA	1:D:189:TRP:CE3	2.53	0.43
1:A:167:LEU:O	1:A:170:CYS:N	2.51	0.43
1:A:188:ILE:H	1:A:188:ILE:HG12	1.54	0.43
1:A:10:THR:HG22	1:A:42:THR:HA	2.01	0.42
1:D:128:LYS:HB3	1:D:129:PRO:CD	2.49	0.42
1:C:189:TRP:CD1	2:G:2:GAL:H62	2.54	0.42
1:B:111:PRO:HB2	1:B:114:SER:OG	2.19	0.42
1:B:189:TRP:CZ2	2:F:2:GAL:H5	2.54	0.42
1:C:82:GLU:H	1:C:82:GLU:HG2	1.63	0.42
1:D:44:SER:HA	1:D:45:PRO:HD3	1.74	0.42
1:C:130:ASN:HB2	1:C:133:PHE:CD2	2.54	0.42
1:A:61:GLN:NE2	1:A:76:ILE:HG23	2.35	0.42
1:B:214:TYR:CE1	1:C:221:PRO:HB3	2.54	0.42
2:G:1:BGC:HC	2:G:2:GAL:HO6	1.62	0.42
1:A:225:ILE:N	1:A:225:ILE:HD13	2.33	0.42
1:A:110:PRO:HB3	1:A:116:GLY:CA	2.50	0.42
1:A:137:ARG:NH1	1:A:147:GLU:HA	2.34	0.42
1:C:125:PHE:CD1	1:C:125:PHE:N	2.87	0.42
1:D:128:LYS:CB	1:D:129:PRO:CD	2.98	0.42
1:D:26:ARG:NH1	1:D:26:ARG:CG	2.80	0.42
1:A:110:PRO:HB3	1:A:116:GLY:HA3	2.02	0.42
1:D:127:ASN:OD1	1:D:127:ASN:N	2.51	0.42
1:A:174:CYS:O	1:A:177:VAL:HB	2.20	0.42
1:B:139:ASP:N	1:B:139:ASP:OD1	2.52	0.42
1:B:9:CYS:HB2	1:B:14:ASP:HB3	2.01	0.42
1:B:12:LYS:O	1:B:15:ILE:HG13	2.19	0.42
1:A:130:ASN:HB2	1:A:133:PHE:CE2	2.55	0.41
1:B:53:ASN:O	1:B:54:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PRO:HA	1:C:111:PRO:HD3	1.97	0.41
1:D:60:LYS:O	1:D:79:ARG:NH2	2.54	0.41
1:B:105:GLY:H	1:B:107:GLU:CD	2.20	0.41
1:B:166:TYR:O	1:B:169:LEU:HB3	2.20	0.41
2:G:1:BGC:O3	2:G:2:GAL:O6	2.27	0.41
1:A:231:LYS:H	1:A:231:LYS:CD	2.26	0.41
1:B:29:MET:CB	1:B:36:ILE:HD11	2.45	0.41
1:C:26:ARG:HG2	1:C:27:TYR:CZ	2.56	0.41
1:C:5:ILE:HD11	1:C:28:PHE:CD2	2.55	0.41
1:D:110:PRO:CB	1:D:116:GLY:HA2	2.50	0.41
1:C:95:ASN:N	1:C:98:LEU:HD22	2.36	0.41
1:D:213:LEU:HA	1:D:213:LEU:HD23	1.85	0.41
1:A:75:HIS:HD2	1:A:174:CYS:SG	2.43	0.41
1:C:233:LYS:HA	1:C:233:LYS:CE	2.46	0.41
1:A:2:ARG:NH1	1:A:86:ARG:O	2.53	0.41
1:B:233:LYS:HB2	1:B:234:PRO:CD	2.50	0.41
1:B:89:ASP:C	1:B:163:THR:OG1	2.59	0.41
1:C:72:LYS:HD2	1:C:75:HIS:CE1	2.56	0.41
1:D:17:TRP:O	1:D:18:LYS:C	2.58	0.41
1:D:46:LYS:HB3	1:D:46:LYS:HE2	1.82	0.41
1:A:3:ILE:HB	1:A:36:ILE:HG13	2.02	0.41
1:B:144:TYR:CE2	1:B:146:PRO:HG3	2.56	0.41
1:C:133:PHE:HD2	1:C:135:TYR:HH	1.68	0.41
1:C:66:TRP:CG	1:C:67:PRO:HA	2.56	0.41
1:A:215:PRO:HB2	1:A:218:TRP:CG	2.56	0.41
1:B:223:GLU:HB2	1:B:225:ILE:CD1	2.51	0.41
1:D:173:ILE:O	1:D:174:CYS:C	2.59	0.41
1:D:220:LEU:HD23	1:D:222:PHE:CE1	2.56	0.41
1:B:44:SER:OG	1:B:45:PRO:HD2	2.21	0.41
1:C:37:GLU:OE1	1:C:57:HIS:NE2	2.50	0.41
1:D:16:PHE:HB3	1:D:96:ALA:O	2.21	0.41
1:A:213:LEU:O	1:A:228:ILE:CD1	2.69	0.41
1:C:154:TYR:O	1:C:196:ASN:ND2	2.54	0.41
1:C:53:ASN:OD1	1:C:55:HIS:HB2	2.21	0.41
1:D:120:THR:HG23	1:D:208:LEU:HB2	2.03	0.41
1:A:74:PHE:CE1	1:A:173:ILE:HG21	2.56	0.40
1:A:192:GLU:O	1:A:195:ILE:HG22	2.21	0.40
1:B:135:TYR:O	1:B:137:ARG:HG2	2.21	0.40
1:C:156:GLY:H	1:C:192:GLU:HG3	1.87	0.40
1:D:66:TRP:CG	1:D:67:PRO:CA	3.00	0.40
1:A:110:PRO:CB	1:A:116:GLY:HA3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:O	1:D:160:GLY:CA	2.69	0.40
1:D:199:PHE:HA	1:D:199:PHE:HD1	1.75	0.40
1:D:22:LEU:HA	1:D:22:LEU:HD12	1.92	0.40
1:D:31:ASP:HB2	1:D:34:PHE:HD2	1.85	0.40
1:D:84:LEU:HG	1:D:91:LEU:HD11	2.03	0.40
1:B:57:HIS:CD2	1:B:57:HIS:N	2.89	0.40
1:B:136:GLU:HG2	1:B:141:SER:HB3	2.04	0.40
1:D:123:PRO:CA	1:D:210:PRO:HB3	2.51	0.40
1:D:70:THR:CG2	1:D:71:LEU:N	2.84	0.40
1:A:74:PHE:HD2	1:A:170:CYS:SG	2.45	0.40
1:D:80:ILE:O	1:D:81:LYS:C	2.60	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:NZ	1:D:200:LEU:O[2_645]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	229/246 (93%)	225 (98%)	4 (2%)	0	100	100
1	B	233/246 (95%)	221 (95%)	11 (5%)	1 (0%)	34	72
1	C	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
1	D	234/246 (95%)	223 (95%)	11 (5%)	0	100	100
All	All	927/984 (94%)	888 (96%)	38 (4%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	PRO

5.3.2   Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/221 (94%)	191 (92%)	17 (8%)	11	39
1	B	212/221 (96%)	190 (90%)	22 (10%)	7	27
1	C	210/221 (95%)	189 (90%)	21 (10%)	7	29
1	D	213/221 (96%)	192 (90%)	21 (10%)	8	30
All	All	843/884 (95%)	762 (90%)	81 (10%)	8	32

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	42	THR
1	A	52	ASN
1	A	54	LYS
1	A	84	LEU
1	A	102	SER
1	A	113	ASP
1	A	130	ASN
1	A	132	GLU
1	A	142	THR
1	A	151	ARG
1	A	159	SER
1	A	174	CYS
1	A	179	ARG
1	A	188	ILE
1	A	227	LEU
1	A	231	LYS
1	B	9	CYS
1	B	15	ILE
1	B	31	ASP
1	B	33	SER

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Mol	Chain	Res	Type
1	B	49	ASP
1	B	62	LYS
1	B	68	ASP
1	B	70	THR
1	B	84	LEU
1	B	86	ARG
1	B	98	LEU
1	B	112	SER
1	B	113	ASP
1	B	114	SER
1	B	130	ASN
1	B	142	THR
1	B	151	ARG
1	B	159	SER
1	B	180	ASP
1	B	188	ILE
1	B	219	LEU
1	B	220	LEU
1	C	2	ARG
1	C	9	CYS
1	C	52	ASN
1	C	57	HIS
1	C	64	LEU
1	C	82	GLU
1	C	98	LEU
1	C	101	THR
1	C	108	ILE
1	C	112	SER
1	C	113	ASP
1	C	130	ASN
1	C	139	ASP
1	C	142	THR
1	C	151	ARG
1	C	175	SER
1	C	180	ASP
1	C	188	ILE
1	C	196	ASN
1	C	227	LEU
1	C	231	LYS
1	D	15	ILE
1	D	26	ARG
1	D	29	MET

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Mol	Chain	Res	Type
1	D	42	THR
1	D	49	ASP
1	D	66	TRP
1	D	84	LEU
1	D	85	GLU
1	D	112	SER
1	D	113	ASP
1	D	126	TYR
1	D	139	ASP
1	D	142	THR
1	D	171	THR
1	D	174	CYS
1	D	180	ASP
1	D	188	ILE
1	D	199	PHE
1	D	222	PHE
1	D	231	LYS
1	D	236	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	75	HIS
1	B	75	HIS
1	B	130	ASN
1	C	75	HIS
1	C	196	ASN
1	D	75	HIS
1	D	190	HIS

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)

12 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	BGC	E	1	2	12,12,12	1.32	2 (16%)	17,17,17	1.38	3 (17%)
2	GAL	E	2	2	11,11,12	1.88	1 (9%)	15,15,17	1.58	3 (20%)
2	FUC	E	3	2	10,10,11	2.35	4 (40%)	14,14,16	2.28	4 (28%)
2	BGC	F	1	2	12,12,12	1.23	2 (16%)	17,17,17	1.51	3 (17%)
2	GAL	F	2	2	11,11,12	1.84	1 (9%)	15,15,17	1.85	3 (20%)
2	FUC	F	3	2	10,10,11	2.54	5 (50%)	14,14,16	2.39	3 (21%)
2	BGC	G	1	2	12,12,12	1.05	2 (16%)	17,17,17	1.89	5 (29%)
2	GAL	G	2	2	11,11,12	1.82	1 (9%)	15,15,17	1.88	6 (40%)
2	FUC	G	3	2	10,10,11	2.36	5 (50%)	14,14,16	2.60	4 (28%)
2	BGC	H	1	2	12,12,12	1.45	2 (16%)	17,17,17	0.93	0
2	GAL	H	2	2	11,11,12	2.23	1 (9%)	15,15,17	2.06	3 (20%)
2	FUC	H	3	2	10,10,11	2.69	5 (50%)	14,14,16	2.38	2 (14%)

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	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2	-	2/2/19/22	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	H	1	2	-	2/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	FUC	H	3	2	-	-	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GAL	C2-C3	6.71	1.62	1.52
2	E	2	GAL	C2-C3	5.73	1.61	1.52
2	G	2	GAL	C2-C3	5.37	1.60	1.52
2	F	2	GAL	C2-C3	5.20	1.60	1.52
2	H	3	FUC	O5-C5	4.88	1.54	1.43
2	E	3	FUC	O5-C5	4.75	1.53	1.43
2	F	3	FUC	O5-C5	4.61	1.53	1.43
2	G	3	FUC	O5-C5	4.56	1.53	1.43
2	H	3	FUC	C2-C3	4.05	1.58	1.52
2	F	3	FUC	C2-C3	3.71	1.58	1.52
2	E	1	BGC	O4-C4	3.39	1.51	1.43
2	H	1	BGC	O4-C4	3.29	1.50	1.43
2	F	3	FUC	O5-C1	3.24	1.48	1.43
2	H	3	FUC	O5-C1	3.13	1.48	1.43
2	H	3	FUC	C6-C5	3.02	1.58	1.51
2	G	3	FUC	O5-C1	3.01	1.48	1.43
2	E	3	FUC	O5-C1	2.90	1.48	1.43
2	G	3	FUC	C2-C3	2.88	1.56	1.52
2	G	3	FUC	C6-C5	2.84	1.58	1.51
2	E	3	FUC	C2-C3	2.80	1.56	1.52
2	F	3	FUC	C6-C5	2.74	1.58	1.51
2	F	3	FUC	C4-C3	2.68	1.59	1.52
2	E	3	FUC	C6-C5	2.64	1.57	1.51
2	H	1	BGC	O5-C1	2.64	1.49	1.42
2	H	3	FUC	C4-C3	2.57	1.58	1.52
2	F	1	BGC	O4-C4	2.53	1.48	1.43
2	G	3	FUC	C4-C3	2.37	1.58	1.52
2	F	1	BGC	O5-C1	2.33	1.48	1.42
2	G	1	BGC	O4-C4	2.21	1.48	1.43
2	G	1	BGC	O5-C1	2.18	1.48	1.42
2	E	1	BGC	O5-C1	2.00	1.47	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	3	FUC	C1-C2-C3	7.62	119.03	109.67
2	H	3	FUC	C1-C2-C3	7.29	118.62	109.67
2	F	3	FUC	C1-C2-C3	6.83	118.07	109.67
2	H	2	GAL	C1-C2-C3	-6.70	101.43	109.67
2	E	3	FUC	C1-C2-C3	6.40	117.53	109.67
2	F	2	GAL	C1-C2-C3	-4.77	103.80	109.67
2	G	1	BGC	C1-C2-C3	-4.74	100.49	110.31
2	E	2	GAL	C1-C2-C3	-4.07	104.67	109.67
2	F	3	FUC	O2-C2-C3	4.02	118.19	110.14
2	F	1	BGC	C3-C4-C5	3.98	117.35	110.24
2	H	3	FUC	O2-C2-C3	3.74	117.62	110.14
2	E	3	FUC	O2-C2-C3	3.47	117.08	110.14
2	G	1	BGC	O5-C1-C2	-3.43	104.16	110.28
2	G	3	FUC	O2-C2-C3	3.42	116.99	110.14
2	E	1	BGC	C1-C2-C3	-3.31	103.46	110.31
2	G	2	GAL	C1-C2-C3	-3.13	105.82	109.67
2	G	2	GAL	O5-C1-C2	3.10	115.56	110.77
2	G	1	BGC	O2-C2-C1	3.07	116.28	109.16
2	E	1	BGC	O5-C1-C2	-2.76	105.36	110.28
2	G	2	GAL	C2-C3-C4	-2.71	106.20	110.89
2	G	3	FUC	O5-C1-C2	2.60	114.79	110.77
2	G	2	GAL	C3-C4-C5	-2.60	105.60	110.24
2	G	2	GAL	O2-C2-C1	-2.58	103.87	109.15
2	H	2	GAL	O2-C2-C1	-2.58	103.88	109.15
2	F	2	GAL	O5-C1-C2	2.53	114.67	110.77
2	E	3	FUC	O2-C2-C1	2.49	114.24	109.15
2	E	2	GAL	C3-C4-C5	-2.43	105.90	110.24
2	G	1	BGC	C4-C3-C2	-2.37	106.69	110.82
2	F	1	BGC	O2-C2-C1	2.30	114.50	109.16
2	G	3	FUC	O3-C3-C2	-2.30	105.60	109.99
2	G	1	BGC	O4-C4-C5	-2.20	103.83	109.30
2	E	2	GAL	O6-C6-C5	-2.16	103.88	111.29
2	F	2	GAL	O3-C3-C2	-2.14	105.89	109.99
2	F	3	FUC	O5-C1-C2	2.10	114.00	110.77
2	H	2	GAL	O2-C2-C3	2.08	114.30	110.14
2	E	3	FUC	O3-C3-C2	-2.07	106.03	109.99
2	G	2	GAL	O5-C5-C4	-2.05	105.85	110.83
2	E	1	BGC	C3-C4-C5	2.04	113.88	110.24
2	F	1	BGC	O2-C2-C3	-2.02	105.67	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	BGC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	H	1	BGC	O5-C5-C6-O6
2	E	2	GAL	C4-C5-C6-O6
2	H	1	BGC	C4-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	F	1	BGC	C4-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GAL	4	0
2	G	2	GAL	4	0
2	H	1	BGC	1	0
2	E	1	BGC	5	0
2	G	1	BGC	6	0
2	F	2	GAL	2	0
2	H	3	FUC	1	0
2	H	2	GAL	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H
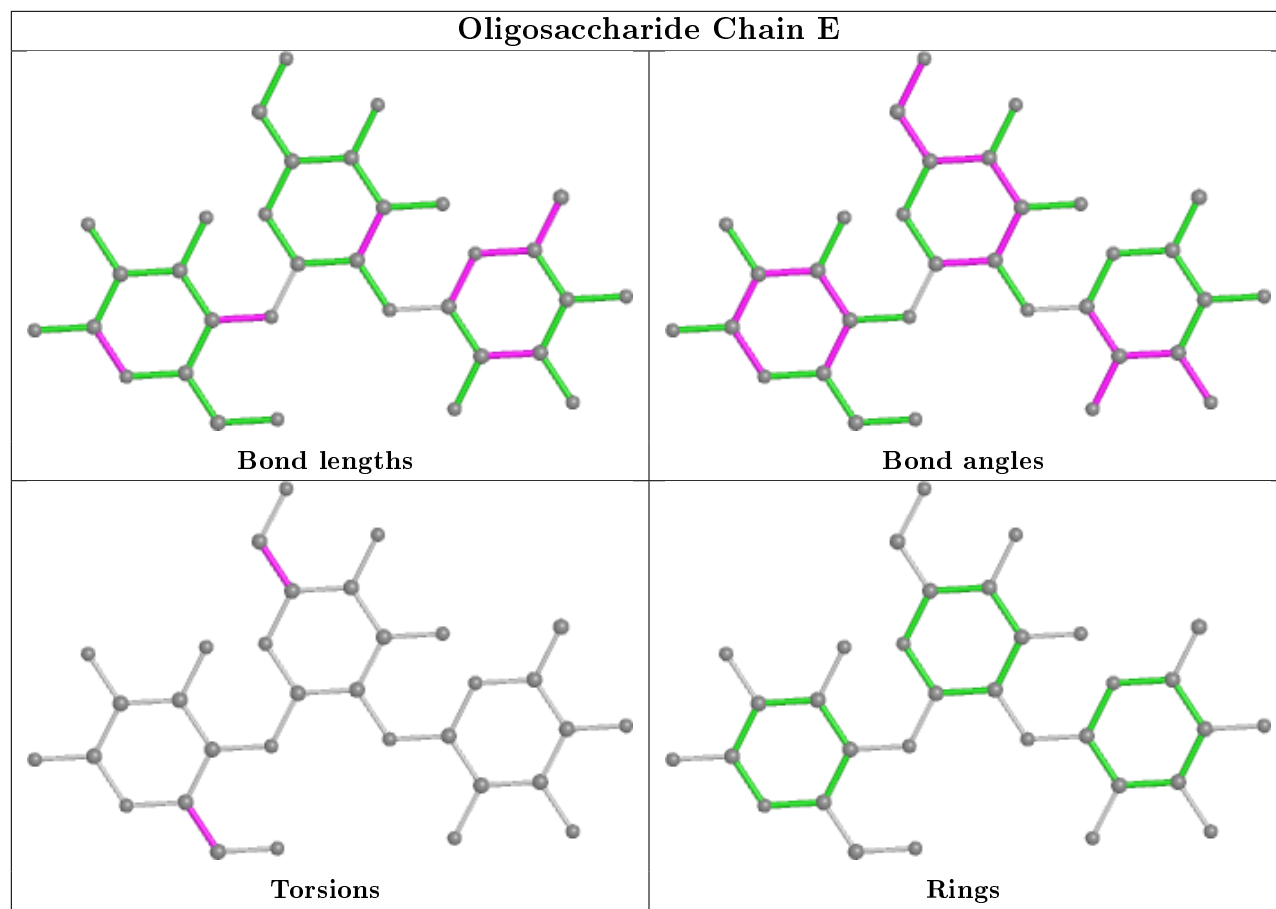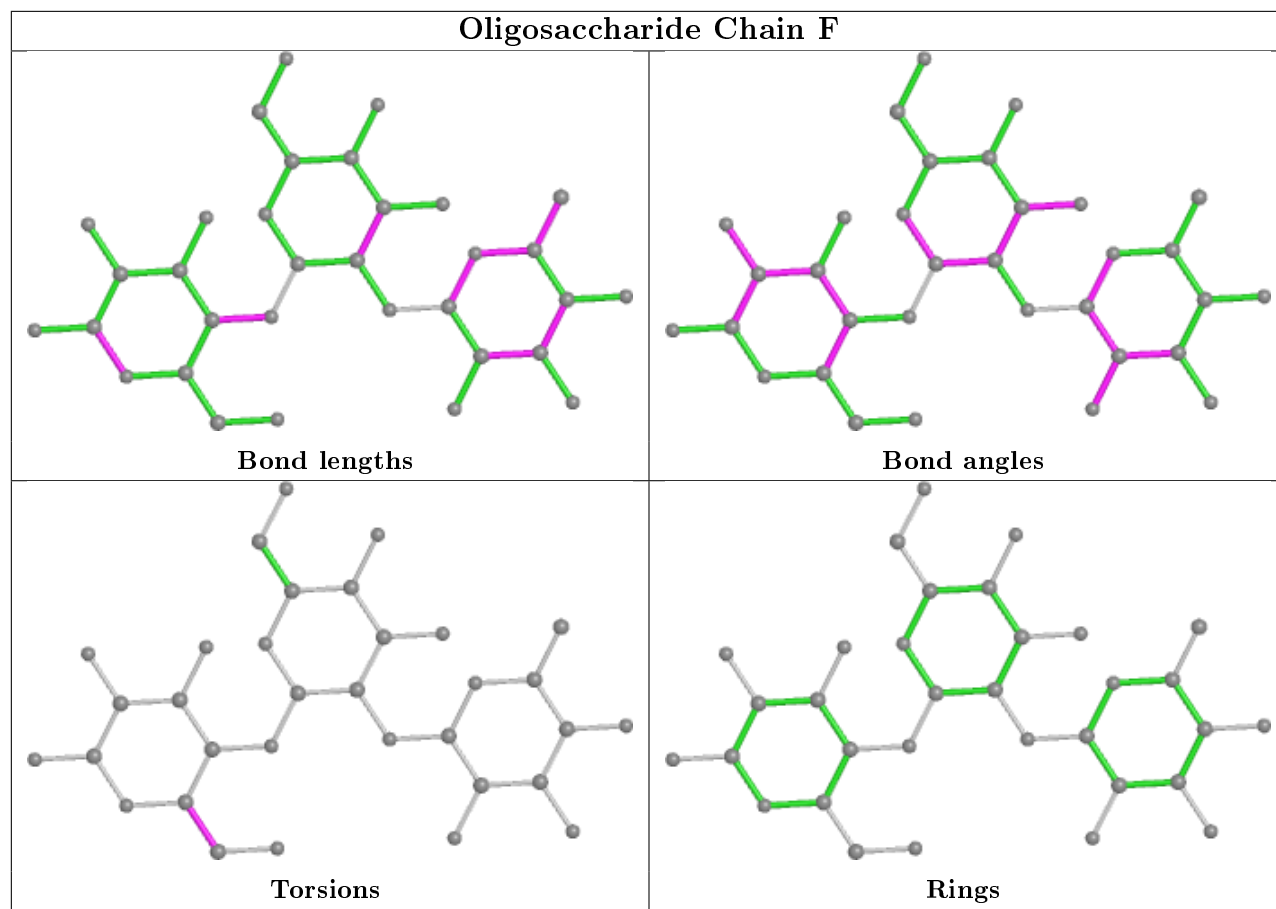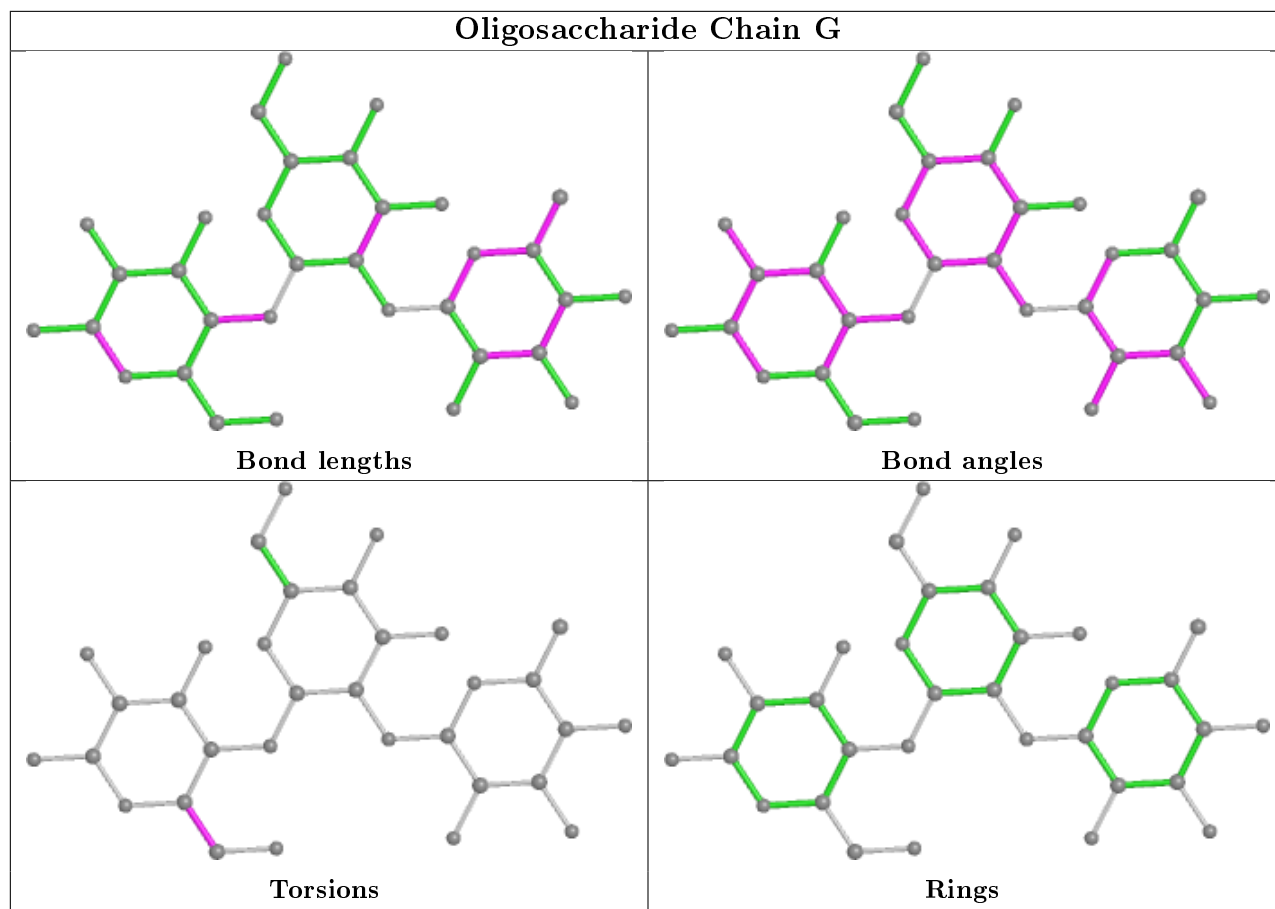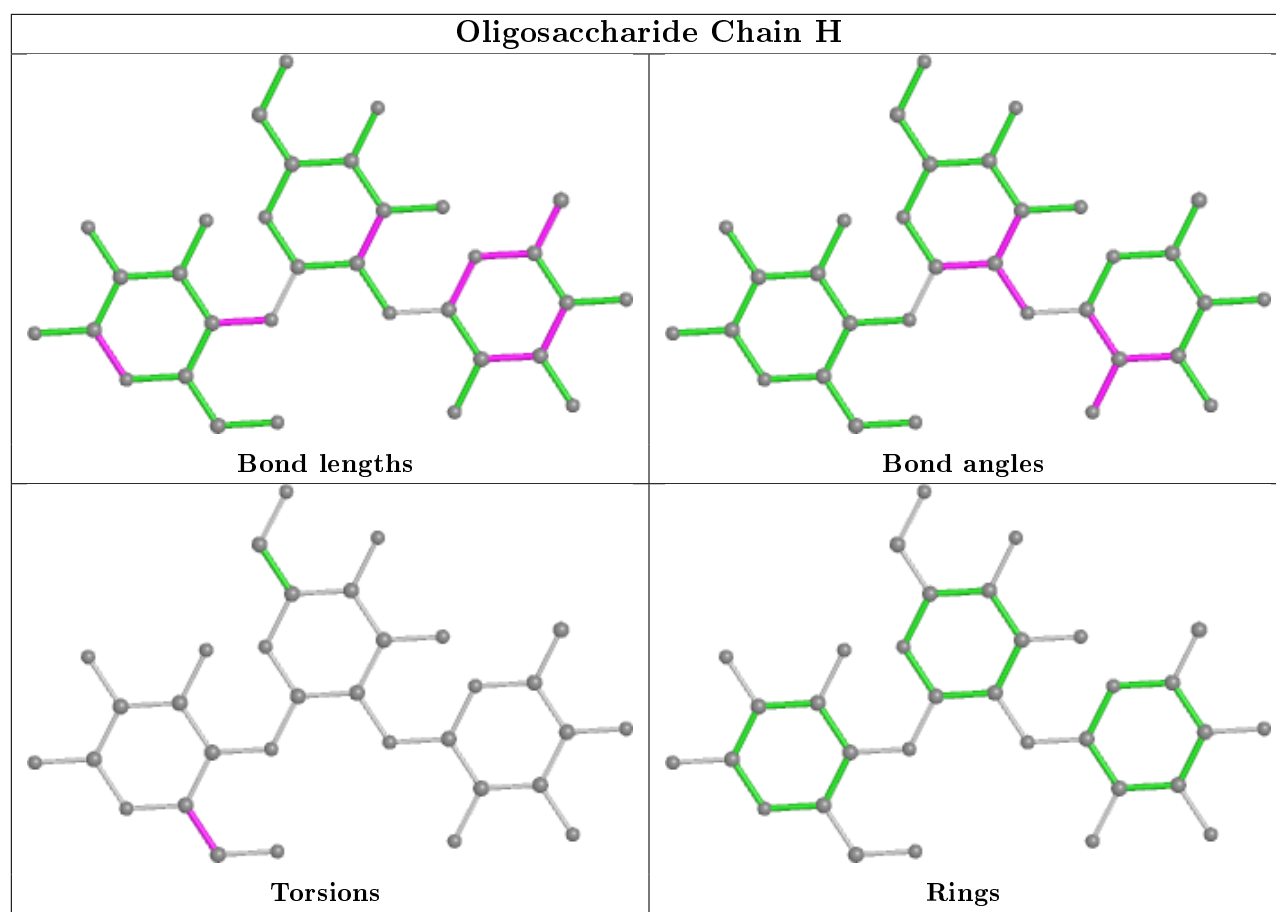
5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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


Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
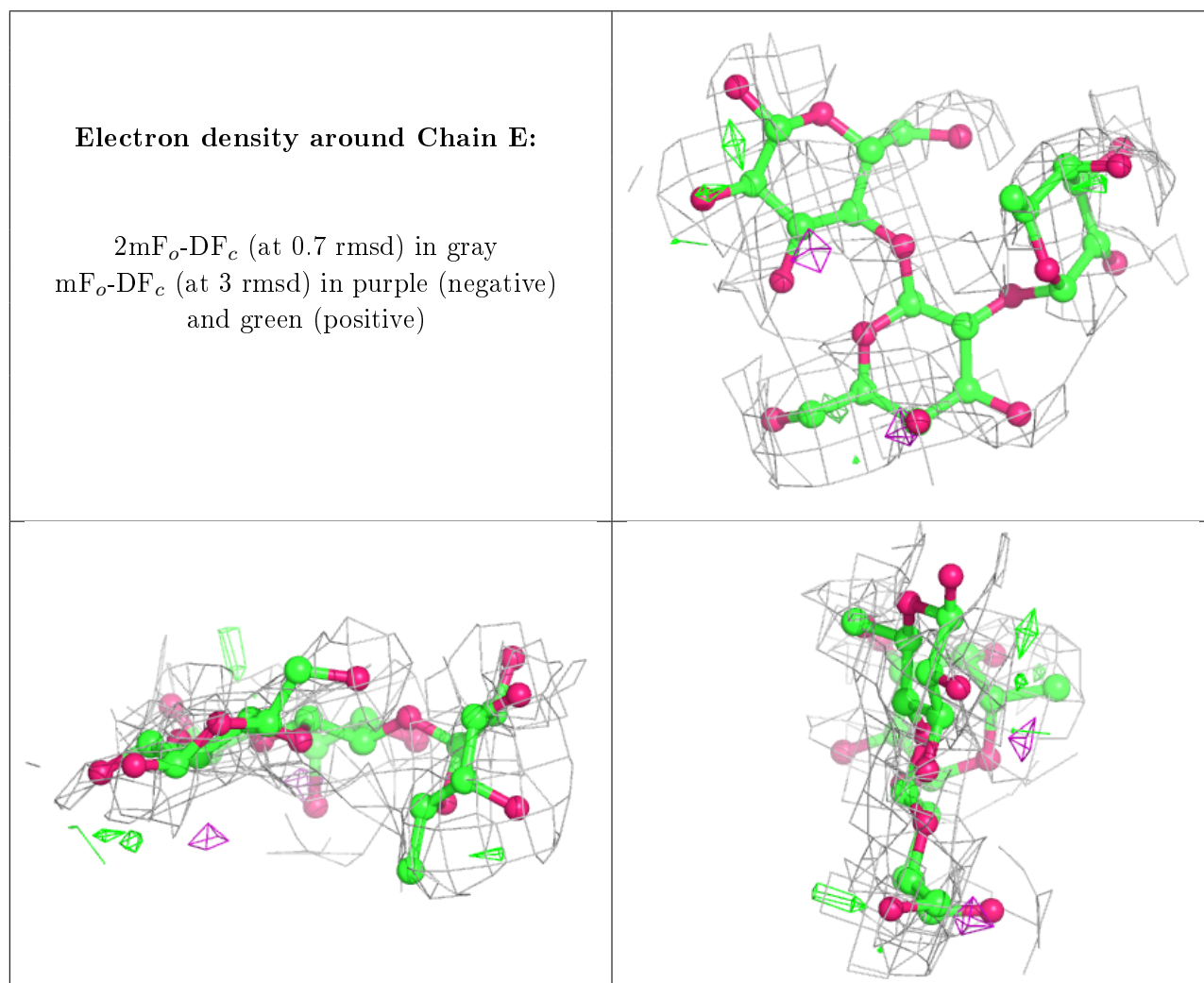
Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
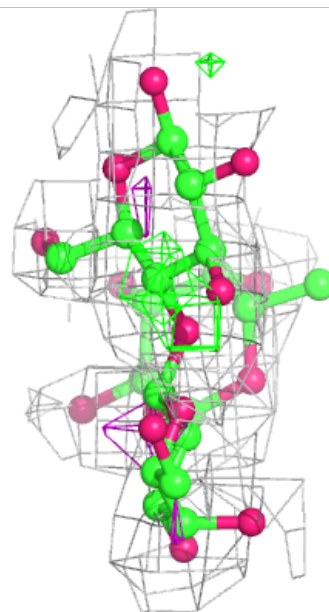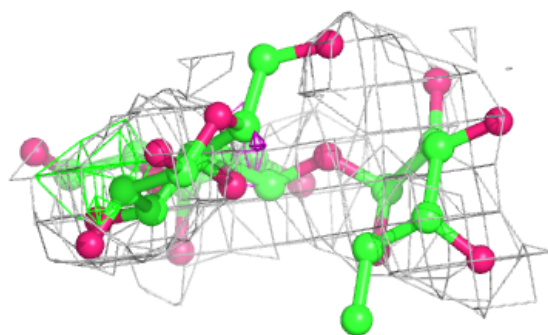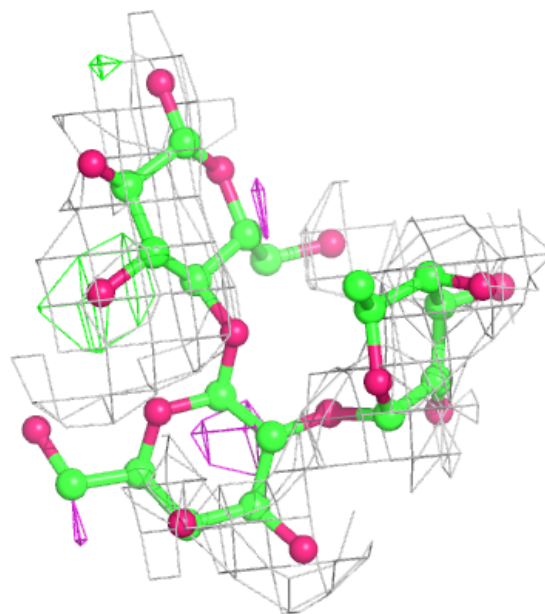
Electron density around Chain G:

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

Electron density around Chain H:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
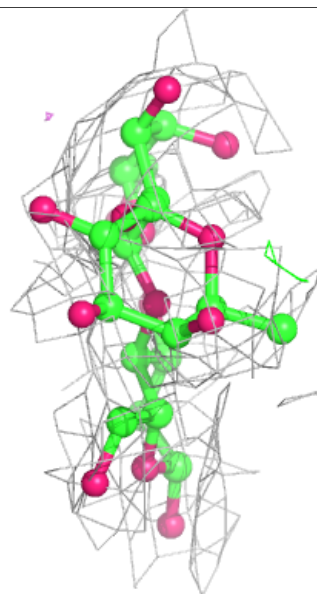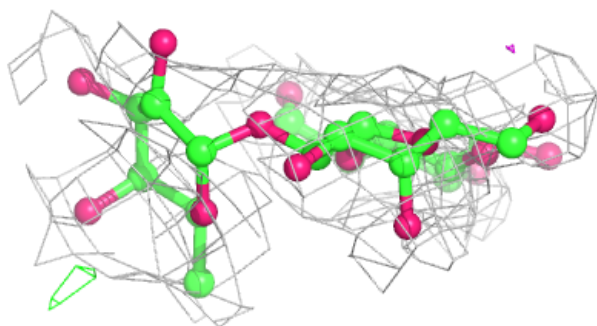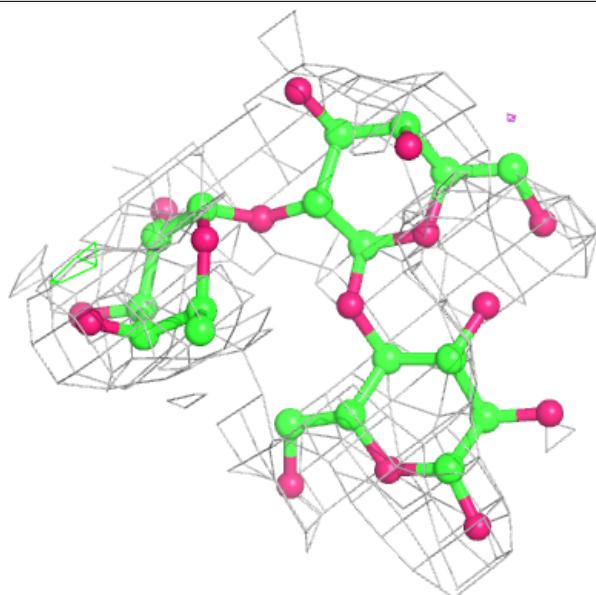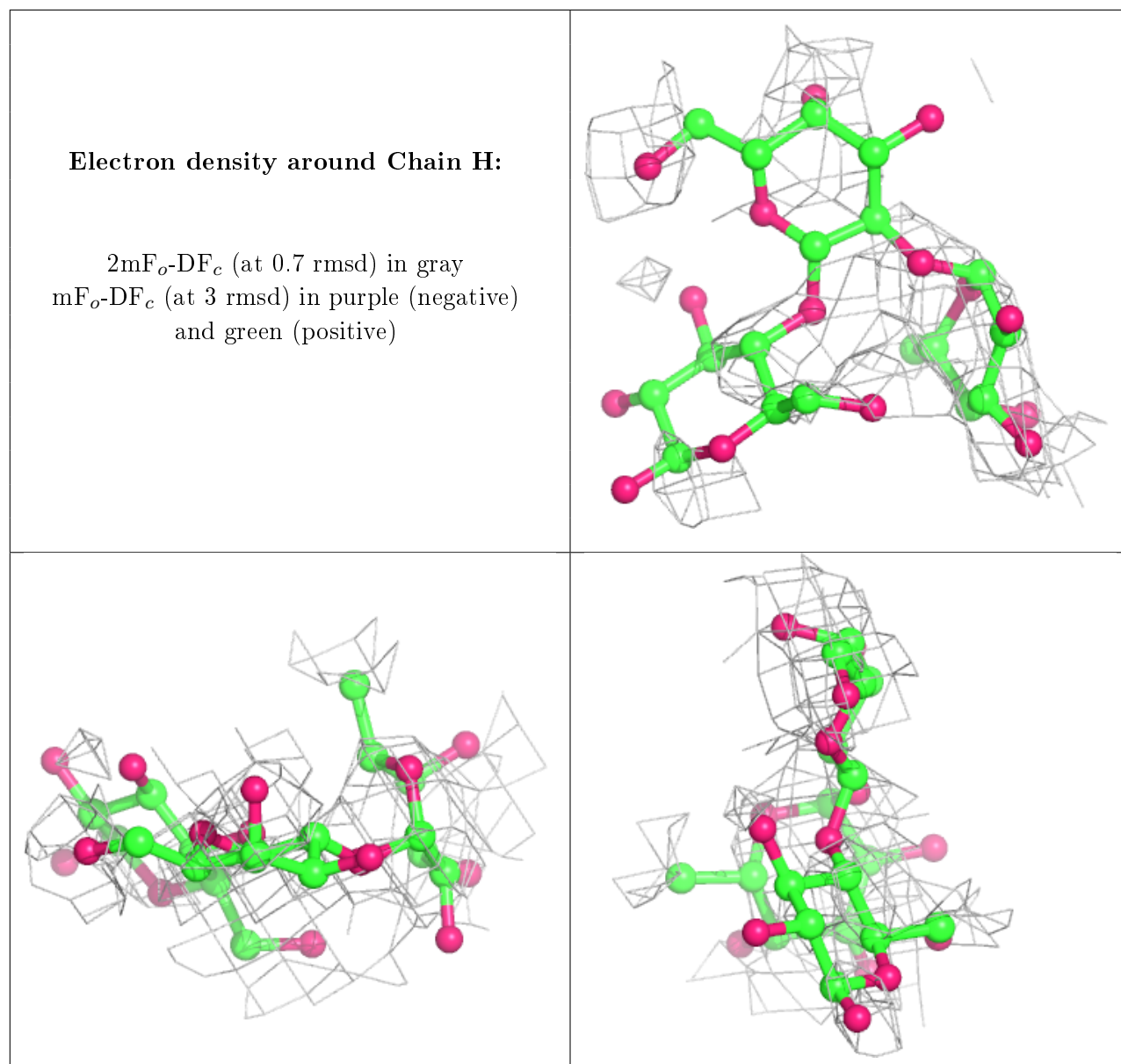
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.