



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:16 PM EDT

PDB ID : 7EIM / pdb_00007eim
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 types of validation reports are described at

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

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

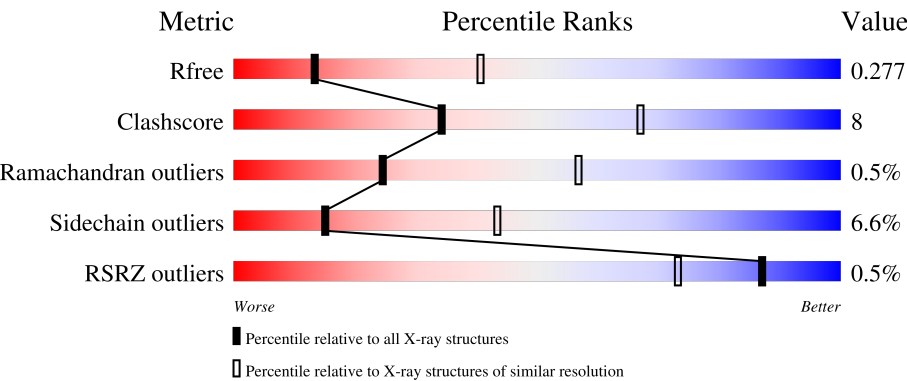
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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	77%21%..
1	B	1536	% 77%21%..
2	C	5	60%40%
2	D	5	40%60%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	 50%50%
3	G	2	 50%50%
3	H	2	 100%

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.

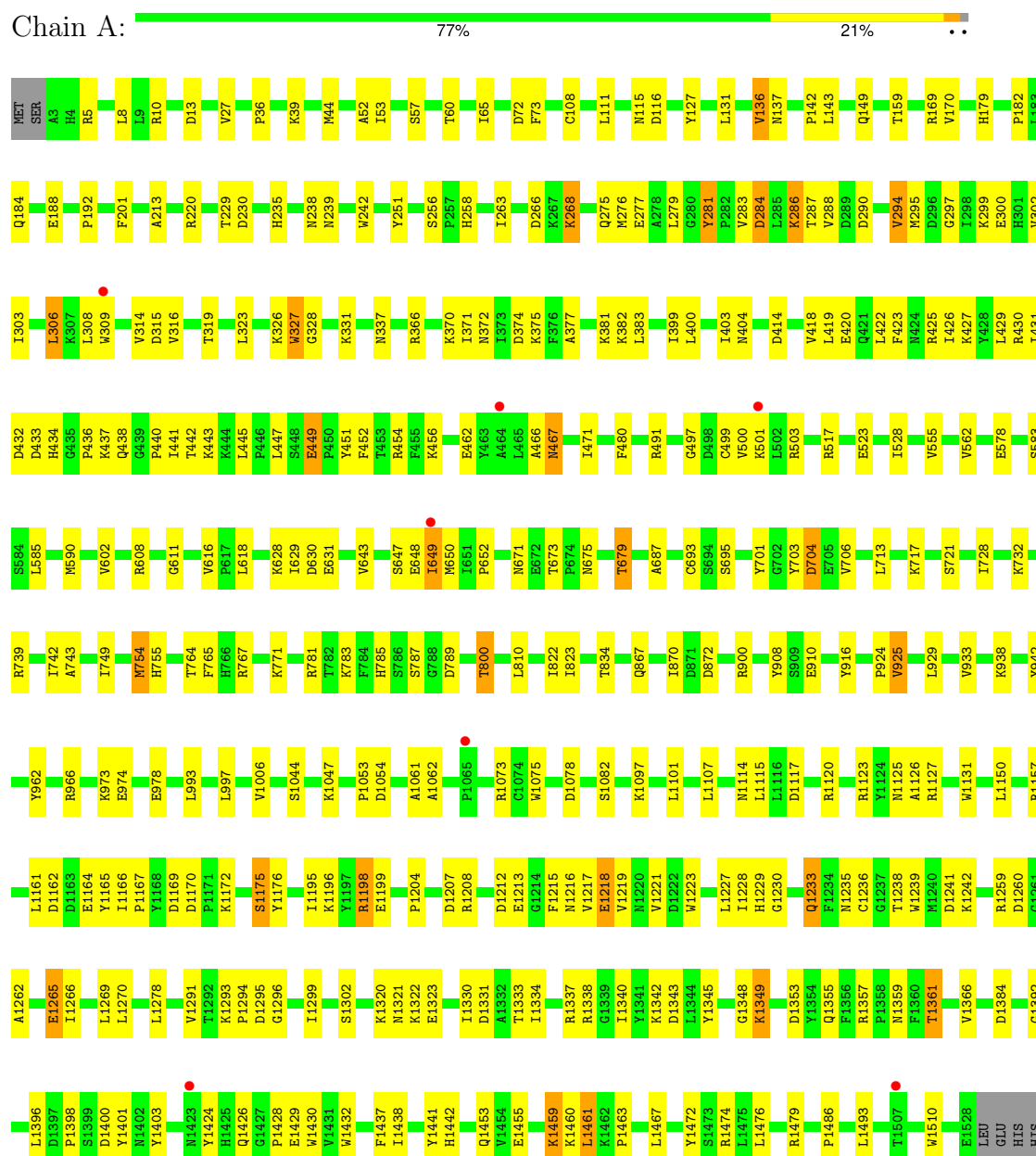


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			
3	G	2	Total	C	O	0	0	0
			23	12	11			
3	H	2	Total	C	O	0	0	0
			23	12	11			

3 Residue-property plots

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.

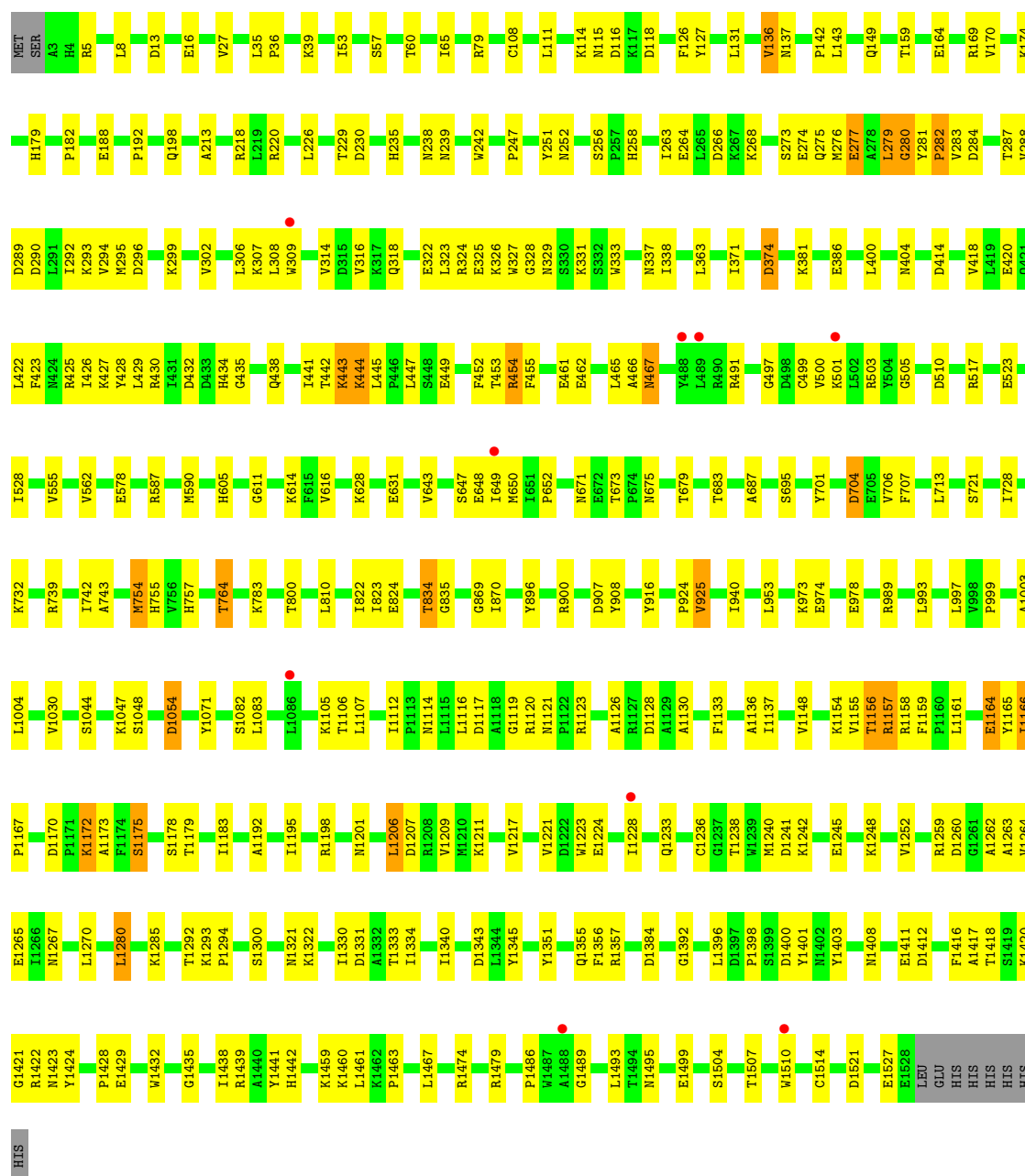
- Molecule 1: 4-alpha-glucanotransferase



HIS
HIS
HIS
HIS

• Molecule 1: 4-alpha-glucanotransferase

Chain B: 



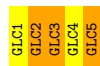
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C: 



- 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:



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

Chain E:



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

Chain F:



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

Chain G:



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

Chain H:



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 , 0.277	Depositor DCC
R_{free} test set	3632 reflections (4.96%)	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)	0.28 , 40.6	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	0.94	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	0.16	0/12578	0.38	0/17055
1	B	0.16	0/12578	0.39	2/17055 (0.0%)
All	All	0.16	0/25156	0.39	2/34110 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1206	LEU	N-CA-C	5.91	113.63	108.78
1	B	1206	LEU	CB-CA-C	-5.28	109.47	117.07

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	193	0
1	B	12269	0	11955	176	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	23	0	21	2	0
All	All	24742	0	24090	373	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 8.

All (373) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:242:TRP:CG	1:A:517:ARG:HH12	2.17	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
1:A:115:ASN:OD1	1:A:116:ASP:N	2.34	0.60
1:A:295:MET:HE1	1:A:419:LEU:HB2	1.83	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:B:242:TRP:CG	1:B:517:ARG:HH12	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1242:LYS:HE2	1:B:1421:GLY:C	2.32	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
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:A:1223:TRP:CD1	1:A:1293:LYS:HZ3	2.27	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:B:1259:ARG:HH12	1:B:1343:ASP:CG	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:H:1:GLC:O6	3:H:2:GLC:O5	2.31	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:B:754:MET:HG2	1:B:755:HIS:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:292:ILE:HA	1:B:295:MET:HE2	1.99	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
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
3:H:1:GLC:HO6	3:H:2:GLC:C5	2.31	0.43
1:A:1165:TYR:O	1:A:1167:PRO:HD3	2.18	0.43
1:B:721:SER:OG	1:B:823:ILE:O	2.21	0.43
1:B:1240:MET:HE1	1:B:1357:ARG:HD3	2.01	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:242:TRP:NE1	1:A:517:ARG:HH22	2.16	0.42
1:A:630:ASP:OD1	1:A:650:MET:HE3	2.19	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:242:TRP:NE1	1:B:517:ARG:HH22	2.17	0.42
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:276:MET:HE3	1:A:294:VAL:HG21	2.01	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:57:SER:O	1:A:60:THR:OG1	2.36	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1392:GLY:C	1:A:1429:GLU:HB3	2.45	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
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:A:1259:ARG:HH12	1:A:1343:ASP:CG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1392:GLY:C	1:B:1429:GLU:HB3	2.46	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 [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	1524/1536 (99%)	1414 (93%)	103 (7%)	7 (0%)	24	57
1	B	1524/1536 (99%)	1412 (93%)	103 (7%)	9 (1%)	21	52
All	All	3048/3072 (99%)	2826 (93%)	206 (7%)	16 (0%)	24	57

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

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Mol	Chain	Res	Type
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%)	1264 (94%)	79 (6%)	18	48
1	B	1343/1353 (99%)	1245 (93%)	98 (7%)	13	40
All	All	2686/2706 (99%)	2509 (93%)	177 (7%)	15	43

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	159	THR
1	A	220	ARG
1	A	229	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	290	ASP
1	A	294	VAL

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Mol	Chain	Res	Type
1	A	302	VAL
1	A	306	LEU
1	A	308	LEU
1	A	316	VAL
1	A	331	LYS
1	A	337	ASN
1	A	374	ASP
1	A	383	LEU
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	456	LYS
1	A	462	GLU
1	A	467	ASN
1	A	500	VAL
1	A	562	VAL
1	A	583	SER
1	A	585	LEU
1	A	616	VAL
1	A	629	ILE
1	A	631	GLU
1	A	649	ILE
1	A	679	THR
1	A	704	ASP
1	A	742	ILE
1	A	754	MET
1	A	764	THR
1	A	785	HIS
1	A	787	SER
1	A	800	THR
1	A	834	THR
1	A	910	GLU
1	A	925	VAL
1	A	973	LYS
1	A	974	GLU
1	A	978	GLU
1	A	1044	SER

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Mol	Chain	Res	Type
1	A	1082	SER
1	A	1127	ARG
1	A	1162	ASP
1	A	1166	ILE
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	1233	GLN
1	A	1265	GLU
1	A	1321	ASN
1	A	1322	LYS
1	A	1323	GLU
1	A	1330	ILE
1	A	1334	ILE
1	A	1349	LYS
1	A	1361	THR
1	A	1424	TYR
1	A	1442	HIS
1	A	1455	GLU
1	A	1459	LYS
1	A	1460	LYS
1	A	1461	LEU
1	B	136	VAL
1	B	159	THR
1	B	220	ARG
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	289	ASP
1	B	290	ASP
1	B	308	LEU
1	B	316	VAL
1	B	324	ARG

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Mol	Chain	Res	Type
1	B	325	GLU
1	B	326	LYS
1	B	333	TRP
1	B	337	ASN
1	B	363	LEU
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	447	LEU
1	B	449	GLU
1	B	454	ARG
1	B	461	GLU
1	B	462	GLU
1	B	467	ASN
1	B	500	VAL
1	B	562	VAL
1	B	616	VAL
1	B	631	GLU
1	B	649	ILE
1	B	704	ASP
1	B	742	ILE
1	B	754	MET
1	B	764	THR
1	B	800	THR
1	B	834	THR
1	B	925	VAL
1	B	974	GLU
1	B	978	GLU
1	B	1030	VAL
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

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Mol	Chain	Res	Type
1	B	1157	ARG
1	B	1159	PHE
1	B	1161	LEU
1	B	1164	GLU
1	B	1166	ILE
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	1236	CYS
1	B	1241	ASP
1	B	1248	LYS
1	B	1252	VAL
1	B	1260	ASP
1	B	1264	VAL
1	B	1265	GLU
1	B	1280	LEU
1	B	1292	THR
1	B	1300	SER
1	B	1321	ASN
1	B	1330	ILE
1	B	1334	ILE
1	B	1340	ILE
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	1459	LYS
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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	223	HIS
1	A	329	ASN
1	A	354	ASN
1	A	785	HIS
1	A	943	ASN
1	A	952	ASN
1	A	1109	HIS
1	A	1201	ASN
1	B	37	GLN
1	B	184	GLN
1	B	223	HIS
1	B	354	ASN
1	B	434	HIS
1	B	525	ASN
1	B	866	GLN
1	B	943	ASN
1	B	1056	ASN
1	B	1109	HIS
1	B	1191	HIS
1	B	1267	ASN
1	B	1309	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.89	1 (8%)	17,17,17	0.98	0
2	GLC	C	2	2	11,11,12	0.97	1 (9%)	15,15,17	1.23	1 (6%)
2	GLC	C	3	2	11,11,12	0.91	1 (9%)	15,15,17	1.42	3 (20%)
2	GLC	C	4	2	11,11,12	1.29	1 (9%)	15,15,17	1.04	1 (6%)
2	GLC	C	5	2	11,11,12	0.62	0	15,15,17	1.32	2 (13%)
2	GLC	D	1	2	12,12,12	1.00	1 (8%)	17,17,17	1.10	1 (5%)
2	GLC	D	2	2	11,11,12	1.57	2 (18%)	15,15,17	1.34	1 (6%)
2	GLC	D	3	2	11,11,12	1.27	2 (18%)	15,15,17	1.35	2 (13%)
2	GLC	D	4	2	11,11,12	1.08	1 (9%)	15,15,17	1.27	3 (20%)
2	GLC	D	5	2	11,11,12	0.57	0	15,15,17	1.23	2 (13%)
3	GLC	E	1	3	12,12,12	0.84	1 (8%)	17,17,17	1.14	1 (5%)
3	GLC	E	2	3	11,11,12	1.37	2 (18%)	15,15,17	2.20	7 (46%)
3	GLC	F	1	3	12,12,12	0.71	0	17,17,17	1.10	1 (5%)
3	GLC	F	2	3	11,11,12	0.55	0	15,15,17	0.78	0
3	GLC	G	1	3	12,12,12	0.70	0	17,17,17	0.63	0
3	GLC	G	2	3	11,11,12	0.62	0	15,15,17	0.79	0
3	GLC	H	1	3	12,12,12	1.01	0	17,17,17	1.14	2 (11%)
3	GLC	H	2	3	11,11,12	1.24	1 (9%)	15,15,17	1.56	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C4-C5	3.68	1.60	1.53
2	C	4	GLC	O4-C4	2.91	1.50	1.43
3	E	2	GLC	C4-C5	2.76	1.58	1.53
2	D	2	GLC	O4-C4	2.75	1.49	1.43
3	E	2	GLC	C1-C2	2.60	1.58	1.52
2	C	2	GLC	O4-C4	2.59	1.49	1.43
2	D	4	GLC	O4-C4	2.41	1.48	1.43
2	D	3	GLC	O4-C4	2.36	1.48	1.43
2	D	1	GLC	O4-C4	2.19	1.48	1.43
3	E	1	GLC	O4-C4	2.17	1.48	1.43
2	C	1	GLC	O4-C4	2.12	1.48	1.43
2	D	3	GLC	C4-C3	2.10	1.57	1.52
3	H	2	GLC	C4-C5	-2.09	1.48	1.53
2	C	3	GLC	O4-C4	2.05	1.48	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	GLC	C2-C3-C4	-4.19	103.50	110.86
3	E	2	GLC	C3-C4-C5	-3.79	103.37	110.23
3	H	2	GLC	C1-O5-C5	3.75	117.21	112.19
2	D	2	GLC	O4-C4-C5	3.68	118.39	109.32
3	E	2	GLC	C1-C2-C3	3.27	114.40	109.64
2	C	2	GLC	O4-C4-C3	3.09	117.66	110.38
2	C	3	GLC	O5-C1-C2	-2.78	104.16	110.79
2	D	4	GLC	O4-C4-C3	2.74	116.84	110.38
2	C	5	GLC	C2-C3-C4	-2.71	106.10	110.86
3	E	2	GLC	O3-C3-C4	2.69	116.71	110.38
2	D	3	GLC	C1-O5-C5	-2.67	108.61	112.19
2	D	5	GLC	C2-C3-C4	-2.60	106.28	110.86
3	E	1	GLC	C1-O5-C5	-2.58	108.66	113.65
3	H	2	GLC	O3-C3-C4	-2.44	104.63	110.38
2	D	5	GLC	C1-C2-C3	-2.41	106.14	109.64
3	F	1	GLC	O5-C5-C6	2.35	112.26	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	GLC	C1-O5-C5	-2.32	109.16	113.65
2	D	4	GLC	C2-C3-C4	-2.30	106.81	110.86
3	H	1	GLC	C3-C4-C5	-2.29	106.08	110.23
3	H	2	GLC	O4-C4-C3	-2.25	105.08	110.38
3	E	2	GLC	O5-C5-C4	2.20	116.18	110.83
3	E	2	GLC	O3-C3-C2	-2.18	105.61	110.05
2	D	3	GLC	O3-C3-C4	2.15	115.44	110.38
2	C	5	GLC	O5-C5-C6	-2.13	103.52	107.66
2	C	3	GLC	O5-C5-C6	2.13	111.81	107.66
3	E	2	GLC	O4-C4-C3	2.13	115.39	110.38
2	C	3	GLC	C1-O5-C5	2.12	115.03	112.19
2	C	4	GLC	O4-C4-C3	2.10	115.33	110.38
2	D	1	GLC	C3-C4-C5	-2.07	106.47	110.23
2	D	4	GLC	C6-C5-C4	-2.02	108.06	113.02

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	H	2	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
3	F	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.

8 monomers are involved in 8 short contacts:

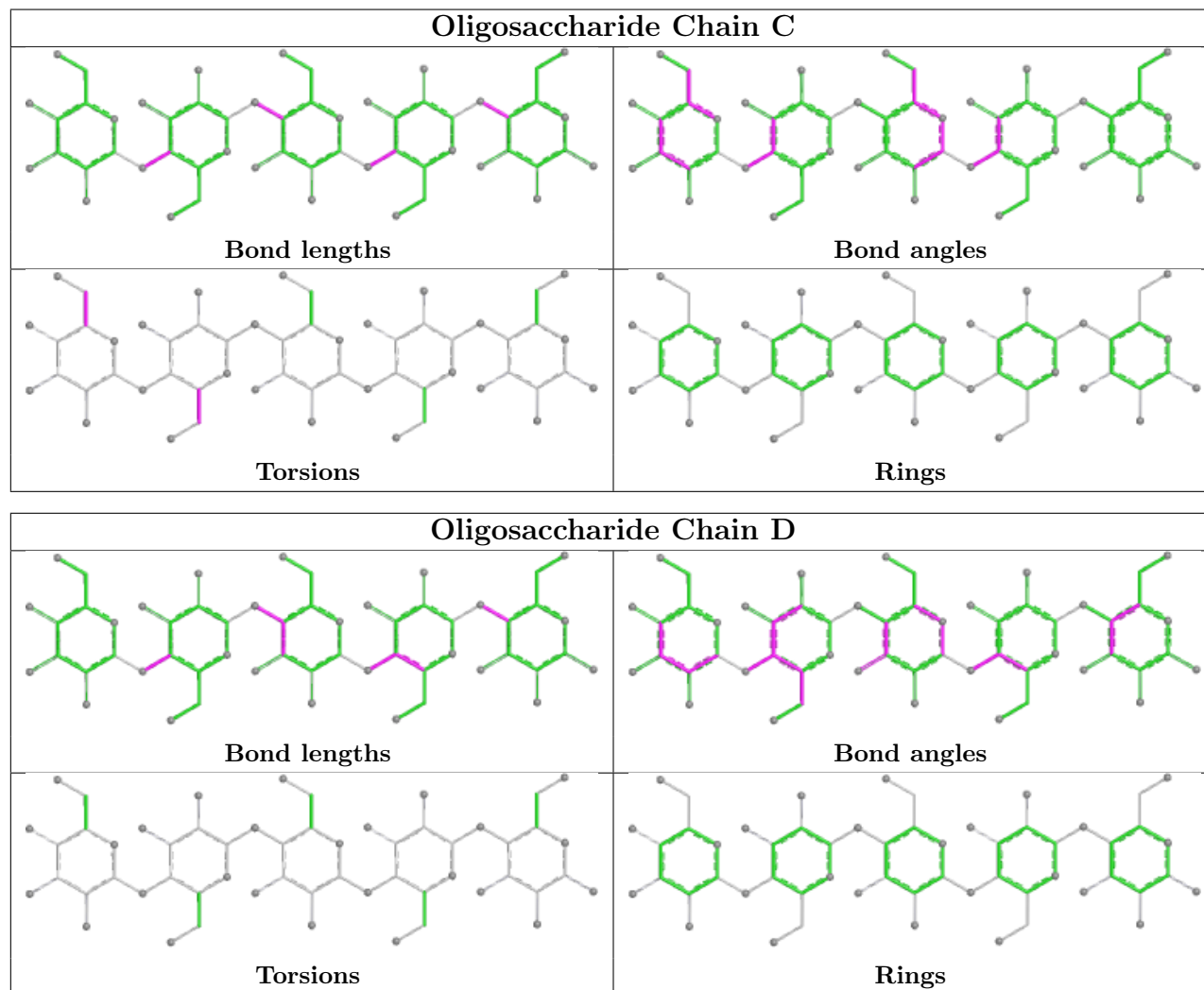
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5	GLC	1	0
3	H	1	GLC	2	0
2	D	2	GLC	1	0
2	C	2	GLC	1	0
2	D	3	GLC	1	0
2	C	3	GLC	2	0

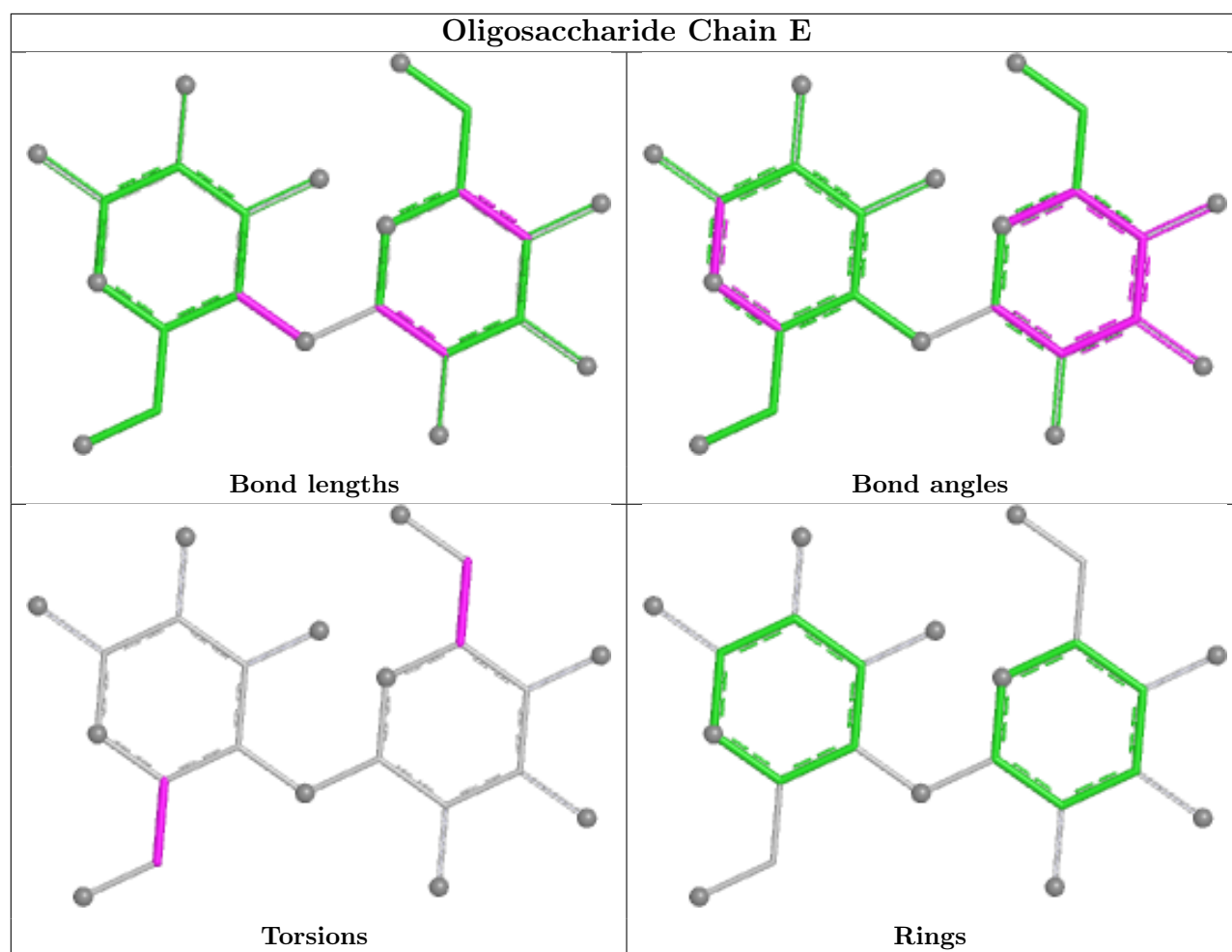
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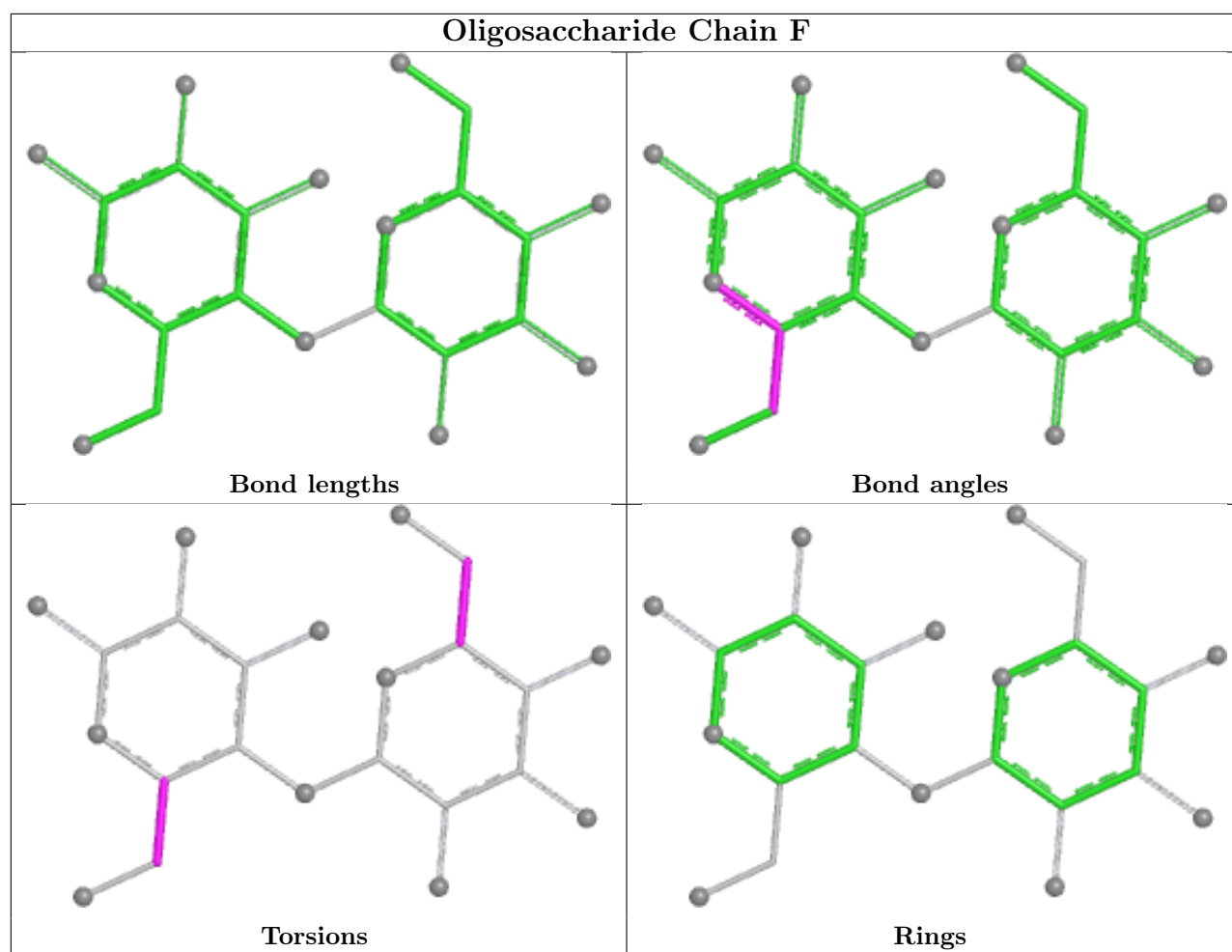
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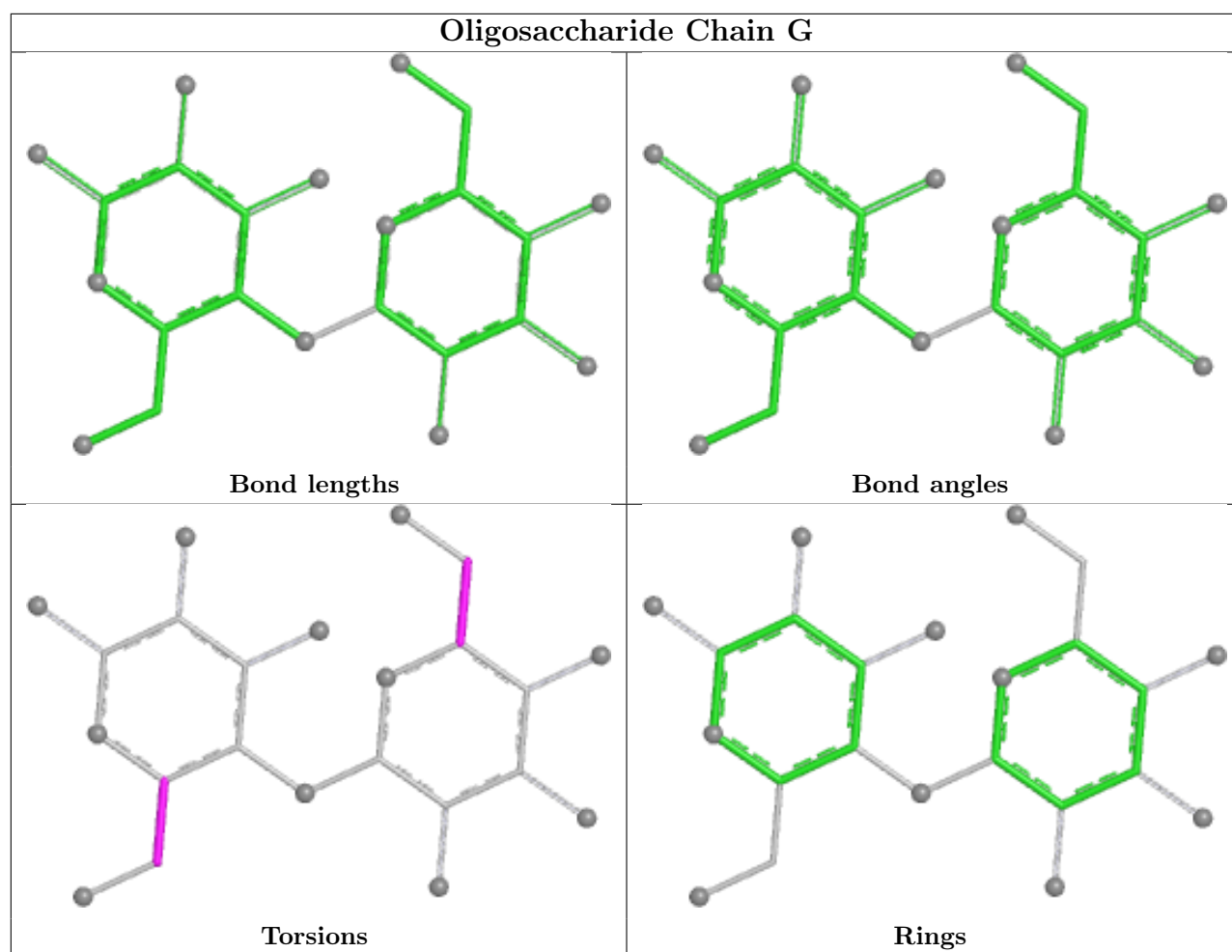
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2	GLC	2	0
3	G	2	GLC	1	0

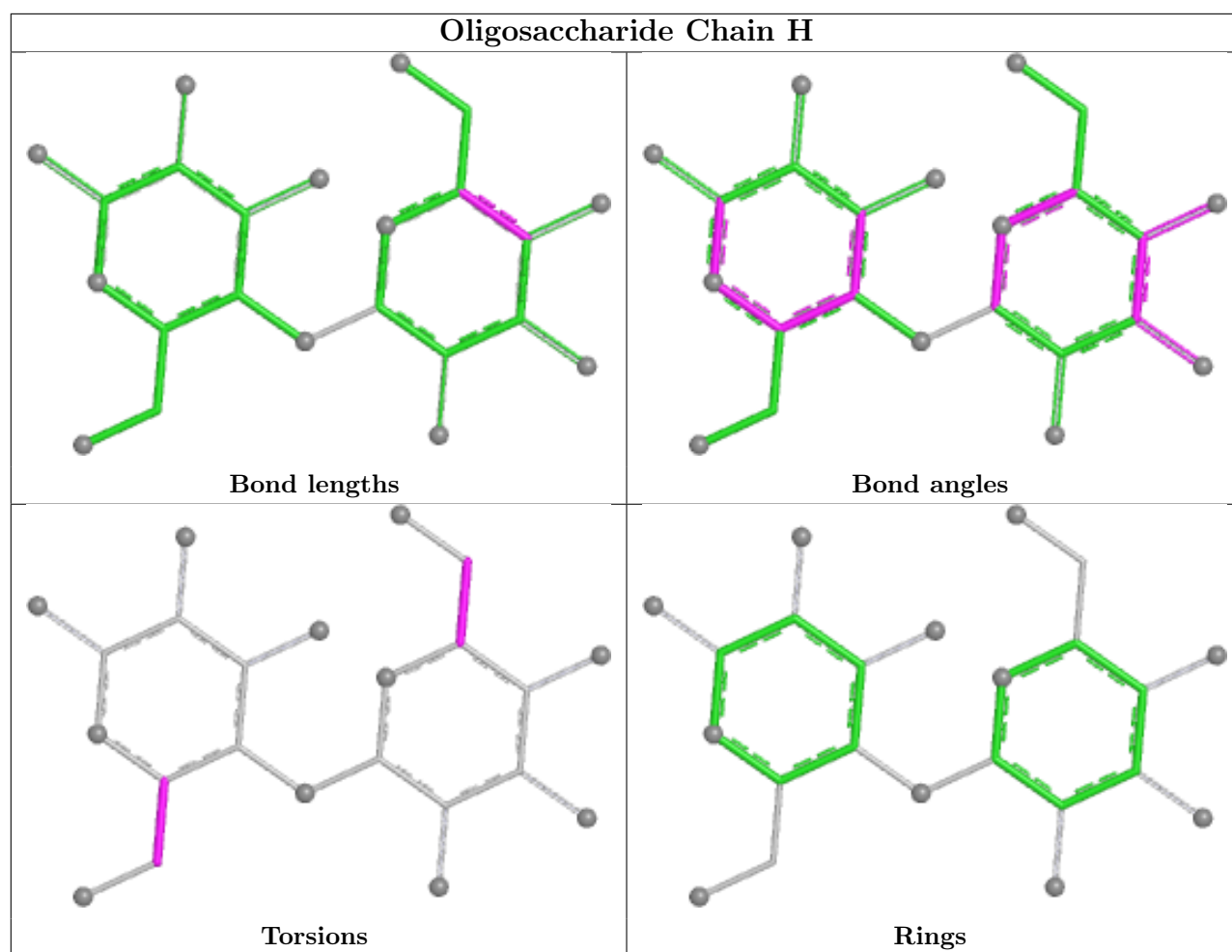
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.29	7 (0%) 87 73	61, 109, 163, 189	0
1	B	1526/1536 (99%)	-0.27	9 (0%) 85 70	55, 112, 176, 211	0
All	All	3052/3072 (99%)	-0.28	16 (0%) 87 73	55, 111, 170, 211	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	LYS	3.3
1	A	1065	PRO	2.6
1	B	309	TRP	2.5
1	B	1510	TRP	2.3
1	A	1423	ASN	2.3
1	A	464	ALA	2.2
1	A	1507	THR	2.2
1	B	1086	LEU	2.2
1	A	649	ILE	2.1
1	B	1228	ILE	2.1
1	A	309	TRP	2.1
1	B	489	LEU	2.1
1	B	488	TYR	2.1
1	A	501	LYS	2.0
1	B	1488	ALA	2.0
1	B	649	ILE	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

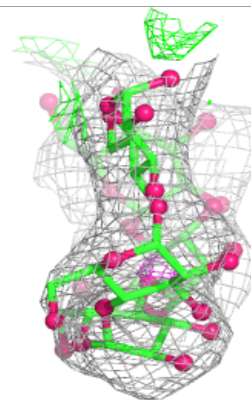
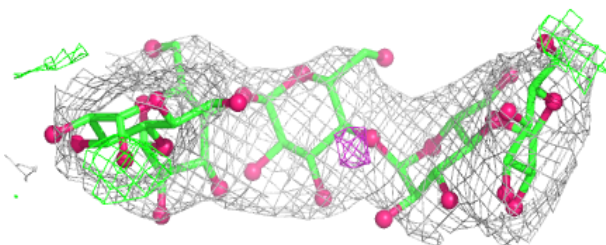
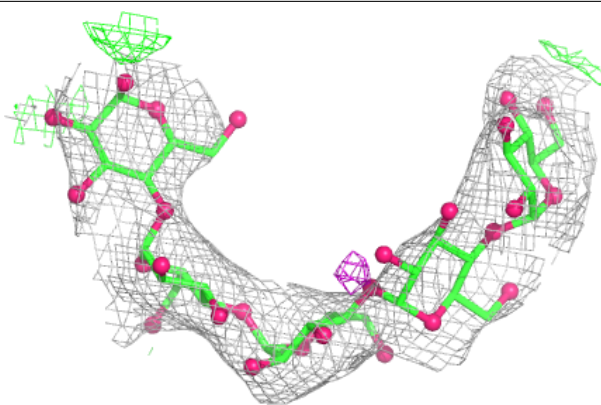
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	5	11/12	0.44	0.09	125,141,159,166	0
2	GLC	D	5	11/12	0.45	0.10	132,149,163,163	0
3	GLC	G	2	11/12	0.53	0.12	106,123,140,143	0
3	GLC	H	2	11/12	0.55	0.07	145,162,170,172	0
3	GLC	F	2	11/12	0.57	0.11	121,143,158,161	0
3	GLC	F	1	12/12	0.60	0.07	122,150,169,173	0
3	GLC	G	1	12/12	0.63	0.10	125,139,147,151	0
2	GLC	D	1	12/12	0.65	0.11	111,139,149,150	0
3	GLC	E	2	11/12	0.73	0.11	100,117,133,135	0
2	GLC	C	1	12/12	0.73	0.12	105,121,136,138	0
3	GLC	E	1	12/12	0.78	0.10	76,90,111,114	0
3	GLC	H	1	12/12	0.82	0.07	122,135,141,146	0
2	GLC	C	2	11/12	0.82	0.10	121,131,142,148	0
2	GLC	D	3	11/12	0.83	0.11	119,132,142,154	0
2	GLC	C	3	11/12	0.84	0.12	116,123,150,152	0
2	GLC	C	4	11/12	0.86	0.09	121,144,158,162	0
2	GLC	D	4	11/12	0.87	0.09	138,157,169,174	0
2	GLC	D	2	11/12	0.89	0.10	125,135,139,144	0

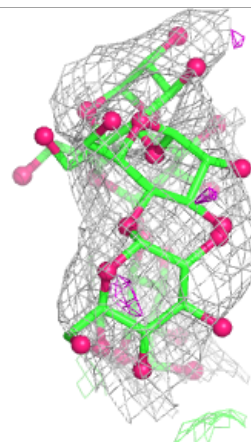
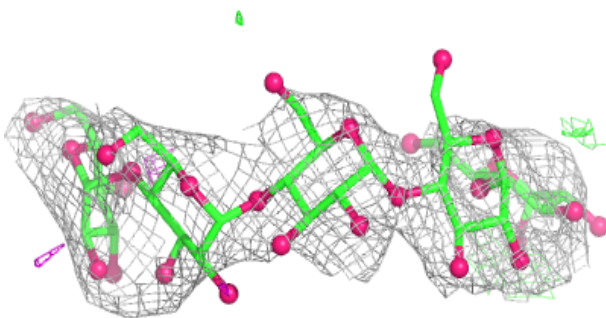
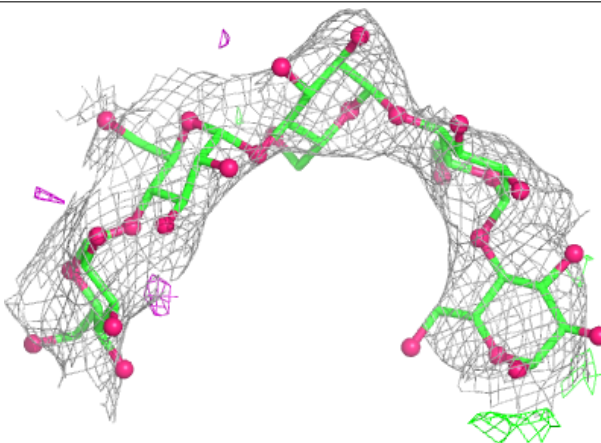
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

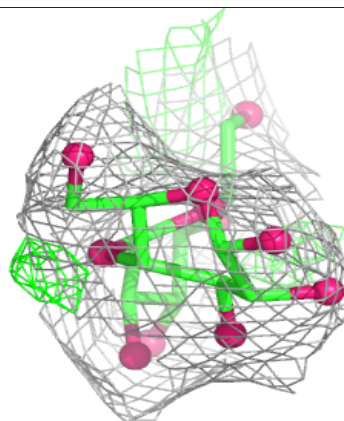
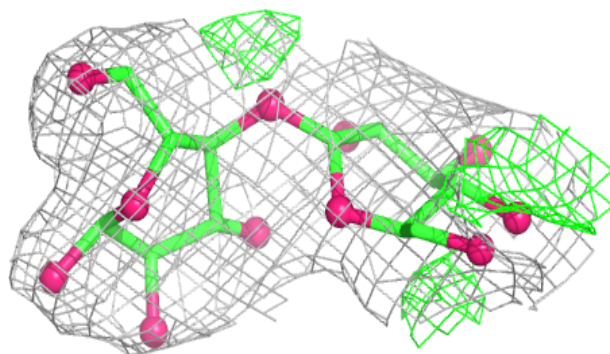
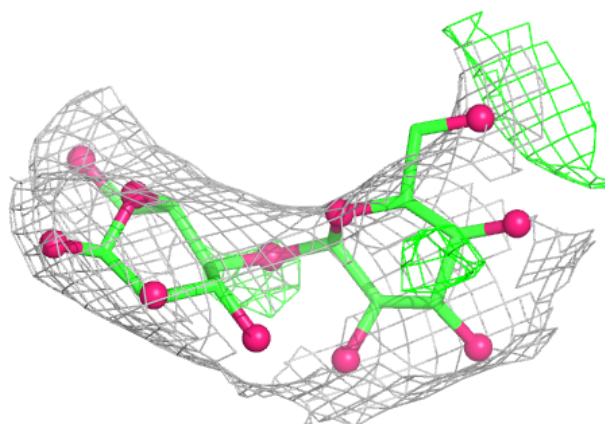
**Electron density around Chain D:**

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



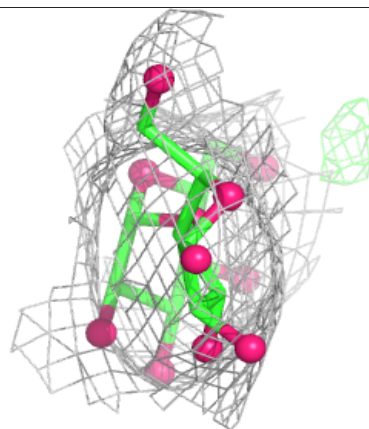
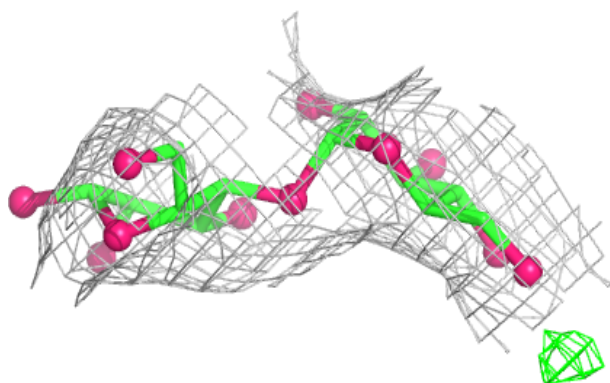
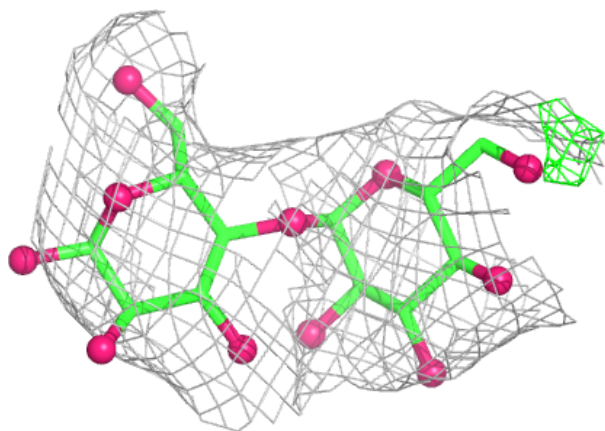
Electron density around Chain E:

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

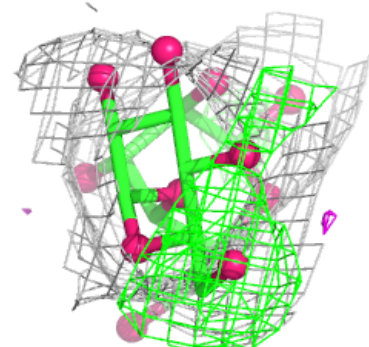
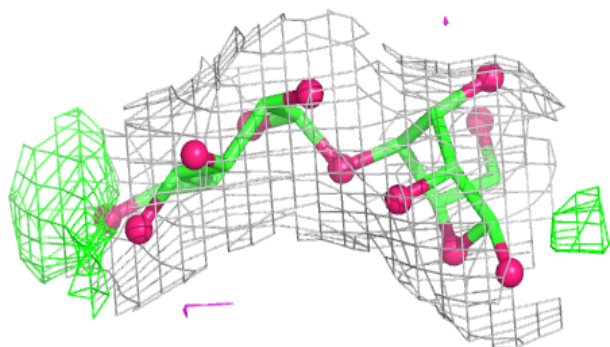
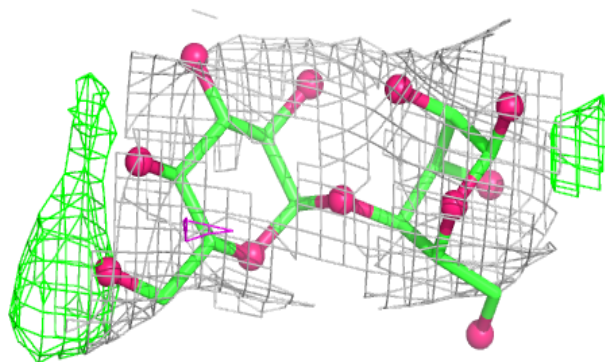


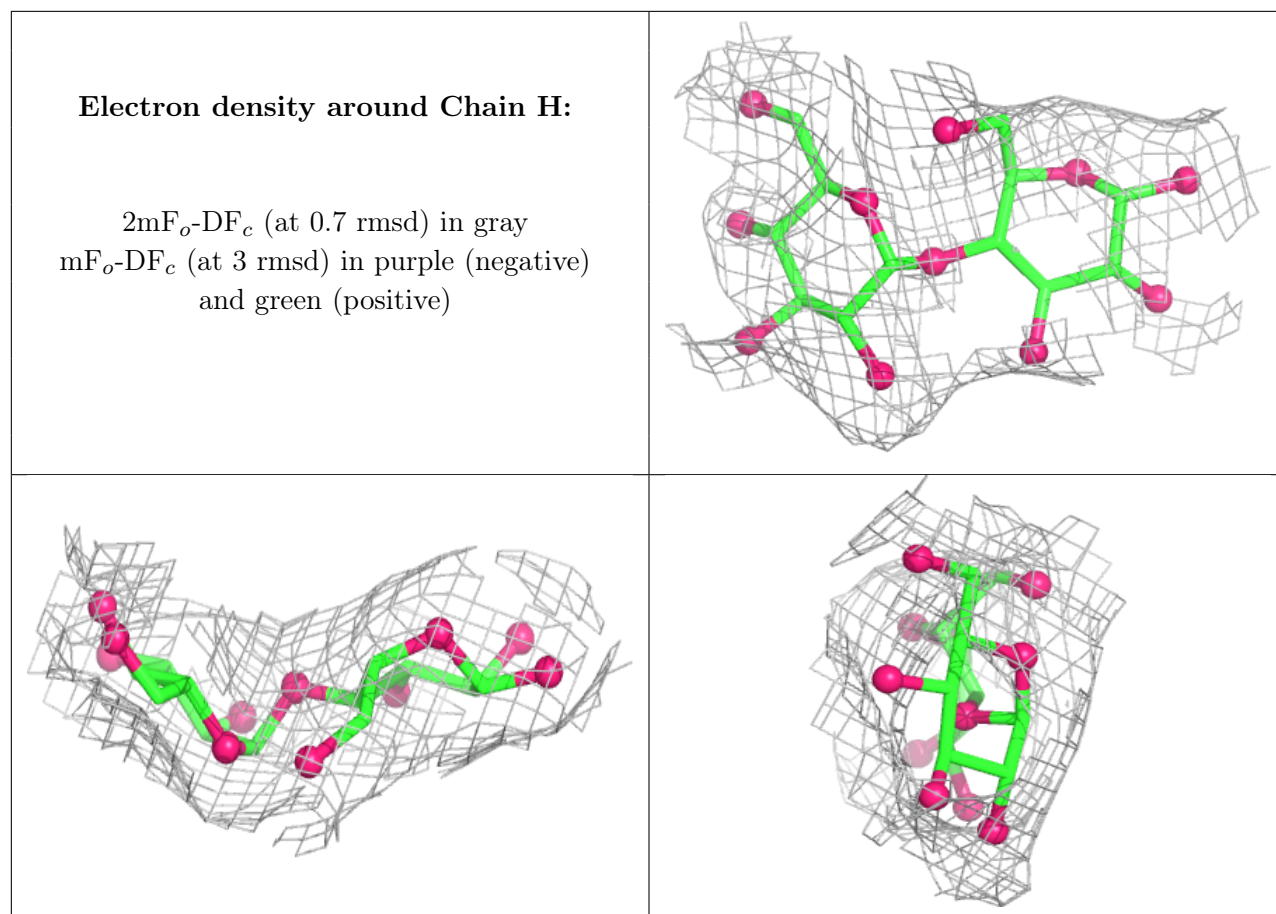
Electron density around Chain F:

$2mF_o - DF_c$ (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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.