



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2021 – 04:11 PM JST

PDB ID : 7EIM
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (W470A) in complex with maltopentaose
Authors : Shen, M.; Xiang, S.
Deposited on : 2021-03-31
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

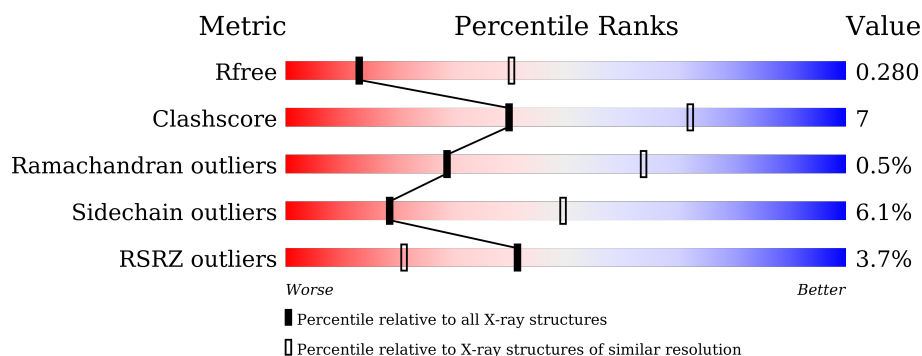
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	1536	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	1536	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>
2	C	5	<div> <div></div> <div> <div>60%</div> <div>40%</div> </div> </div>
2	D	5	<div> <div></div> <div> <div>40%</div> <div>60%</div> </div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
3	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
3	H	2	<div><div></div><div>100%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24742 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.

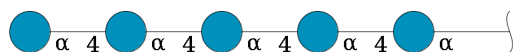
- Molecule 1 is a protein called 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12269	7822	2064	2331	52			
1	B	1526	Total	C	N	O	S	0	0	0
			12269	7822	2064	2331	52			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	ALA	TRP	engineered mutation	UNP Q6FSK0
A	1529	LEU	-	expression tag	UNP Q6FSK0
A	1530	GLU	-	expression tag	UNP Q6FSK0
A	1531	HIS	-	expression tag	UNP Q6FSK0
A	1532	HIS	-	expression tag	UNP Q6FSK0
A	1533	HIS	-	expression tag	UNP Q6FSK0
A	1534	HIS	-	expression tag	UNP Q6FSK0
A	1535	HIS	-	expression tag	UNP Q6FSK0
A	1536	HIS	-	expression tag	UNP Q6FSK0
B	470	ALA	TRP	engineered mutation	UNP Q6FSK0
B	1529	LEU	-	expression tag	UNP Q6FSK0
B	1530	GLU	-	expression tag	UNP Q6FSK0
B	1531	HIS	-	expression tag	UNP Q6FSK0
B	1532	HIS	-	expression tag	UNP Q6FSK0
B	1533	HIS	-	expression tag	UNP Q6FSK0
B	1534	HIS	-	expression tag	UNP Q6FSK0
B	1535	HIS	-	expression tag	UNP Q6FSK0
B	1536	HIS	-	expression tag	UNP Q6FSK0

- Molecule 2 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
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	D	5	Total	C	O	0	0	0
			56	30	26			

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

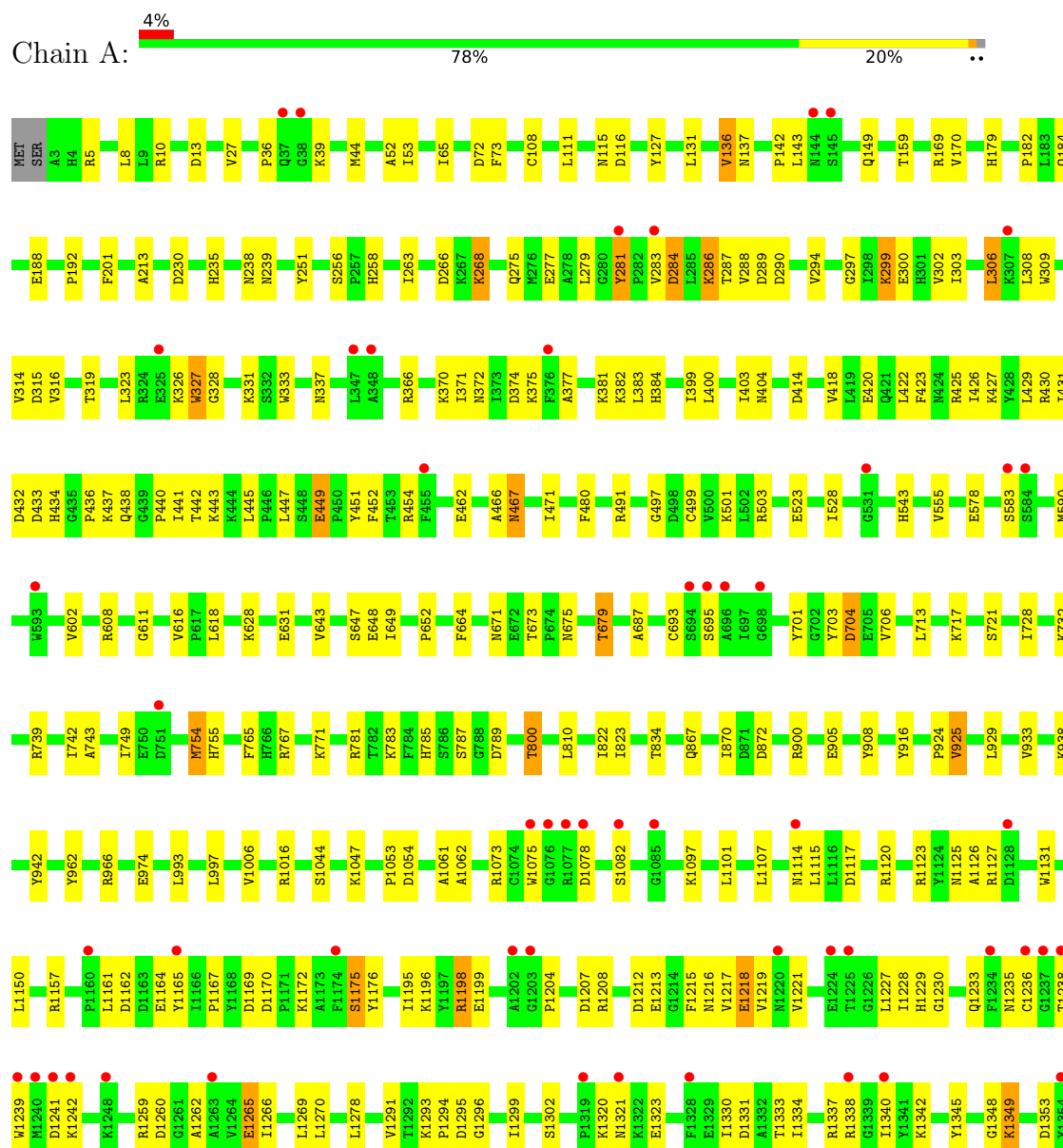


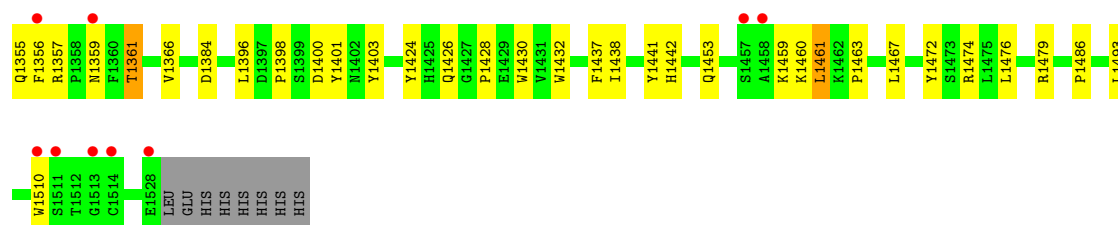
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			
3	G	2	Total	C	O	0	0	0
			23	12	11			
3	H	2	Total	C	O	0	0	0
			23	12	11			

3 Residue-property plots [i](#)

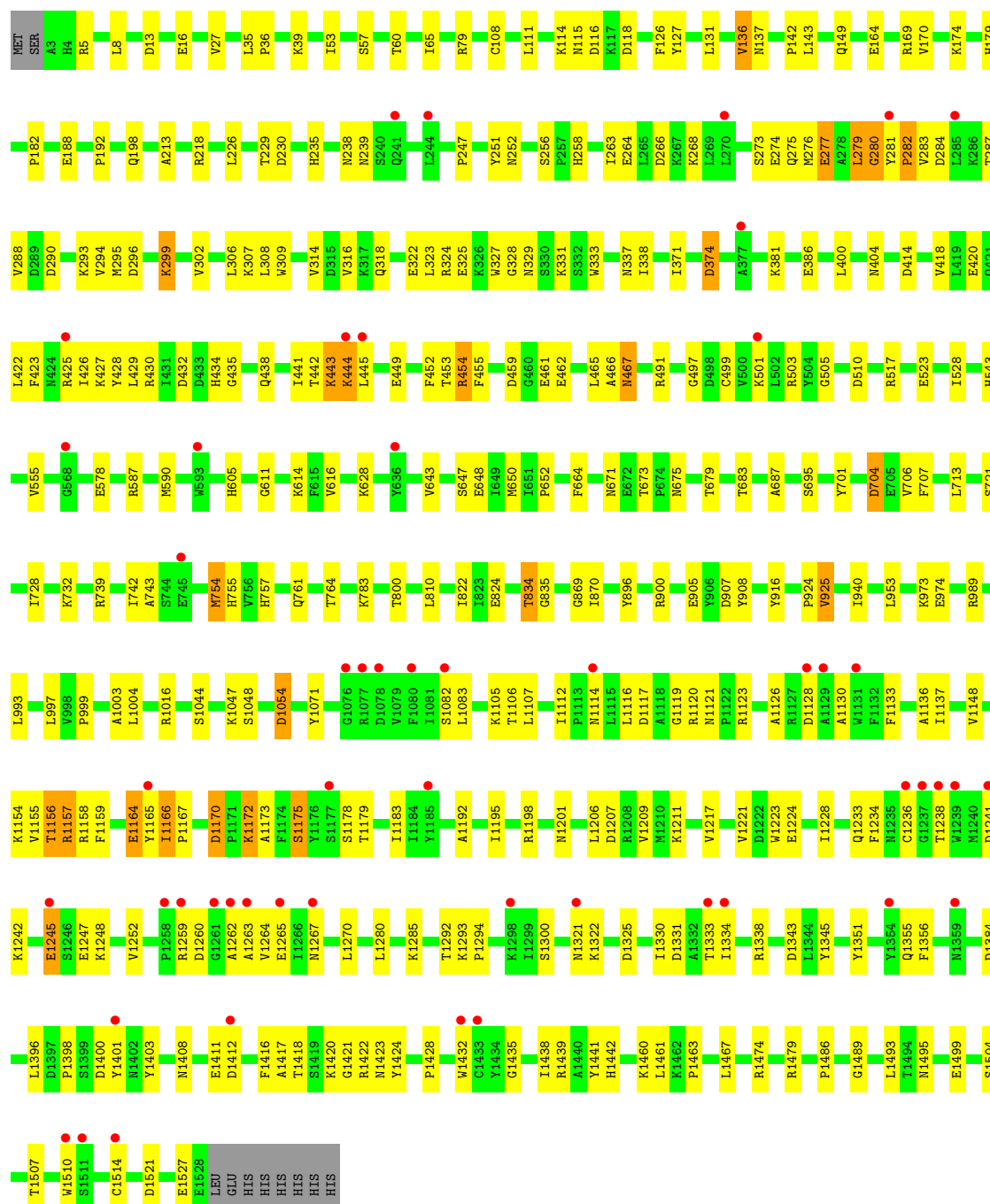
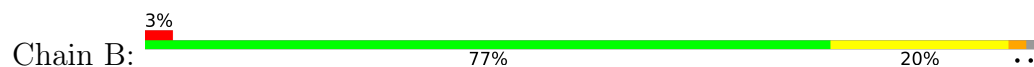
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 4-alpha-glucanotransferase





● Molecule 1: 4-alpha-glucanotransferase



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

Chain C:  60% 40%

GLC1
GLC2
GLC3
GLC4
GLC5

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

Chain D:  40% 60%

GLC1
GLC2
GLC3
GLC4
GLC5

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

Chain E:  100%

GLC1
GLC2

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

Chain F:  50% 50%

GLC1
GLC2

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

Chain G:  50% 50%

GLC1
GLC2

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

Chain H:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.52Å 200.33Å 134.28Å 90.00° 100.84° 90.00°	Depositor
Resolution (Å)	38.77 – 3.10 38.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.77-3.10) 99.1 (38.77-3.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.250 , 0.282 0.249 , 0.280	Depositor DCC
R_{free} test set	3632 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	90.7	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24742	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: 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	0.26	0/12578	0.45	0/17055
1	B	0.26	0/12578	0.45	0/17055
All	All	0.26	0/25156	0.45	0/34110

There are no bond length outliers.

There are no bond angle outliers.

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	12269	0	11955	184	0
1	B	12269	0	11955	170	0
2	C	56	0	48	3	0
2	D	56	0	48	2	0
3	E	23	0	21	0	0
3	F	23	0	21	0	0
3	G	23	0	21	1	0
3	H	23	0	21	0	0
All	All	24742	0	24090	356	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 7.

All (356) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:LYS:HA	1:A:1218:GLU:HG3	1.43	1.00
1:A:182:PRO:HD3	1:A:230:ASP:HB2	1.64	0.79
1:B:328:GLY:H	1:B:331:LYS:HE2	1.48	0.79
1:A:1361:THR:HG21	1:A:1437:PHE:HA	1.66	0.78
1:B:182:PRO:HD3	1:B:230:ASP:HB2	1.65	0.77
1:B:169:ARG:NH1	1:B:721:SER:O	2.18	0.77
1:B:1221:VAL:HG22	1:B:1228:ILE:HG12	1.68	0.76
1:A:286:LYS:HE3	1:A:438:GLN:HE22	1.52	0.75
1:A:8:LEU:HB2	1:A:652:PRO:HG2	1.69	0.74
1:A:1115:LEU:HB3	1:A:1123:ARG:HB3	1.71	0.72
1:A:430:ARG:HB3	1:A:438:GLN:HG3	1.70	0.72
1:A:169:ARG:NH1	1:A:721:SER:O	2.22	0.72
1:B:8:LEU:HB2	1:B:652:PRO:HG2	1.71	0.72
1:B:452:PHE:HA	1:B:466:ALA:HA	1.71	0.72
1:B:428:TYR:HA	1:B:432:ASP:HB2	1.71	0.71
1:A:1355:GLN:OE1	1:A:1357:ARG:NH1	2.24	0.71
1:A:284:ASP:HB2	1:A:440:PRO:HA	1.74	0.70
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.24	0.70
1:A:1123:ARG:HH22	1:A:1207:ASP:HB2	1.57	0.69
1:A:1384:ASP:OD1	1:A:1474:ARG:NH1	2.26	0.69
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.74	0.69
1:B:443:LYS:HD3	1:B:444:LYS:HG2	1.75	0.68
1:A:1259:ARG:NH2	1:A:1265:GLU:OE2	2.26	0.68
1:A:1195:ILE:HD11	1:A:1219:VAL:HB	1.77	0.67
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.78	0.66
1:A:452:PHE:HA	1:A:466:ALA:HA	1.78	0.66
1:B:13:ASP:OD2	1:B:1479:ARG:NH2	2.25	0.66
1:B:1384:ASP:OD1	1:B:1474:ARG:NH1	2.30	0.64
1:A:1342:LYS:HE2	1:A:1353:ASP:HB3	1.79	0.64
1:B:374:ASP:OD1	1:B:374:ASP:N	2.30	0.63
1:B:400:LEU:O	1:B:404:ASN:ND2	2.31	0.63
1:B:331:LYS:HB3	1:B:381:LYS:HD2	1.81	0.63
1:B:430:ARG:HD2	1:B:438:GLN:HA	1.81	0.63
1:A:1170:ASP:HB3	1:A:1172:LYS:HG2	1.82	0.61
1:A:1295:ASP:OD1	1:A:1296:GLY:N	2.33	0.61
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.82	0.61
1:B:1192:ALA:HB1	1:B:1223:TRP:HZ2	1.66	0.61
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.34	0.61
1:A:13:ASP:OD2	1:A:1479:ARG:NH2	2.28	0.61
1:B:1259:ARG:NH1	1:B:1343:ASP:OD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:OD1	1:A:116:ASP:N	2.34	0.60
1:A:728:ILE:HD11	1:A:810:LEU:HD22	1.83	0.60
1:B:268:LYS:HG3	1:B:302:VAL:HG12	1.82	0.60
1:B:131:LEU:HD13	1:B:143:LEU:HD13	1.83	0.60
1:A:1293:LYS:HD2	1:A:1294:PRO:HD2	1.82	0.60
1:B:179:HIS:NE2	1:B:230:ASP:OD1	2.35	0.60
1:A:306:LEU:HD23	1:A:366:ARG:HH22	1.67	0.60
1:A:590:MET:HB2	1:A:671:ASN:HD22	1.67	0.59
1:B:115:ASN:OD1	1:B:116:ASP:N	2.36	0.59
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.35	0.59
1:A:1198:ARG:NH2	1:A:1212:ASP:O	2.36	0.59
1:B:1417:ALA:HB1	1:B:1423:ASN:OD1	2.02	0.59
1:A:430:ARG:HD2	1:A:438:GLN:HA	1.84	0.58
1:A:400:LEU:O	1:A:404:ASN:ND2	2.37	0.58
1:A:721:SER:OG	1:A:823:ILE:O	2.17	0.58
1:A:425:ARG:HH22	1:A:491:ARG:HB3	1.68	0.58
1:A:466:ALA:H	1:A:501:LYS:HD2	1.68	0.58
1:A:1123:ARG:HH11	1:A:1125:ASN:HB3	1.69	0.58
1:B:1107:LEU:O	1:B:1157:ARG:NH1	2.37	0.58
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.86	0.57
1:B:1083:LEU:HD22	1:B:1136:ALA:HB1	1.86	0.57
1:A:1441:TYR:OH	1:A:1474:ARG:NH2	2.38	0.57
1:B:428:TYR:HE1	1:B:434:HIS:HB2	1.70	0.57
1:A:277:GLU:HB3	1:A:283:VAL:HG22	1.87	0.56
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.87	0.56
1:A:1432:TRP:CG	1:A:1510:TRP:HD1	2.24	0.56
1:B:36:PRO:HB2	1:B:39:LYS:HG3	1.87	0.56
1:B:466:ALA:H	1:B:501:LYS:HD2	1.71	0.56
1:B:590:MET:HB2	1:B:671:ASN:HD22	1.70	0.56
1:B:306:LEU:HD13	1:B:309:TRP:HZ2	1.69	0.56
1:A:1221:VAL:HG22	1:A:1228:ILE:HG12	1.88	0.56
1:A:1331:ASP:OD1	1:A:1333:THR:OG1	2.24	0.56
1:A:1218:GLU:HA	1:A:1218:GLU:OE1	2.04	0.56
1:B:273:SER:HA	1:B:276:MET:HB2	1.88	0.55
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.87	0.55
1:A:238:ASN:ND2	1:A:497:GLY:O	2.39	0.55
1:B:430:ARG:HB3	1:B:438:GLN:HG3	1.88	0.55
1:A:721:SER:HA	1:A:822:ILE:HD11	1.88	0.55
1:B:466:ALA:HB3	1:B:501:LYS:HE3	1.88	0.54
1:A:36:PRO:HB2	1:A:39:LYS:HG3	1.89	0.54
1:A:929:LEU:HD22	1:A:1006:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:PRO:HB2	1:A:1208:ARG:NH1	2.22	0.54
1:A:315:ASP:O	1:A:319:THR:OG1	2.24	0.54
1:B:238:ASN:ND2	1:B:497:GLY:O	2.40	0.54
1:B:611:GLY:HA2	1:B:997:LEU:HD23	1.88	0.54
1:B:1165:TYR:O	1:B:1167:PRO:HD3	2.07	0.54
1:A:377:ALA:O	1:A:381:LYS:HG3	2.08	0.54
1:A:1217:VAL:O	1:A:1218:GLU:HG2	2.07	0.53
1:A:870:ILE:HD11	1:A:997:LEU:HD13	1.89	0.53
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.91	0.53
1:A:1167:PRO:HB2	1:A:1170:ASP:HB2	1.91	0.53
1:B:425:ARG:HH22	1:B:491:ARG:HB3	1.74	0.52
1:B:188:GLU:H	1:B:239:ASN:HD21	1.56	0.52
1:B:142:PRO:HG2	1:B:743:ALA:HB1	1.90	0.52
1:A:1219:VAL:HG22	1:A:1230:GLY:HA3	1.91	0.52
1:B:1331:ASP:OD1	1:B:1333:THR:OG1	2.28	0.52
1:B:306:LEU:HD13	1:B:309:TRP:CZ2	2.44	0.52
1:B:1123:ARG:HH11	1:B:1206:LEU:HD23	1.74	0.52
1:A:372:ASN:OD1	1:A:375:LYS:HG3	2.10	0.52
1:B:1351:TYR:O	1:B:1355:GLN:HG3	2.10	0.52
1:B:453:THR:N	1:B:465:LEU:O	2.42	0.52
1:B:757:HIS:HB3	1:B:764:THR:HB	1.91	0.52
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.33	0.51
1:A:327:TRP:CE2	1:A:381:LYS:HE2	2.45	0.51
1:B:238:ASN:HB2	1:B:453:THR:HG21	1.91	0.51
1:B:925:VAL:HG21	1:B:1486:PRO:HB2	1.91	0.51
1:B:1170:ASP:HB3	1:B:1172:LYS:HG2	1.92	0.51
1:A:1075:TRP:CH2	2:C:3:GLC:H62	2.46	0.51
1:B:1432:TRP:CG	1:B:1510:TRP:HD1	2.29	0.51
1:A:1228:ILE:HG13	1:A:1270:LEU:HD22	1.92	0.51
1:A:131:LEU:HD13	1:A:143:LEU:HD13	1.92	0.51
1:A:1131:TRP:CD1	1:A:1266:ILE:HG23	2.46	0.51
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.93	0.51
1:A:695:SER:O	1:A:739:ARG:NH2	2.36	0.51
1:A:938:LYS:HE2	1:A:942:TYR:HE2	1.75	0.51
1:B:1105:LYS:HE2	1:B:1156:THR:H	1.75	0.51
1:B:282:PRO:HG3	1:B:293:LYS:HB2	1.94	0.50
1:B:425:ARG:NH2	1:B:491:ARG:HB3	2.27	0.50
1:B:679:THR:OG1	1:B:783:LYS:HG2	2.11	0.50
1:B:1242:LYS:HE2	1:B:1421:GLY:C	2.32	0.50
1:B:1322:LYS:H	1:B:1322:LYS:HD2	1.75	0.50
1:A:1233:GLN:OE1	1:A:1348:GLY:HA3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:916:TYR:O	1:B:924:PRO:HD2	2.11	0.50
1:A:10:ARG:HA	1:A:52:ALA:HB3	1.93	0.50
1:A:266:ASP:HB3	1:A:454:ARG:HH22	1.77	0.50
1:A:916:TYR:O	1:A:924:PRO:HD2	2.12	0.50
1:B:381:LYS:HG2	1:B:386:GLU:HA	1.93	0.50
1:B:1259:ARG:HH21	1:B:1263:ALA:HB1	1.77	0.50
1:A:53:ILE:HD11	1:A:65:ILE:HD11	1.94	0.50
1:A:466:ALA:HB3	1:A:501:LYS:HE3	1.94	0.50
1:A:1278:LEU:HD11	1:A:1302:SER:HA	1.92	0.50
2:D:2:GLC:H62	2:D:3:GLC:O5	2.11	0.50
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.93	0.49
1:A:5:ARG:HA	1:A:643:VAL:HG12	1.93	0.49
1:A:256:SER:HB2	1:A:258:HIS:CE1	2.47	0.49
1:A:1157:ARG:HG2	1:A:1176:TYR:CZ	2.48	0.49
1:B:721:SER:HA	1:B:822:ILE:HD11	1.94	0.49
1:B:1418:THR:HG22	1:B:1423:ASN:HD21	1.77	0.49
1:A:1219:VAL:HG13	1:A:1229:HIS:O	2.13	0.49
1:B:673:THR:HG22	1:B:675:ASN:H	1.76	0.49
1:A:925:VAL:HG21	1:A:1486:PRO:HB2	1.95	0.49
1:A:425:ARG:NH2	1:A:491:ARG:HB3	2.27	0.49
1:A:1320:LYS:HA	1:A:1338:ARG:HB2	1.95	0.49
1:B:647:SER:OG	1:B:648:GLU:N	2.45	0.49
1:A:647:SER:OG	1:A:648:GLU:N	2.46	0.49
1:A:1204:PRO:O	1:A:1208:ARG:HG2	2.12	0.49
1:B:420:GLU:HA	1:B:423:PHE:CE2	2.48	0.49
1:A:136:VAL:HG13	1:A:137:ASN:H	1.78	0.49
1:B:870:ILE:HD11	1:B:997:LEU:HD13	1.94	0.49
1:B:1172:LYS:HA	1:B:1175:SER:HB2	1.94	0.49
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.13	0.48
1:B:1054:ASP:OD1	1:B:1054:ASP:N	2.45	0.48
1:A:611:GLY:HA2	1:A:997:LEU:HD23	1.94	0.48
1:B:318:GLN:NE2	1:B:322:GLU:OE2	2.46	0.48
1:B:331:LYS:HD2	1:B:381:LYS:HE3	1.93	0.48
1:A:1204:PRO:HB2	1:A:1208:ARG:HH11	1.79	0.48
1:A:1239:TRP:HE1	1:A:1359:ASN:HD21	1.61	0.48
1:A:1428:PRO:HB3	1:A:1493:LEU:HD21	1.94	0.48
1:A:263:ILE:HG23	1:A:454:ARG:HH21	1.79	0.48
1:A:306:LEU:HD13	1:A:309:TRP:CZ2	2.48	0.48
1:A:471:ILE:HD11	1:A:480:PHE:HB3	1.96	0.48
1:B:5:ARG:HA	1:B:643:VAL:HG12	1.95	0.48
1:B:467:ASN:HB3	1:B:499:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD1	1:A:73:PHE:N	2.43	0.48
1:A:687:ALA:HB2	1:A:703:TYR:HE2	1.78	0.48
1:B:422:LEU:HD23	1:B:425:ARG:HE	1.78	0.48
1:A:452:PHE:CD1	1:A:466:ALA:HB2	2.49	0.48
1:B:427:LYS:HE2	1:B:427:LYS:HB3	1.63	0.47
1:B:256:SER:HB2	1:B:258:HIS:CE1	2.49	0.47
1:A:382:LYS:HD2	1:A:382:LYS:HA	1.63	0.47
1:A:466:ALA:HB3	1:A:501:LYS:CE	2.45	0.47
1:B:426:ILE:O	1:B:430:ARG:HG2	2.14	0.47
1:B:136:VAL:HG13	1:B:137:ASN:H	1.79	0.47
1:A:466:ALA:N	1:A:501:LYS:HD2	2.29	0.47
1:B:452:PHE:CD1	1:B:466:ALA:HB2	2.49	0.47
1:A:673:THR:HG22	1:A:675:ASN:H	1.80	0.47
1:A:1054:ASP:OD1	1:A:1054:ASP:N	2.43	0.47
1:B:296:ASP:HA	1:B:299:LYS:HB3	1.97	0.47
1:B:466:ALA:HB3	1:B:501:LYS:CE	2.45	0.47
1:B:870:ILE:HG12	1:B:993:LEU:HD22	1.97	0.47
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.96	0.47
1:B:277:GLU:HA	1:B:280:GLY:HA3	1.96	0.47
1:B:1228:ILE:H	1:B:1267:ASN:ND2	2.13	0.47
1:B:1259:ARG:HH12	1:B:1343:ASP:CG	2.18	0.47
1:B:1396:LEU:HD21	1:B:1400:ASP:HB3	1.97	0.47
1:B:1435:GLY:HA3	1:B:1514:CYS:HB3	1.97	0.47
1:B:1242:LYS:HE2	1:B:1421:GLY:O	2.15	0.47
1:A:142:PRO:HG2	1:A:743:ALA:HB1	1.97	0.46
1:A:275:GLN:O	1:A:279:LEU:HB2	2.14	0.46
1:A:1217:VAL:HG12	1:A:1235:ASN:OD1	2.15	0.46
1:B:314:VAL:HG11	1:B:371:ILE:HD13	1.97	0.46
1:B:940:ILE:HD11	1:B:1003:ALA:HB1	1.97	0.46
1:A:649:ILE:H	1:A:649:ILE:HG13	1.51	0.46
1:B:266:ASP:HB3	1:B:454:ARG:HH22	1.80	0.46
1:B:614:LYS:HB2	1:B:1004:LEU:HD13	1.96	0.46
1:A:182:PRO:HG2	1:A:192:PRO:O	2.15	0.46
1:A:467:ASN:N	1:A:467:ASN:OD1	2.48	0.46
1:A:188:GLU:H	1:A:239:ASN:HD21	1.62	0.46
1:A:427:LYS:O	1:A:431:ILE:N	2.48	0.46
1:A:1172:LYS:HA	1:A:1175:SER:HB2	1.97	0.46
1:A:1198:ARG:HH21	1:A:1215:PHE:HB2	1.81	0.46
1:A:1453:GLN:HB3	1:A:1461:LEU:HG	1.95	0.46
1:B:198:GLN:HG2	1:B:517:ARG:HH21	1.79	0.46
1:A:1053:PRO:O	1:A:1120:ARG:NH2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:MET:O	1:B:299:LYS:N	2.48	0.46
1:B:523:GLU:HB2	1:B:555:VAL:HG21	1.98	0.46
1:A:679:THR:OG1	1:A:783:LYS:HG2	2.16	0.46
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.50	0.46
1:A:431:ILE:O	1:A:433:ASP:N	2.49	0.45
1:B:323:LEU:O	1:B:327:TRP:HB2	2.16	0.45
1:B:466:ALA:N	1:B:501:LYS:HD2	2.31	0.45
1:B:695:SER:O	1:B:739:ARG:NH2	2.42	0.45
1:B:1438:ILE:HA	1:B:1441:TYR:HB3	1.98	0.45
1:A:1199:GLU:HG3	1:A:1215:PHE:O	2.16	0.45
1:A:754:MET:HG2	1:A:755:HIS:N	2.32	0.45
1:B:1245:GLU:HG3	1:B:1420:LYS:HB3	1.98	0.45
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.97	0.45
1:A:149:GLN:HG2	1:A:170:VAL:HG11	1.99	0.45
1:A:467:ASN:HB3	1:A:499:CYS:O	2.17	0.45
1:B:264:GLU:O	1:B:268:LYS:HB2	2.16	0.45
1:A:268:LYS:HA	1:A:268:LYS:HD2	1.57	0.45
1:B:754:MET:HG2	1:B:755:HIS:N	2.30	0.45
1:A:27:VAL:HG22	1:A:578:GLU:HG3	1.99	0.45
1:A:426:ILE:HA	1:A:429:LEU:HB3	1.99	0.45
1:A:713:LEU:H	1:A:713:LEU:HD12	1.81	0.45
1:B:252:ASN:HB3	1:B:465:LEU:HD23	1.98	0.45
1:B:869:GLY:O	1:B:989:ARG:NH1	2.42	0.45
1:A:213:ALA:HA	1:A:528:ILE:HG23	1.98	0.45
1:A:452:PHE:CE1	1:A:466:ALA:HB2	2.52	0.45
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.52	0.45
1:B:307:LYS:HE3	1:B:307:LYS:HB3	1.78	0.45
1:A:420:GLU:HA	1:A:423:PHE:CE2	2.52	0.44
1:B:53:ILE:HD11	1:B:65:ILE:HD11	1.98	0.44
1:B:282:PRO:HG2	1:B:294:VAL:HG22	1.98	0.44
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.53	0.44
1:A:235:HIS:HB2	1:A:499:CYS:HB3	1.99	0.44
1:A:314:VAL:HG11	1:A:371:ILE:HD13	2.00	0.44
1:B:1117:ASP:O	1:B:1119:GLY:N	2.50	0.44
1:A:1061:ALA:HB2	1:A:1073:ARG:CZ	2.48	0.44
1:B:1158:ARG:HD3	1:B:1173:ALA:O	2.18	0.44
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.18	0.44
1:A:870:ILE:HG12	1:A:993:LEU:HD22	1.99	0.44
1:B:213:ALA:HA	1:B:528:ILE:HG23	1.99	0.44
1:A:299:LYS:HB3	1:A:299:LYS:HE3	1.72	0.43
1:B:704:ASP:OD1	1:B:704:ASP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:LEU:HD12	1:B:713:LEU:H	1.83	0.43
1:A:370:LYS:HD2	1:A:370:LYS:HA	1.52	0.43
1:A:451:TYR:CZ	1:A:491:ARG:HD3	2.53	0.43
1:A:523:GLU:HB2	1:A:555:VAL:HG21	2.00	0.43
1:A:1260:ASP:OD1	1:A:1260:ASP:N	2.48	0.43
1:B:182:PRO:HG2	1:B:192:PRO:O	2.19	0.43
1:A:1075:TRP:HB2	1:A:1078:ASP:HB2	2.00	0.43
1:B:1133:PHE:CZ	1:B:1137:ILE:HD11	2.54	0.43
1:A:1438:ILE:HA	1:A:1441:TYR:HB3	2.00	0.43
1:B:1164:GLU:HB3	1:B:1165:TYR:H	1.46	0.43
1:B:1400:ASP:OD1	1:B:1401:TYR:N	2.52	0.43
1:A:1165:TYR:O	1:A:1167:PRO:HD3	2.18	0.43
1:B:1293:LYS:HB2	1:B:1294:PRO:HD2	2.01	0.43
1:B:953:LEU:HD13	1:B:999:PRO:HA	2.01	0.43
1:B:266:ASP:OD2	1:B:452:PHE:N	2.52	0.43
1:A:1357:ARG:NH2	1:A:1426:GLN:OE1	2.52	0.42
1:B:235:HIS:HB2	1:B:499:CYS:HB3	2.01	0.42
1:B:673:THR:HG21	1:B:707:PHE:O	2.19	0.42
1:A:184:GLN:HA	1:A:201:PHE:HA	2.00	0.42
1:A:1164:GLU:HB3	1:A:1165:TYR:H	1.76	0.42
1:A:1349:LYS:H	1:A:1349:LYS:HG2	1.50	0.42
1:B:1107:LEU:HD22	1:B:1183:ILE:HG23	2.00	0.42
1:A:326:LYS:O	1:A:328:GLY:N	2.52	0.42
1:B:1206:LEU:HB3	1:B:1207:ASP:H	1.44	0.42
1:A:765:PHE:HE2	1:A:767:ARG:HB2	1.84	0.42
1:B:114:LYS:NZ	1:B:118:ASP:OD1	2.52	0.42
1:B:136:VAL:HA	1:B:226:LEU:HD21	2.02	0.42
1:B:1495:ASN:HB2	1:B:1499:GLU:HB3	2.01	0.42
1:A:1161:LEU:HD12	1:A:1161:LEU:HA	1.91	0.42
1:A:1239:TRP:HE1	1:A:1359:ASN:ND2	2.18	0.42
1:B:164:GLU:OE2	1:B:218:ARG:NH1	2.52	0.42
1:B:628:LYS:O	1:B:650:MET:HB2	2.18	0.42
1:A:962:TYR:CZ	1:A:966:ARG:HD3	2.53	0.42
1:A:1472:TYR:CZ	1:A:1476:LEU:HD21	2.55	0.42
1:B:247:PRO:HB3	1:B:455:PHE:HZ	1.84	0.42
1:B:263:ILE:HG23	1:B:454:ARG:HH21	1.83	0.42
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.83	0.42
1:A:422:LEU:HD23	1:A:425:ARG:HE	1.83	0.42
1:A:1196:LYS:HD2	1:A:1218:GLU:HG3	2.01	0.42
1:A:1236:CYS:HB3	1:A:1241:ASP:HA	2.02	0.42
1:A:1291:VAL:HB	1:A:1299:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:ALA:HB1	1:B:732:LYS:HE3	2.00	0.42
1:B:1238:THR:OG1	1:B:1259:ARG:HD3	2.19	0.42
1:A:425:ARG:O	1:A:429:LEU:N	2.44	0.42
1:A:1062:ALA:HB2	1:A:1075:TRP:HD1	1.85	0.42
1:A:1459:LYS:HA	1:A:1459:LYS:HD2	1.73	0.42
1:A:399:ILE:O	1:A:403:ILE:HG13	2.20	0.42
1:B:414:ASP:O	1:B:418:VAL:HG23	2.20	0.42
1:B:683:THR:HG22	1:B:728:ILE:HG13	2.02	0.42
1:A:687:ALA:HB1	1:A:732:LYS:HE3	2.01	0.42
1:A:781:ARG:HH22	1:A:789:ASP:HA	1.84	0.42
1:A:1117:ASP:O	1:A:1120:ARG:HG2	2.20	0.42
1:A:1400:ASP:OD1	1:A:1401:TYR:N	2.53	0.42
1:B:587:ARG:HG3	1:B:605:HIS:CE1	2.55	0.42
1:B:1155:VAL:HG22	1:B:1178:SER:O	2.20	0.42
1:B:1192:ALA:O	1:B:1294:PRO:HD3	2.20	0.42
1:B:1493:LEU:HB3	1:B:1504:SER:HB2	2.02	0.42
1:A:1269:LEU:HD23	1:A:1366:VAL:HG21	2.02	0.41
1:A:1075:TRP:HH2	2:C:3:GLC:H62	1.83	0.41
1:B:505:GLY:HA3	1:B:510:ASP:HB2	2.02	0.41
1:B:1105:LYS:HG2	1:B:1155:VAL:HB	2.02	0.41
1:A:299:LYS:HA	1:A:303:ILE:HB	2.02	0.41
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	2.20	0.41
1:B:174:LYS:HD3	1:B:174:LYS:HA	1.94	0.41
1:B:251:TYR:CE2	1:B:503:ARG:HG3	2.56	0.41
1:A:251:TYR:HB2	1:A:501:LYS:NZ	2.35	0.41
1:A:1117:ASP:HB3	1:A:1120:ARG:O	2.21	0.41
1:A:1242:LYS:NZ	2:C:2:GLC:O2	2.53	0.41
1:B:16:GLU:HG2	1:B:126:PHE:HZ	1.85	0.41
1:B:822:ILE:HG23	1:B:824:GLU:HG3	2.01	0.41
1:B:1112:ILE:H	1:B:1130:ALA:HB2	1.85	0.41
1:A:608:ARG:HD2	1:A:749:ILE:HG12	2.02	0.41
1:B:79:ARG:HA	1:B:79:ARG:HD2	1.87	0.41
1:B:896:TYR:CE2	1:B:973:LYS:HD2	2.56	0.41
1:B:1228:ILE:HG13	1:B:1270:LEU:HD22	2.03	0.41
1:A:297:GLY:HA2	1:A:300:GLU:HG2	2.02	0.41
1:A:449:GLU:H	1:A:449:GLU:HG2	1.56	0.41
1:A:618:LEU:HD13	1:A:933:VAL:HG13	2.03	0.41
1:B:57:SER:O	1:B:60:THR:OG1	2.38	0.41
1:B:338:ILE:H	1:B:338:ILE:HG13	1.63	0.41
1:A:36:PRO:HG2	1:A:44:MET:SD	2.61	0.41
1:A:628:LYS:HE2	1:A:628:LYS:HB2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:TYR:CE2	1:A:1047:LYS:HE2	2.56	0.41
1:A:1097:LYS:O	1:A:1101:LEU:HG	2.21	0.41
1:B:27:VAL:HG22	1:B:578:GLU:HG3	2.03	0.41
1:B:279:LEU:H	1:B:279:LEU:HG	1.56	0.41
1:B:907:ASP:OD2	1:B:1048:SER:OG	2.33	0.41
1:B:908:TYR:CE2	1:B:1047:LYS:HE2	2.55	0.41
1:B:1071:TYR:CE1	2:D:5:GLC:H61	2.56	0.41
1:B:1280:LEU:HG	1:B:1285:LYS:HB2	2.01	0.41
1:A:717:LYS:HD3	1:A:717:LYS:HA	1.92	0.41
1:B:35:LEU:H	1:B:35:LEU:HD12	1.86	0.41
1:B:251:TYR:HB2	1:B:501:LYS:CE	2.51	0.41
1:B:953:LEU:HB2	1:B:999:PRO:HG3	2.03	0.41
1:A:1337:ARG:HB2	1:A:1340:ILE:HD12	2.01	0.40
3:G:2:GLC:O6	3:G:2:GLC:O4	2.31	0.40
1:A:251:TYR:CE2	1:A:503:ARG:HG3	2.57	0.40
1:A:800:THR:HG23	1:A:867:GLN:HA	2.02	0.40
1:A:1097:LYS:HG3	1:A:1150:LEU:HD13	2.03	0.40
1:A:1107:LEU:HB3	1:A:1157:ARG:CZ	2.51	0.40
1:B:149:GLN:HG2	1:B:170:VAL:HG11	2.03	0.40
1:B:1154:LYS:HG2	1:B:1179:THR:HG22	2.03	0.40
1:A:602:VAL:HG13	1:A:693:CYS:SG	2.61	0.40
1:A:1238:THR:OG1	1:A:1259:ARG:HD3	2.21	0.40
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.56	0.40
1:B:1166:ILE:HG12	1:B:1201:ASN:HD21	1.87	0.40
1:A:414:ASP:O	1:A:418:VAL:HG23	2.22	0.40
1:A:771:LYS:NZ	1:A:872:ASP:O	2.47	0.40
1:A:1430:TRP:CE2	1:A:1493:LEU:HD12	2.56	0.40
1:B:1489:GLY:HA3	1:B:1507:THR:HG23	2.03	0.40
1:B:834:THR:HG22	1:B:835:GLY:H	1.86	0.40

There are no symmetry-related clashes.

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	1524/1536 (99%)	1414 (93%)	103 (7%)	7 (0%)	29	64
1	B	1524/1536 (99%)	1412 (93%)	103 (7%)	9 (1%)	25	59
All	All	3048/3072 (99%)	2826 (93%)	206 (7%)	16 (0%)	29	64

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	TRP
1	B	282	PRO
1	B	283	VAL
1	B	329	ASN
1	A	281	TYR
1	A	1175	SER
1	B	435	GLY
1	B	1175	SER
1	A	436	PRO
1	A	900	ARG
1	B	900	ARG
1	A	432	ASP
1	B	280	GLY
1	B	1121	ASN
1	A	706	VAL
1	B	706	VAL

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	1343/1353 (99%)	1272 (95%)	71 (5%)	22	54
1	B	1343/1353 (99%)	1249 (93%)	94 (7%)	15	45
All	All	2686/2706 (99%)	2521 (94%)	165 (6%)	18	49

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	159	THR
1	A	268	LYS
1	A	281	TYR
1	A	284	ASP
1	A	286	LYS
1	A	287	THR
1	A	288	VAL
1	A	289	ASP
1	A	290	ASP
1	A	294	VAL
1	A	299	LYS
1	A	302	VAL
1	A	306	LEU
1	A	308	LEU
1	A	316	VAL
1	A	331	LYS
1	A	333	TRP
1	A	337	ASN
1	A	374	ASP
1	A	383	LEU
1	A	384	HIS
1	A	434	HIS
1	A	437	LYS
1	A	441	ILE
1	A	442	THR
1	A	443	LYS
1	A	445	LEU
1	A	447	LEU
1	A	449	GLU
1	A	462	GLU
1	A	467	ASN
1	A	543	HIS
1	A	583	SER
1	A	616	VAL
1	A	631	GLU
1	A	664	PHE
1	A	679	THR
1	A	704	ASP
1	A	742	ILE
1	A	754	MET
1	A	785	HIS
1	A	787	SER

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Mol	Chain	Res	Type
1	A	800	THR
1	A	834	THR
1	A	905	GLU
1	A	925	VAL
1	A	974	GLU
1	A	1016	ARG
1	A	1044	SER
1	A	1082	SER
1	A	1127	ARG
1	A	1162	ASP
1	A	1169	ASP
1	A	1198	ARG
1	A	1213	GLU
1	A	1216	ASN
1	A	1218	GLU
1	A	1227	LEU
1	A	1265	GLU
1	A	1321	ASN
1	A	1323	GLU
1	A	1330	ILE
1	A	1334	ILE
1	A	1349	LYS
1	A	1356	PHE
1	A	1361	THR
1	A	1424	TYR
1	A	1442	HIS
1	A	1460	LYS
1	A	1461	LEU
1	B	136	VAL
1	B	229	THR
1	B	274	GLU
1	B	275	GLN
1	B	277	GLU
1	B	279	LEU
1	B	281	TYR
1	B	284	ASP
1	B	287	THR
1	B	288	VAL
1	B	290	ASP
1	B	299	LYS
1	B	308	LEU
1	B	316	VAL

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Mol	Chain	Res	Type
1	B	324	ARG
1	B	325	GLU
1	B	333	TRP
1	B	337	ASN
1	B	374	ASP
1	B	429	LEU
1	B	441	ILE
1	B	442	THR
1	B	443	LYS
1	B	444	LYS
1	B	445	LEU
1	B	449	GLU
1	B	454	ARG
1	B	459	ASP
1	B	461	GLU
1	B	462	GLU
1	B	467	ASN
1	B	543	HIS
1	B	616	VAL
1	B	664	PHE
1	B	704	ASP
1	B	742	ILE
1	B	754	MET
1	B	761	GLN
1	B	800	THR
1	B	834	THR
1	B	905	GLU
1	B	925	VAL
1	B	974	GLU
1	B	1016	ARG
1	B	1044	SER
1	B	1054	ASP
1	B	1082	SER
1	B	1106	THR
1	B	1116	LEU
1	B	1120	ARG
1	B	1128	ASP
1	B	1148	VAL
1	B	1156	THR
1	B	1157	ARG
1	B	1159	PHE
1	B	1164	GLU

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Mol	Chain	Res	Type
1	B	1166	ILE
1	B	1170	ASP
1	B	1172	LYS
1	B	1195	ILE
1	B	1198	ARG
1	B	1209	VAL
1	B	1211	LYS
1	B	1217	VAL
1	B	1224	GLU
1	B	1233	GLN
1	B	1234	PHE
1	B	1236	CYS
1	B	1241	ASP
1	B	1245	GLU
1	B	1247	GLU
1	B	1248	LYS
1	B	1252	VAL
1	B	1260	ASP
1	B	1264	VAL
1	B	1265	GLU
1	B	1292	THR
1	B	1300	SER
1	B	1321	ASN
1	B	1325	ASP
1	B	1330	ILE
1	B	1334	ILE
1	B	1338	ARG
1	B	1356	PHE
1	B	1408	ASN
1	B	1411	GLU
1	B	1412	ASP
1	B	1416	PHE
1	B	1422	ARG
1	B	1424	TYR
1	B	1442	HIS
1	B	1460	LYS
1	B	1461	LEU
1	B	1527	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	438	GLN
1	B	1109	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 ⓘ

18 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	C	1	2	12,12,12	0.91	1 (8%)	17,17,17	1.00	0
2	GLC	C	2	2	11,11,12	1.00	1 (9%)	15,15,17	1.32	2 (13%)
2	GLC	C	3	2	11,11,12	0.94	1 (9%)	15,15,17	1.75	4 (26%)
2	GLC	C	4	2	11,11,12	1.32	1 (9%)	15,15,17	1.10	1 (6%)
2	GLC	C	5	2	11,11,12	0.64	0	15,15,17	1.43	4 (26%)
2	GLC	D	1	2	12,12,12	1.02	1 (8%)	17,17,17	1.12	1 (5%)
2	GLC	D	2	2	11,11,12	1.60	2 (18%)	15,15,17	1.43	2 (13%)
2	GLC	D	3	2	11,11,12	1.31	2 (18%)	15,15,17	1.41	3 (20%)
2	GLC	D	4	2	11,11,12	1.11	1 (9%)	15,15,17	1.34	3 (20%)
2	GLC	D	5	2	11,11,12	0.58	0	15,15,17	1.32	2 (13%)
3	GLC	E	1	3	12,12,12	0.86	1 (8%)	17,17,17	1.17	1 (5%)
3	GLC	E	2	3	11,11,12	1.40	3 (27%)	15,15,17	2.33	7 (46%)
3	GLC	F	1	3	12,12,12	0.71	0	17,17,17	1.11	1 (5%)
3	GLC	F	2	3	11,11,12	0.55	0	15,15,17	0.91	0
3	GLC	G	1	3	12,12,12	0.70	0	17,17,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	G	2	3	11,11,12	0.62	0	15,15,17	0.89	0
3	GLC	H	1	3	12,12,12	1.02	0	17,17,17	1.15	2 (11%)
3	GLC	H	2	3	11,11,12	1.25	2 (18%)	15,15,17	1.65	4 (26%)

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	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	1/2/19/22	0/1/1/1
2	GLC	C	5	2	-	1/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
3	GLC	E	1	3	-	1/2/22/22	0/1/1/1
3	GLC	E	2	3	-	1/2/19/22	0/1/1/1
3	GLC	F	1	3	-	1/2/22/22	0/1/1/1
3	GLC	F	2	3	-	1/2/19/22	0/1/1/1
3	GLC	G	1	3	-	1/2/22/22	0/1/1/1
3	GLC	G	2	3	-	2/2/19/22	0/1/1/1
3	GLC	H	1	3	-	1/2/22/22	0/1/1/1
3	GLC	H	2	3	-	1/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C4-C5	3.72	1.60	1.53
2	C	4	GLC	O4-C4	3.06	1.50	1.43
2	D	2	GLC	O4-C4	2.88	1.49	1.43
3	E	2	GLC	C4-C5	2.79	1.58	1.53
3	E	2	GLC	C1-C2	2.72	1.58	1.52
2	C	2	GLC	O4-C4	2.72	1.49	1.43
2	D	4	GLC	O4-C4	2.53	1.48	1.43
2	D	3	GLC	O4-C4	2.47	1.48	1.43
2	D	1	GLC	O4-C4	2.30	1.48	1.43
3	E	1	GLC	O4-C4	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GLC	O4-C4	2.22	1.48	1.43
2	C	3	GLC	O4-C4	2.14	1.48	1.43
2	D	3	GLC	C4-C3	2.14	1.57	1.52
3	H	2	GLC	C4-C5	-2.12	1.48	1.53
3	H	2	GLC	O3-C3	2.07	1.47	1.43
3	E	2	GLC	O5-C1	2.04	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLC	O5-C1-C2	-4.28	104.16	110.77
3	E	2	GLC	C2-C3-C4	-4.28	103.50	110.89
3	E	2	GLC	C3-C4-C5	-3.85	103.37	110.24
3	E	2	GLC	C1-C2-C3	3.85	114.40	109.67
3	H	2	GLC	C1-O5-C5	3.70	117.21	112.19
2	D	2	GLC	O4-C4-C5	3.66	118.39	109.30
2	C	2	GLC	O4-C4-C3	3.16	117.66	110.35
2	C	3	GLC	O5-C5-C6	2.94	111.81	107.20
2	D	5	GLC	C1-C2-C3	-2.87	106.14	109.67
2	D	4	GLC	O4-C4-C3	2.81	116.84	110.35
2	C	5	GLC	C2-C3-C4	-2.77	106.10	110.89
3	E	2	GLC	O3-C3-C4	2.75	116.71	110.35
2	D	5	GLC	C2-C3-C4	-2.67	106.28	110.89
3	E	1	GLC	C1-O5-C5	-2.65	108.66	113.66
2	D	3	GLC	C1-O5-C5	-2.65	108.61	112.19
3	H	2	GLC	O3-C3-C4	-2.47	104.63	110.35
3	H	1	GLC	C1-O5-C5	-2.38	109.16	113.66
2	D	4	GLC	C2-C3-C4	-2.36	106.81	110.89
2	C	5	GLC	O5-C5-C6	-2.35	103.52	107.20
3	F	1	GLC	O5-C5-C6	2.34	112.26	106.44
3	H	1	GLC	C3-C4-C5	-2.33	106.08	110.24
3	E	2	GLC	O3-C3-C2	-2.29	105.61	109.99
3	H	2	GLC	O4-C4-C3	-2.28	105.08	110.35
2	C	5	GLC	C1-C2-C3	-2.21	106.94	109.67
2	D	3	GLC	O3-C3-C4	2.20	115.44	110.35
3	E	2	GLC	O5-C5-C4	2.20	116.18	110.83
3	E	2	GLC	O4-C4-C3	2.18	115.39	110.35
3	H	2	GLC	O5-C1-C2	2.16	114.10	110.77
2	C	4	GLC	O4-C4-C3	2.15	115.33	110.35
2	C	2	GLC	O5-C1-C2	-2.12	107.49	110.77
2	D	1	GLC	C3-C4-C5	-2.11	106.47	110.24
2	D	4	GLC	C6-C5-C4	-2.11	108.06	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLC	C1-O5-C5	2.09	115.03	112.19
2	D	3	GLC	O3-C3-C2	-2.03	106.11	109.99
2	C	5	GLC	C6-C5-C4	-2.03	108.26	113.00
2	D	2	GLC	C1-C2-C3	2.02	112.15	109.67
2	C	3	GLC	C6-C5-C4	-2.01	108.29	113.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

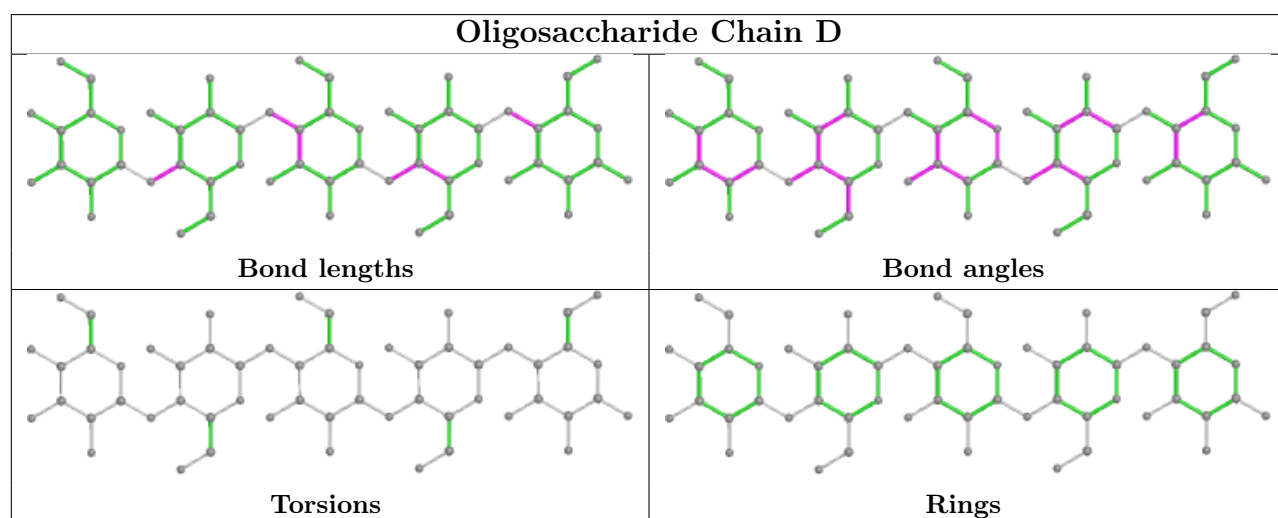
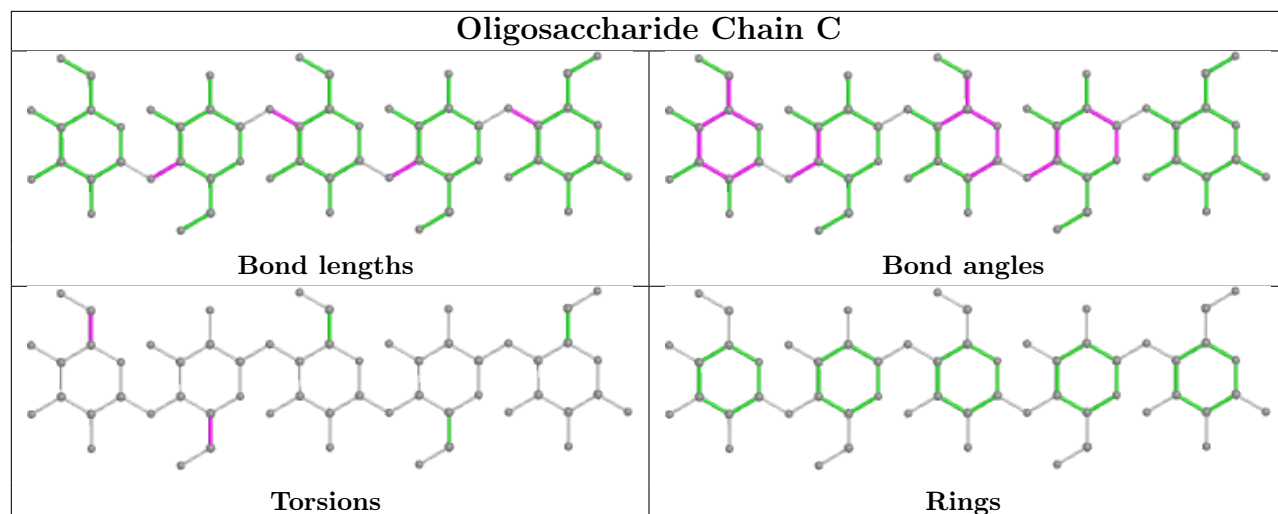
Mol	Chain	Res	Type	Atoms
3	G	2	GLC	O5-C5-C6-O6
3	G	2	GLC	C4-C5-C6-O6
3	H	1	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
3	E	2	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
3	H	2	GLC	O5-C5-C6-O6
2	C	5	GLC	O5-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6

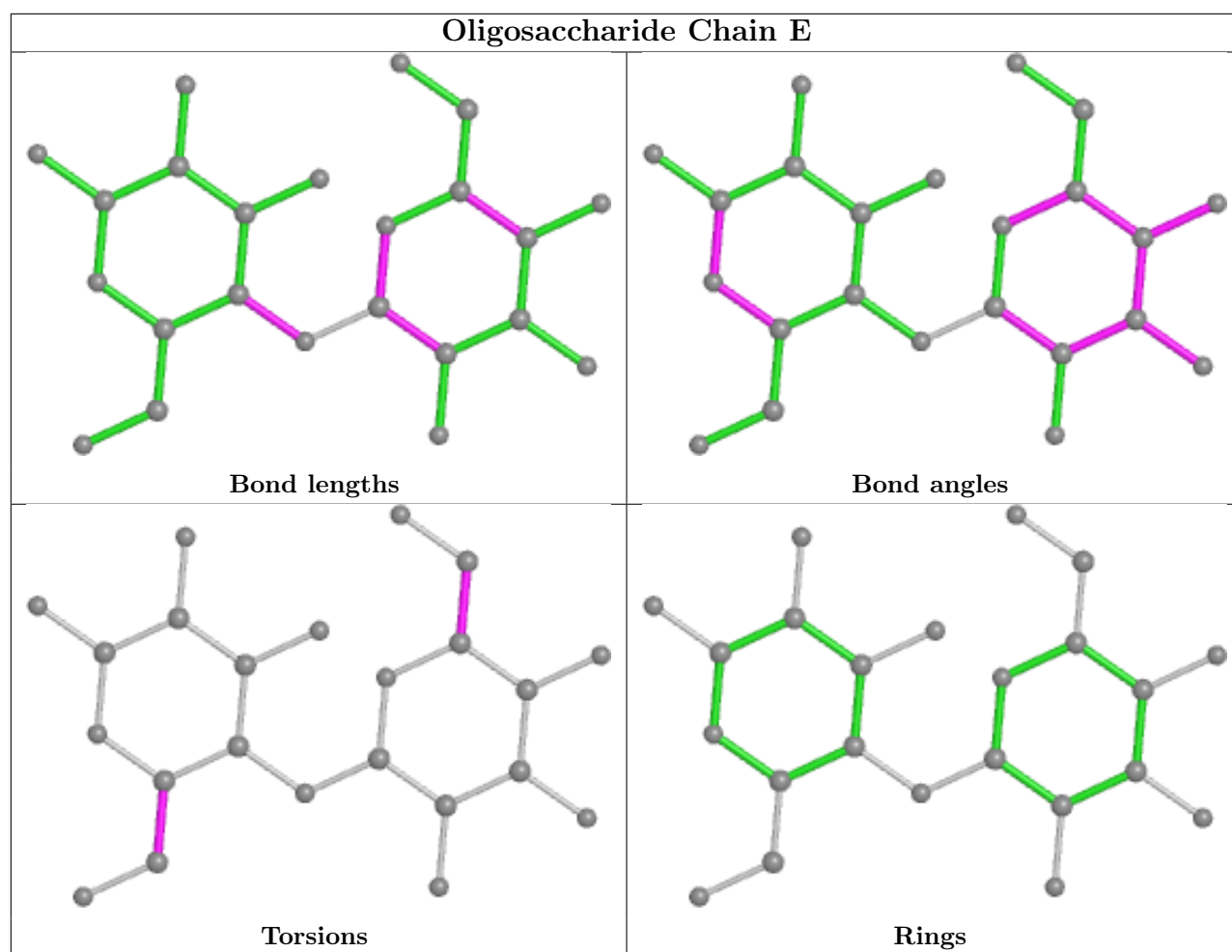
There are no ring outliers.

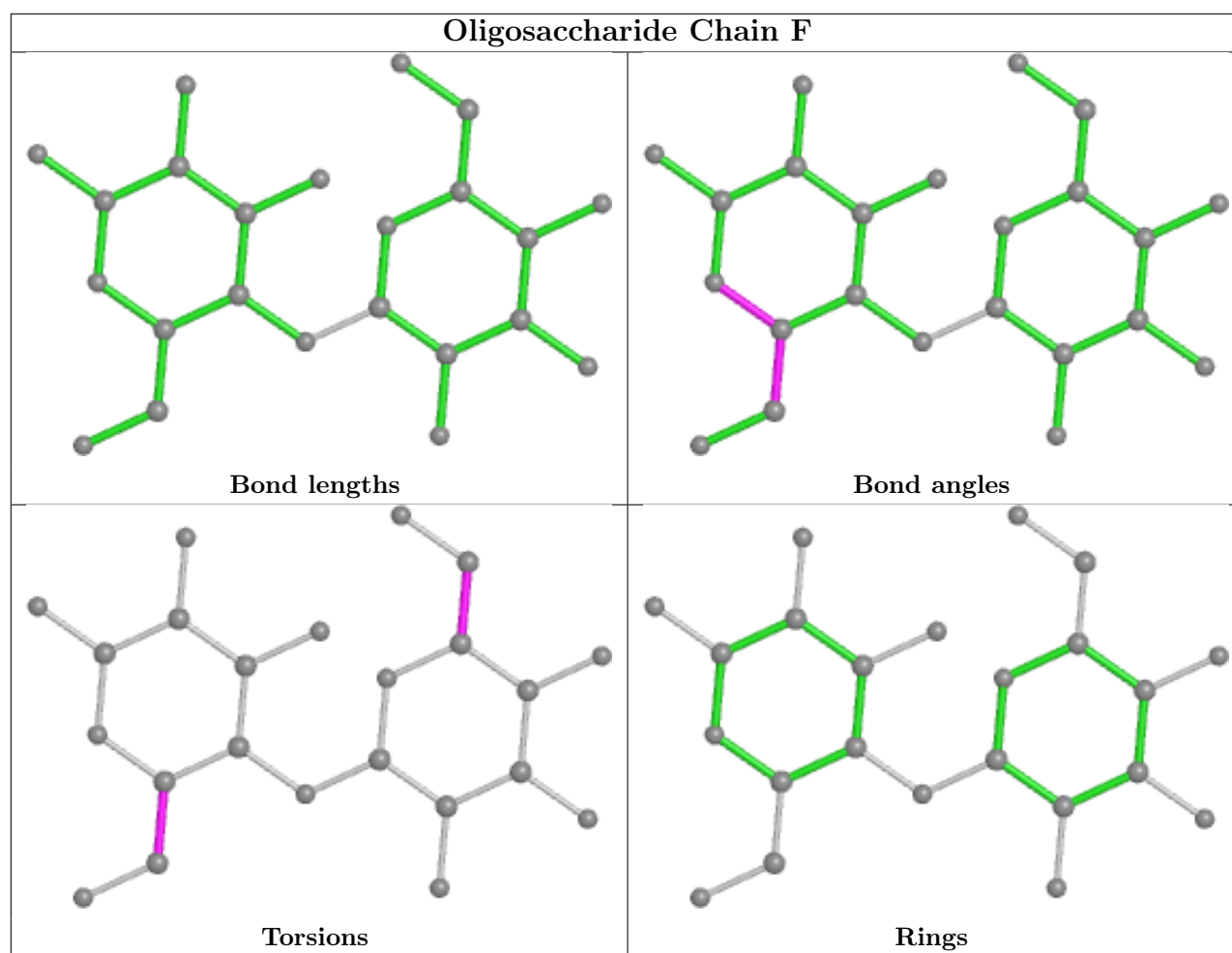
6 monomers are involved in 6 short contacts:

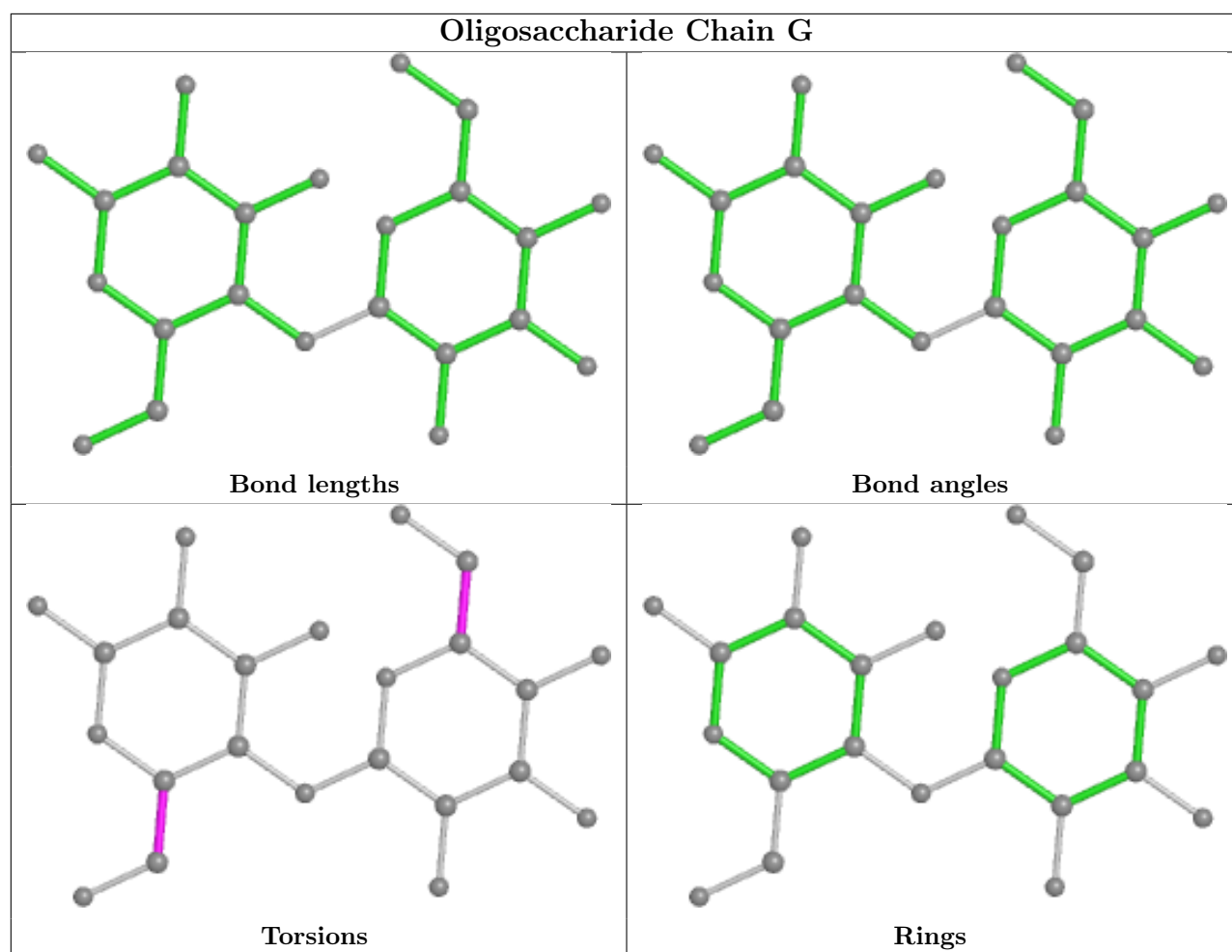
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	1	0
3	G	2	GLC	1	0
2	D	5	GLC	1	0
2	D	3	GLC	1	0
2	C	3	GLC	2	0
2	C	2	GLC	1	0

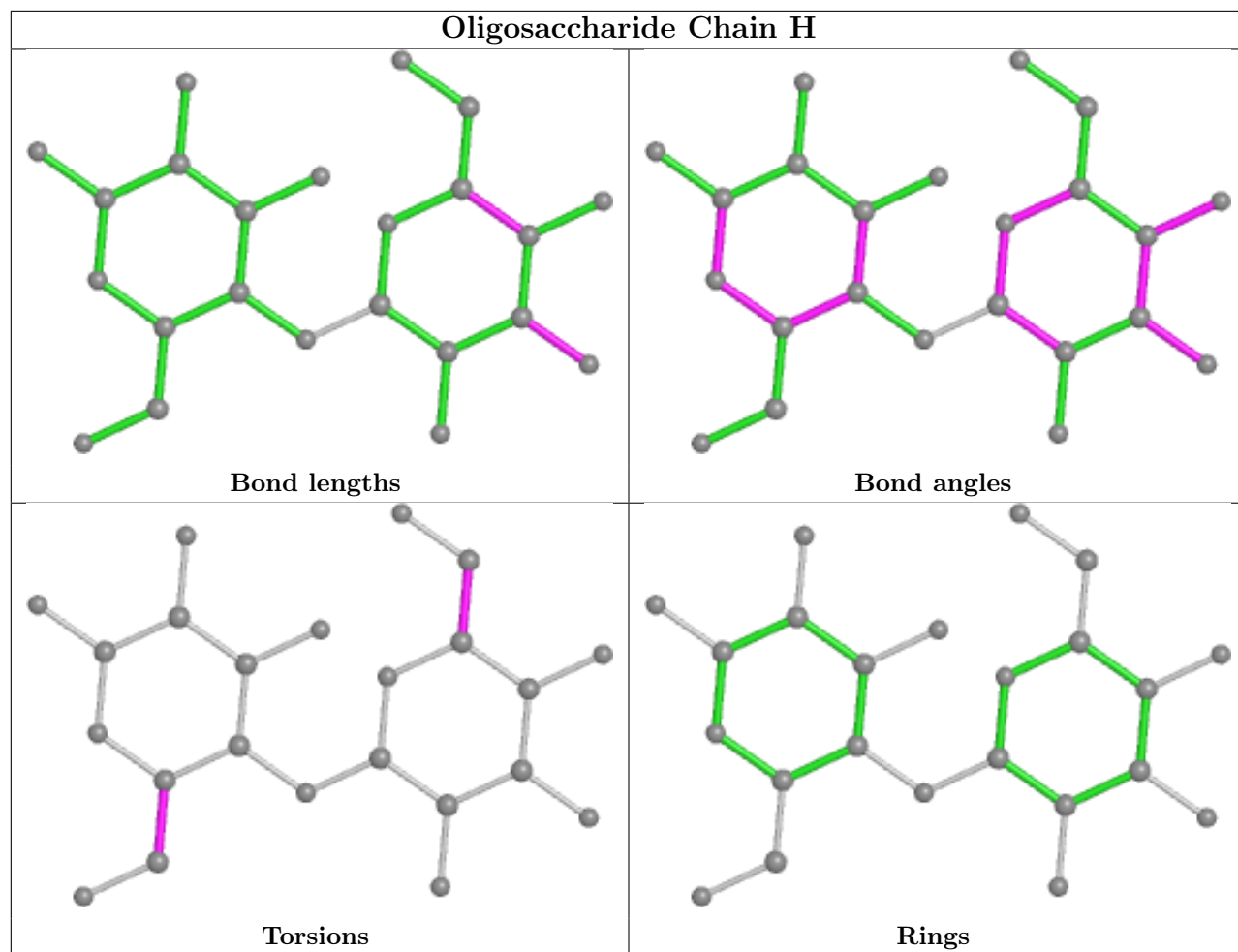
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

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

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	1526/1536 (99%)	0.09	62 (4%)	37	18	61, 109, 163, 189	0
1	B	1526/1536 (99%)	0.12	52 (3%)	45	24	55, 112, 176, 211	0
All	All	3052/3072 (99%)	0.11	114 (3%)	41	21	55, 111, 170, 211	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1238	THR	6.7
1	B	1165	TYR	4.8
1	B	1236	CYS	4.7
1	A	1354	TYR	4.4
1	B	444	LYS	4.4
1	B	1237	GLY	4.4
1	A	1457	SER	4.3
1	B	1239	TRP	4.2
1	A	1321	ASN	4.1
1	A	1128	ASP	3.9
1	B	1263	ALA	3.8
1	A	348	ALA	3.8
1	A	1238	THR	3.7
1	A	1078	ASP	3.6
1	A	37	GLN	3.6
1	A	1236	CYS	3.6
1	A	144	ASN	3.5
1	A	593	TRP	3.5
1	A	1510	TRP	3.5
1	B	1078	ASP	3.5
1	A	1202	ALA	3.5
1	A	1165	TYR	3.3
1	B	1298	LYS	3.3
1	B	1128	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1511	SER	3.3
1	A	38	GLY	3.3
1	A	347	LEU	3.2
1	B	1433	CYS	3.2
1	B	1359	ASN	3.2
1	A	1082	SER	3.2
1	A	1458	ALA	3.2
1	B	1082	SER	3.1
1	B	1412	ASP	3.1
1	B	593	TRP	3.1
1	B	1077	ARG	3.0
1	B	285	LEU	3.0
1	B	1510	TRP	3.0
1	B	1259	ARG	3.0
1	B	1354	TYR	3.0
1	A	696	ALA	2.9
1	B	1265	GLU	2.9
1	A	1077	ARG	2.9
1	A	1528	GLU	2.9
1	A	1114	ASN	2.9
1	A	1224	GLU	2.9
1	A	1511	SER	2.8
1	A	1241	ASP	2.8
1	B	636	TYR	2.8
1	A	283	VAL	2.8
1	A	307	LYS	2.8
1	B	1267	ASN	2.8
1	B	1080	PHE	2.8
1	A	281	TYR	2.7
1	B	1262	ALA	2.7
1	A	698	GLY	2.7
1	B	1333	THR	2.7
1	B	1432	TRP	2.6
1	A	1203	GLY	2.6
1	B	501	LYS	2.6
1	A	376	PHE	2.6
1	A	751	ASP	2.6
1	A	1248	LYS	2.6
1	A	1237	GLY	2.6
1	A	1234	PHE	2.6
1	A	145	SER	2.6
1	B	241	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1240	MET	2.5
1	B	568	GLY	2.5
1	A	584	SER	2.4
1	B	1114	ASN	2.4
1	B	1321	ASN	2.4
1	A	1319	PRO	2.4
1	A	531	GLY	2.4
1	A	1220	ASN	2.3
1	A	1338	ARG	2.3
1	A	1075	TRP	2.3
1	B	445	LEU	2.3
1	A	1242	LYS	2.3
1	B	745	GLU	2.3
1	A	1076	GLY	2.3
1	A	1160	PRO	2.3
1	A	1356	PHE	2.3
1	B	1131	TRP	2.2
1	A	1359	ASN	2.2
1	A	1263	ALA	2.2
1	B	1401	TYR	2.2
1	A	1514	CYS	2.2
1	A	455	PHE	2.2
1	A	1340	ILE	2.2
1	A	695	SER	2.2
1	B	270	LEU	2.2
1	B	1258	PRO	2.2
1	A	1225	THR	2.2
1	B	1261	GLY	2.2
1	B	1241	ASP	2.2
1	A	1239	TRP	2.1
1	B	281	TYR	2.1
1	A	325	GLU	2.1
1	B	1177	SER	2.1
1	A	1328	PHE	2.1
1	A	583	SER	2.1
1	B	425	ARG	2.1
1	B	377	ALA	2.1
1	B	1129	ALA	2.1
1	B	1334	ILE	2.1
1	A	1174	PHE	2.1
1	A	1513	GLY	2.1
1	A	694	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1185	TYR	2.0
1	B	1245	GLU	2.0
1	A	1085	GLY	2.0
1	B	1076	GLY	2.0
1	B	244	LEU	2.0
1	B	1514	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

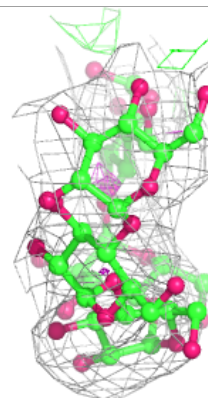
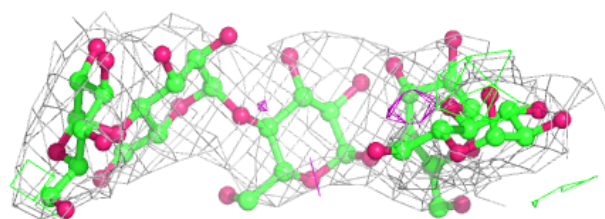
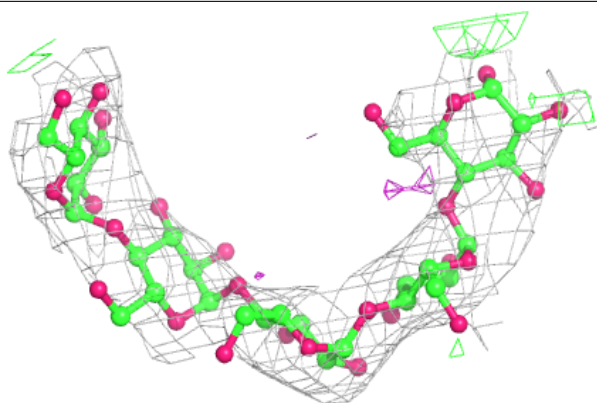
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	G	2	11/12	0.67	0.22	106,123,140,143	0
3	GLC	F	2	11/12	0.72	0.19	121,143,158,161	0
3	GLC	H	2	11/12	0.73	0.24	145,162,170,172	0
2	GLC	D	5	11/12	0.76	0.26	132,149,163,163	0
2	GLC	C	5	11/12	0.81	0.17	125,141,159,166	0
3	GLC	H	1	12/12	0.81	0.14	122,135,141,146	0
3	GLC	G	1	12/12	0.81	0.28	125,139,147,151	0
3	GLC	F	1	12/12	0.82	0.23	122,150,169,173	0
2	GLC	C	2	11/12	0.83	0.22	121,131,142,148	0
3	GLC	E	2	11/12	0.83	0.19	100,117,133,135	0
2	GLC	D	3	11/12	0.84	0.26	119,132,142,154	0
2	GLC	C	1	12/12	0.86	0.21	105,121,136,138	0
2	GLC	D	2	11/12	0.87	0.24	125,135,139,144	0
2	GLC	D	4	11/12	0.87	0.16	138,157,169,174	0
2	GLC	D	1	12/12	0.89	0.24	111,139,149,150	0
3	GLC	E	1	12/12	0.89	0.14	76,90,111,114	0
2	GLC	C	3	11/12	0.89	0.25	116,123,150,152	0
2	GLC	C	4	11/12	0.90	0.19	121,144,158,162	0

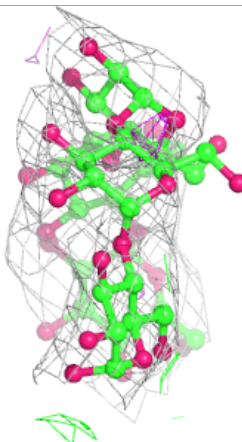
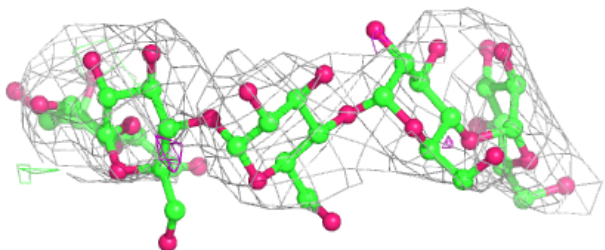
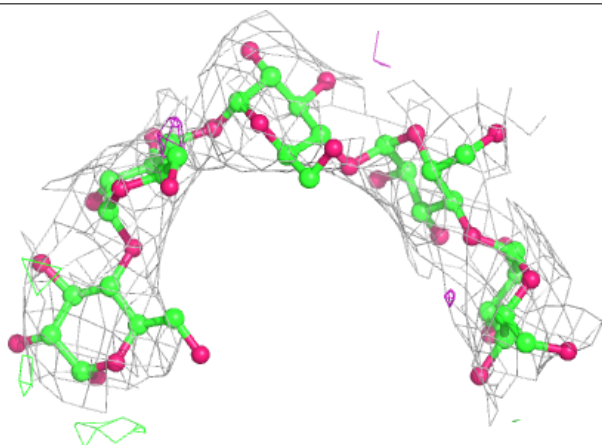
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

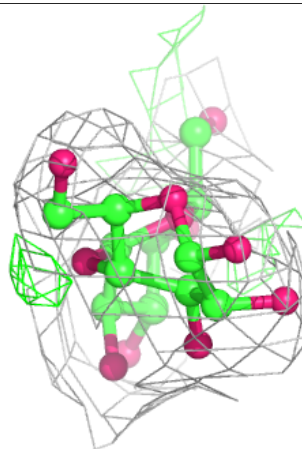
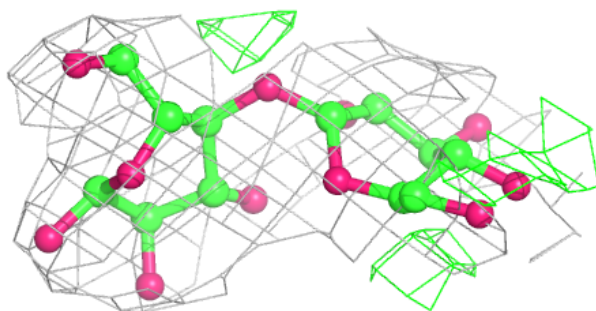
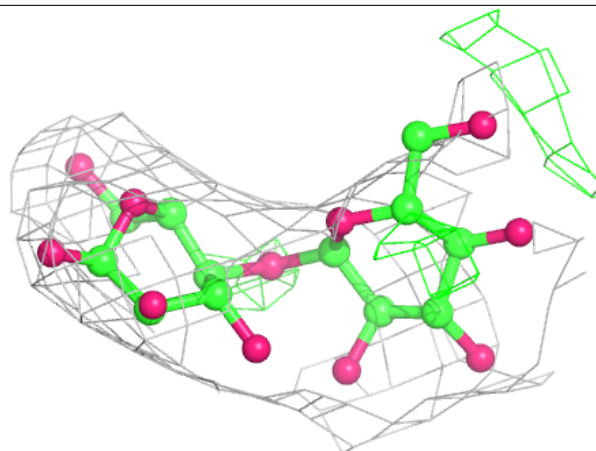
**Electron density around Chain D:**

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

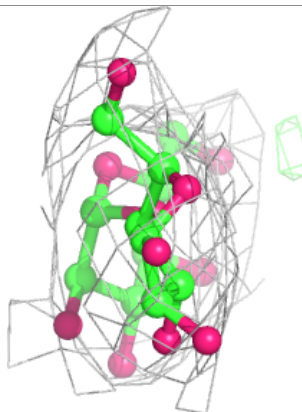
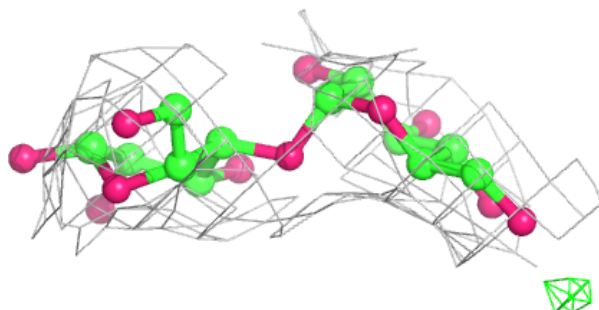
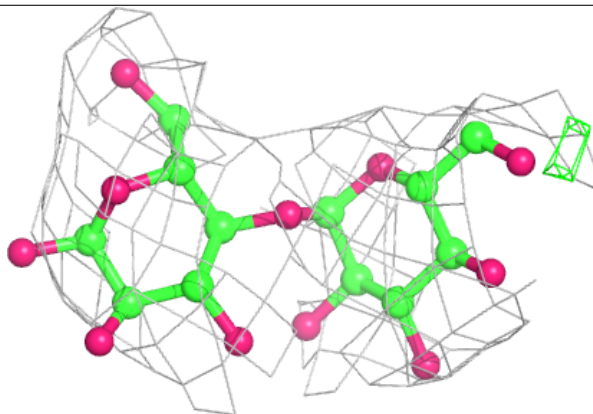


Electron density around Chain E:

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

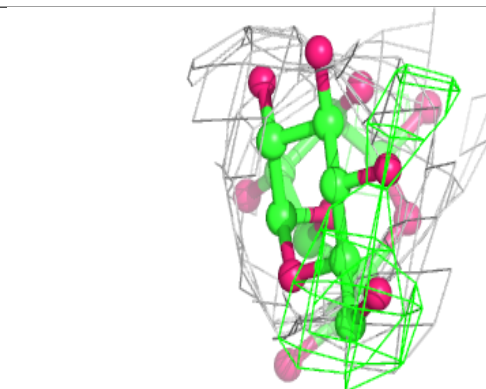
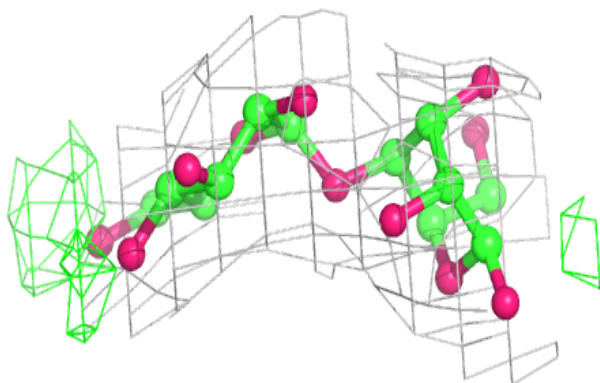
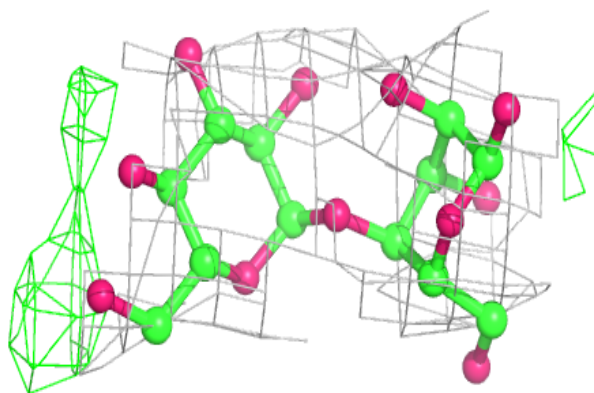
**Electron density around Chain F:**

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

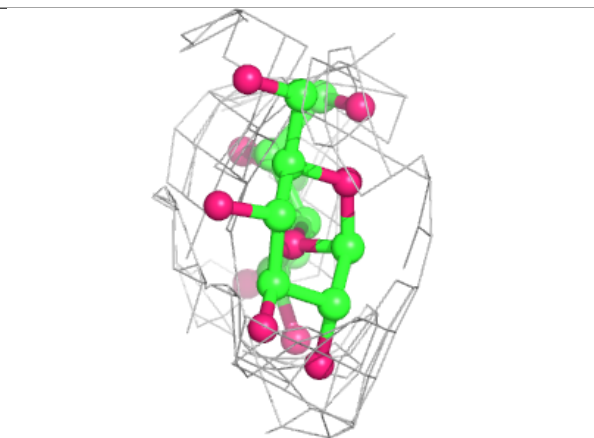
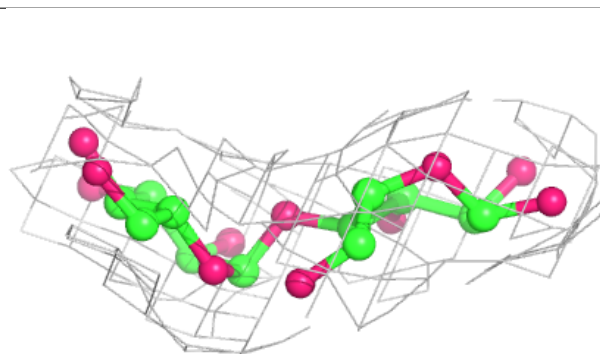
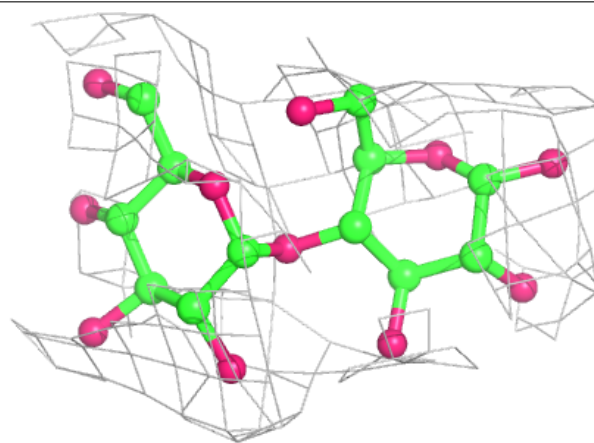


Electron density around Chain G:

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

**Electron density around Chain H:**

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.