



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2021 – 04:11 PM JST

PDB ID : 7EJT
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (W470A) in complex with maltoheptaose
Authors : Shen, M.; Xiang, S.
Deposited on : 2021-04-02
Resolution : 3.20 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

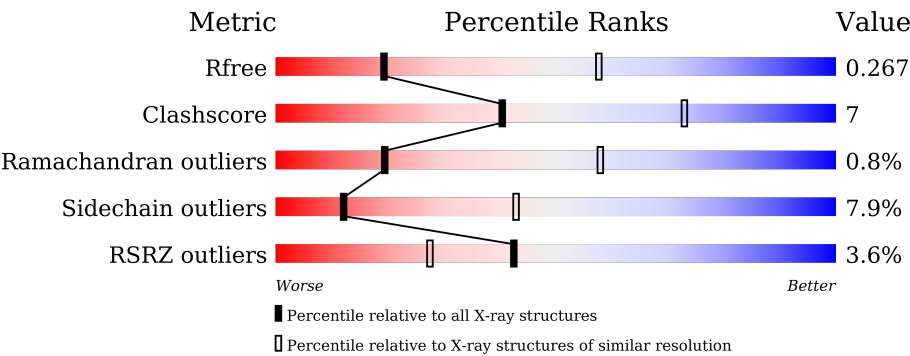
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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>77%</div><div>20%</div><div>..</div></div>
1	B	1536	<div><div>3%</div><div>77%</div><div>21%</div><div>..</div></div>
2	C	2	<div><div>50%</div><div>50%</div></div>
2	D	2	<div><div>50%</div><div>50%</div></div>
2	E	2	<div><div>50%</div><div>50%</div></div>
3	F	3	<div><div>67%</div><div>33%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	5	 20%80%
4	H	5	 40%60%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24753 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:

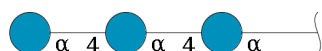
Chain	Residue	Modelled	Actual	Comment	Reference
A	470	ALA	TRP	engineered mutation	UNP Q6FSK0
A	1529	LEU	-	expression tag	UNP Q6FSK0
A	1530	GLU	-	expression tag	UNP Q6FSK0
A	1531	HIS	-	expression tag	UNP Q6FSK0
A	1532	HIS	-	expression tag	UNP Q6FSK0
A	1533	HIS	-	expression tag	UNP Q6FSK0
A	1534	HIS	-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



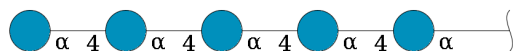
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			

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



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

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

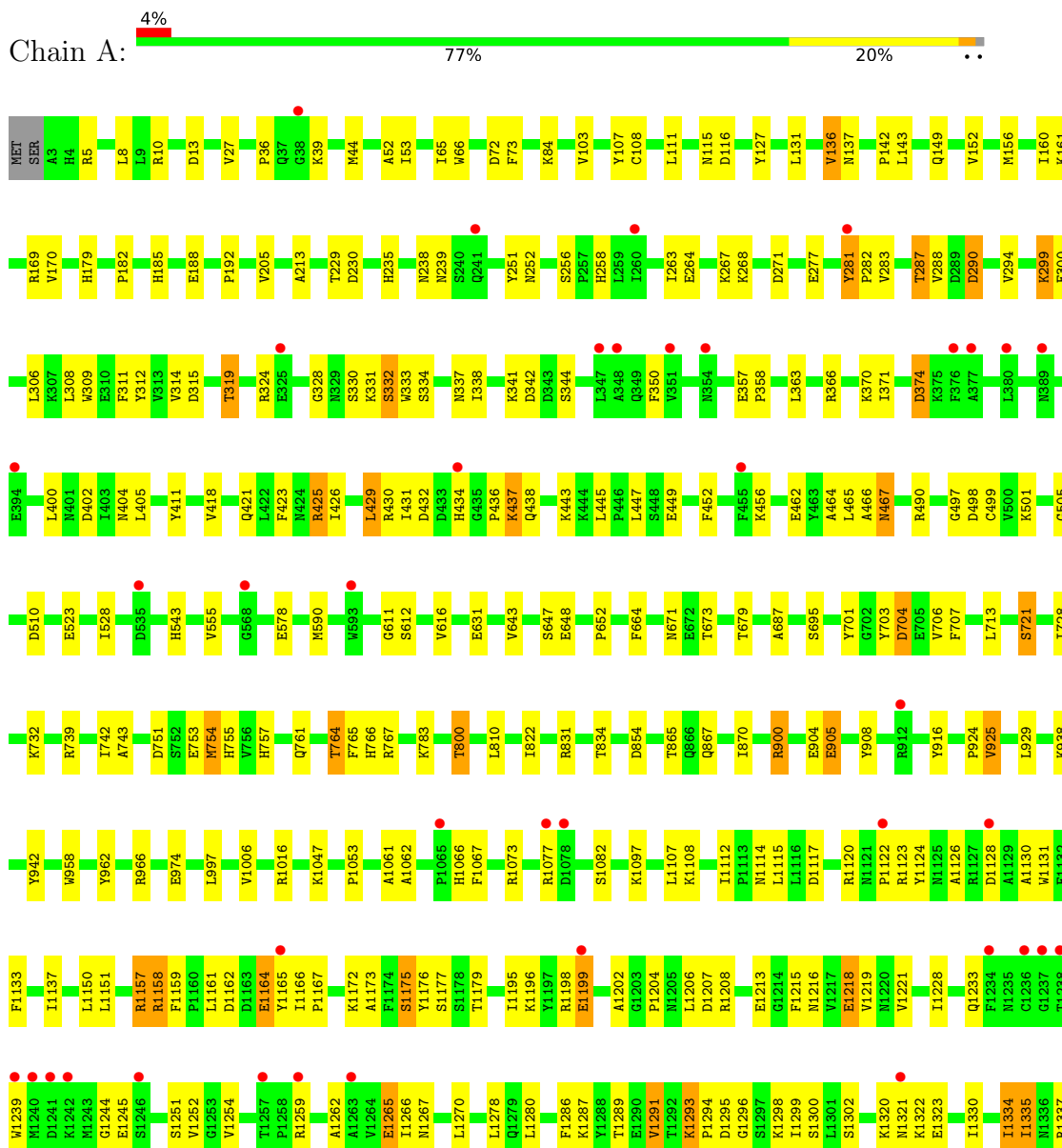


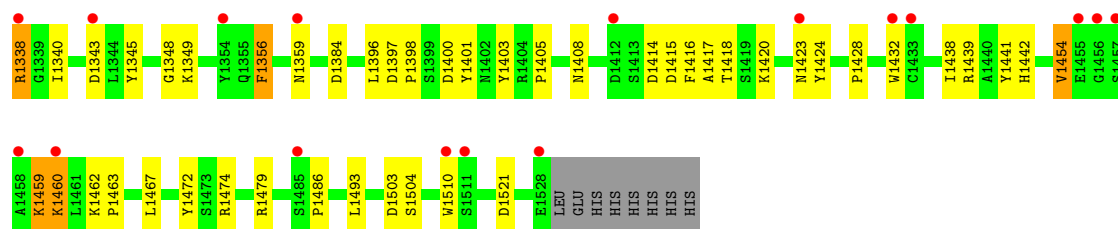
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	5	Total	C	O	0	0	0
			56	30	26			
4	H	5	Total	C	O	0	0	0
			56	30	26			

3 Residue-property plots

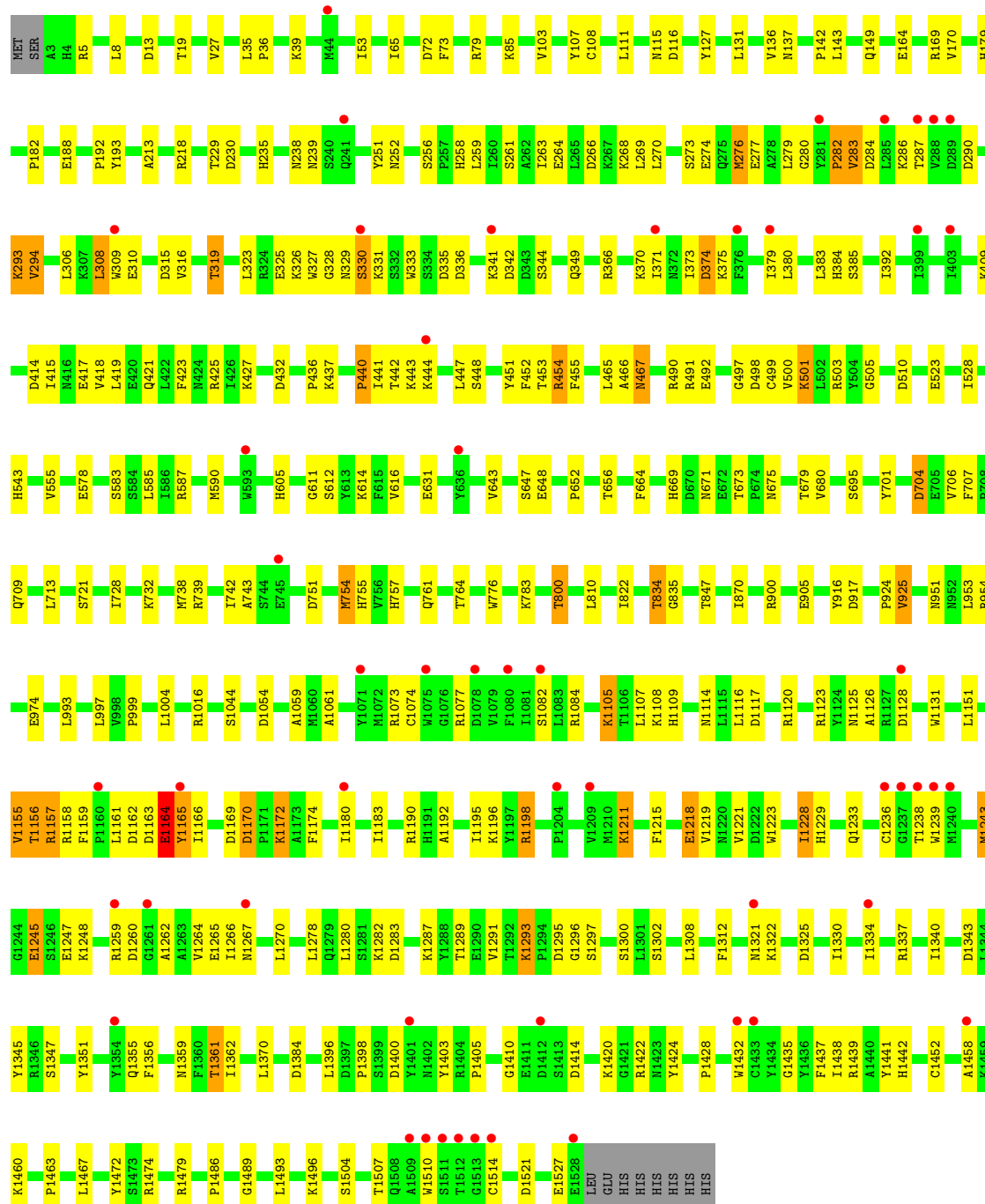
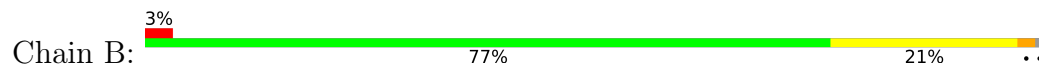
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: 4-alpha-glucanotransferase



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



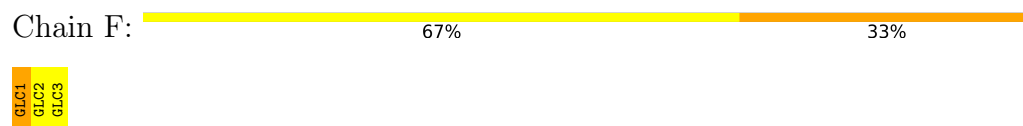
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.39Å 199.27Å 133.74Å 90.00° 100.77° 90.00°	Depositor
Resolution (Å)	40.48 – 3.20 40.48 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.48-3.20) 99.1 (40.48-3.18)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.255 , 0.268 0.255 , 0.267	Depositor DCC
R_{free} test set	3402 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	89.6	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24753	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/12578	0.46	1/17055 (0.0%)
1	B	0.27	0/12578	0.46	0/17055
All	All	0.27	0/25156	0.46	1/34110 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ARG	CG-CD-NE	5.05	122.42	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12269	0	11955	174	0
1	B	12269	0	11955	176	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
2	E	23	0	21	2	0
3	F	34	0	30	2	0
4	G	56	0	48	4	0
4	H	56	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24753	0	24099	353	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 (353) 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)
4:G:2:GLC:HO3	4:G:3:GLC:HO2	1.22	0.84
1:A:182:PRO:HD3	1:A:230:ASP:HB2	1.62	0.80
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.62	0.79
1:B:1107:LEU:O	1:B:1157:ARG:NH1	2.15	0.79
1:A:8:LEU:HB2	1:A:652:PRO:HG2	1.65	0.77
1:B:1361:THR:HG21	1:B:1437:PHE:HA	1.65	0.77
1:B:182:PRO:HD3	1:B:230:ASP:HB2	1.67	0.76
1:A:1293:LYS:HG3	1:A:1294:PRO:HD2	1.67	0.76
4:H:2:GLC:O3	4:H:3:GLC:O2	2.03	0.75
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.70	0.73
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.71	0.73
1:A:328:GLY:H	1:A:331:LYS:HE2	1.55	0.72
1:B:282:PRO:HG2	1:B:294:VAL:HG13	1.72	0.72
1:B:8:LEU:HB2	1:B:652:PRO:HG2	1.72	0.72
1:B:169:ARG:NH1	1:B:721:SER:O	2.24	0.70
1:B:452:PHE:HA	1:B:466:ALA:HA	1.73	0.70
1:A:1123:ARG:HH22	1:A:1207:ASP:HB2	1.56	0.70
1:B:282:PRO:HG3	1:B:293:LYS:HB3	1.74	0.69
1:A:169:ARG:NH1	1:A:721:SER:O	2.26	0.69
1:A:1384:ASP:OD1	1:A:1474:ARG:NH1	2.25	0.69
1:A:1259:ARG:NH2	1:A:1265:GLU:OE2	2.26	0.69
1:A:452:PHE:HA	1:A:466:ALA:HA	1.75	0.68
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.27	0.68
1:A:466:ALA:H	1:A:501:LYS:HD2	1.60	0.67
1:A:1221:VAL:HG22	1:A:1228:ILE:HG12	1.77	0.67
1:A:374:ASP:OD1	1:A:374:ASP:N	2.20	0.66
1:A:1245:GLU:HG3	1:A:1420:LYS:HB3	1.77	0.65
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.78	0.65
1:B:466:ALA:H	1:B:501:LYS:HD2	1.63	0.64
1:B:1384:ASP:OD1	1:B:1474:ARG:NH1	2.30	0.63
1:A:66:TRP:CZ3	1:A:84:LYS:HG2	2.32	0.63
1:A:1356:PHE:HB3	1:A:1397:ASP:HB2	1.81	0.62
1:B:36:PRO:HB2	1:B:39:LYS:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:LYS:HD2	1:A:1218:GLU:HG2	1.81	0.61
1:B:1198:ARG:HH21	1:B:1215:PHE:HB2	1.64	0.61
1:A:1115:LEU:HB3	1:A:1123:ARG:HB3	1.83	0.61
1:B:1239:TRP:HE1	1:B:1359:ASN:HD21	1.48	0.61
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.34	0.60
1:B:319:THR:HG23	1:B:370:LYS:HE3	1.83	0.60
1:B:590:MET:HB2	1:B:671:ASN:HD22	1.67	0.60
1:A:1206:LEU:O	4:G:4:GLC:H4	2.02	0.59
1:A:766:HIS:HE1	1:A:865:THR:HG21	1.67	0.59
1:B:466:ALA:HB3	1:B:501:LYS:HE3	1.84	0.59
1:A:1503:ASP:O	4:G:1:GLC:O2	2.20	0.59
1:A:466:ALA:HB3	1:A:501:LYS:HE3	1.83	0.59
1:B:238:ASN:ND2	1:B:497:GLY:O	2.35	0.59
1:A:1432:TRP:CG	1:A:1510:TRP:HD1	2.21	0.59
1:A:306:LEU:HD13	1:A:309:TRP:HZ2	1.67	0.58
1:B:179:HIS:NE2	1:B:230:ASP:OD1	2.36	0.58
1:A:958:TRP:HB3	3:F:3:GLC:H61	1.83	0.58
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.36	0.58
1:A:1228:ILE:HG13	1:A:1270:LEU:HD22	1.86	0.58
1:B:266:ASP:HB3	1:B:454:ARG:HH22	1.67	0.58
1:B:131:LEU:HD13	1:B:143:LEU:HD13	1.86	0.58
1:A:36:PRO:HB2	1:A:39:LYS:HG3	1.86	0.58
1:A:728:ILE:HD11	1:A:810:LEU:HD22	1.85	0.58
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.85	0.58
1:A:456:LYS:HG3	1:A:462:GLU:HG2	1.86	0.57
1:A:430:ARG:HB3	1:A:438:GLN:HG3	1.86	0.57
1:A:1077:ARG:HH21	1:A:1128:ASP:HB2	1.69	0.57
1:A:115:ASN:OD1	1:A:116:ASP:N	2.37	0.57
1:A:1239:TRP:HE1	1:A:1359:ASN:HD21	1.52	0.56
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.87	0.56
1:A:721:SER:HA	1:A:822:ILE:HD11	1.87	0.56
1:A:590:MET:HB2	1:A:671:ASN:HD22	1.70	0.56
1:B:1293:LYS:HD3	1:B:1297:SER:HB2	1.87	0.56
1:A:53:ILE:HD11	1:A:65:ILE:HD11	1.87	0.56
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.85	0.56
1:B:671:ASN:OD1	1:B:671:ASN:N	2.38	0.55
1:A:1278:LEU:HD11	1:A:1302:SER:HA	1.88	0.55
1:A:695:SER:O	1:A:739:ARG:NH2	2.33	0.55
1:A:916:TYR:O	1:A:924:PRO:HD2	2.07	0.55
1:A:131:LEU:HD13	1:A:143:LEU:HD13	1.88	0.55
1:A:264:GLU:HA	1:A:267:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HB3	1:B:448:SER:HB3	1.90	0.54
1:B:1059:ALA:HB1	1:B:1074:CYS:SG	2.47	0.54
1:A:238:ASN:ND2	1:A:497:GLY:O	2.40	0.54
1:B:13:ASP:OD2	1:B:1479:ARG:NH2	2.28	0.53
1:B:5:ARG:HA	1:B:643:VAL:HG12	1.90	0.53
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.89	0.53
1:B:916:TYR:O	1:B:924:PRO:HD2	2.08	0.53
1:B:1262:ALA:HB1	1:B:1267:ASN:HD21	1.72	0.53
1:B:115:ASN:OD1	1:B:116:ASP:N	2.40	0.53
1:B:757:HIS:HB3	1:B:764:THR:HB	1.89	0.53
1:B:261:SER:HB2	1:B:309:TRP:HZ3	1.73	0.53
1:A:929:LEU:HD22	1:A:1006:VAL:HG13	1.90	0.53
1:B:164:GLU:OE2	1:B:218:ARG:NH1	2.41	0.53
1:A:5:ARG:HA	1:A:643:VAL:HG12	1.90	0.53
1:A:1198:ARG:HE	1:A:1215:PHE:HB2	1.74	0.53
1:B:1156:THR:HG23	1:B:1174:PHE:HA	1.91	0.53
1:A:315:ASP:O	1:A:319:THR:OG1	2.24	0.53
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.91	0.52
1:B:611:GLY:HA2	1:B:997:LEU:HD23	1.91	0.52
1:A:523:GLU:HB2	1:A:555:VAL:HG21	1.91	0.52
1:B:1107:LEU:HD22	1:B:1183:ILE:HG23	1.92	0.52
1:A:1233:GLN:OE1	1:A:1348:GLY:HA3	2.09	0.52
1:B:380:LEU:HB3	1:B:392:ILE:HD12	1.92	0.52
1:B:1322:LYS:H	1:B:1322:LYS:HD2	1.73	0.52
1:A:1335:ILE:HD11	1:A:1338:ARG:HG2	1.92	0.52
1:A:1441:TYR:OH	1:A:1474:ARG:NH2	2.43	0.51
1:B:1396:LEU:HD21	1:B:1400:ASP:HB3	1.91	0.51
1:B:1229:HIS:HE1	1:B:1345:TYR:HD2	1.58	0.51
1:B:418:VAL:HG22	1:B:490:ARG:HA	1.92	0.51
1:A:466:ALA:N	1:A:501:LYS:HD2	2.25	0.51
1:B:466:ALA:N	1:B:501:LYS:HD2	2.26	0.51
1:A:188:GLU:H	1:A:239:ASN:HD21	1.58	0.51
1:A:870:ILE:HD11	1:A:997:LEU:HD13	1.91	0.51
1:A:10:ARG:HA	1:A:52:ALA:HB3	1.93	0.51
1:A:1454:VAL:HG12	1:A:1462:LYS:HG3	1.92	0.51
1:B:1105:LYS:HG2	1:B:1155:VAL:HB	1.93	0.51
1:B:1108:LYS:HD2	1:B:1159:PHE:HD1	1.76	0.51
1:B:1245:GLU:HG3	1:B:1420:LYS:HB3	1.92	0.51
1:A:72:ASP:OD1	1:A:73:PHE:N	2.40	0.50
1:A:1123:ARG:NH2	1:A:1207:ASP:HB2	2.26	0.50
1:B:679:THR:OG1	1:B:783:LYS:HG2	2.11	0.50

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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	0.50
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.92	0.50
1:B:72:ASP:OD1	1:B:73:PHE:N	2.42	0.50
1:B:256:SER:HB2	1:B:258:HIS:CE1	2.47	0.50
1:A:182:PRO:HG2	1:A:192:PRO:O	2.12	0.50
1:A:136:VAL:HG13	1:A:137:ASN:H	1.77	0.50
1:B:432:ASP:HB2	1:B:436:PRO:HB3	1.94	0.50
1:B:647:SER:OG	1:B:648:GLU:N	2.44	0.50
1:B:1077:ARG:HH21	1:B:1128:ASP:HB2	1.77	0.50
1:B:136:VAL:HG13	1:B:137:ASN:H	1.77	0.50
1:A:306:LEU:HD13	1:A:309:TRP:CZ2	2.47	0.50
1:A:647:SER:OG	1:A:648:GLU:N	2.45	0.50
1:B:870:ILE:HG12	1:B:993:LEU:HD22	1.94	0.50
1:B:925:VAL:HG21	1:B:1486:PRO:HB2	1.93	0.49
1:A:281:TYR:CG	1:A:282:PRO:HD3	2.47	0.49
1:A:679:THR:OG1	1:A:783:LYS:HG2	2.12	0.49
1:B:1243:MET:HB2	4:H:3:GLC:H2	1.94	0.49
1:A:466:ALA:HB3	1:A:501:LYS:CE	2.42	0.49
1:A:754:MET:HG2	1:A:755:HIS:N	2.25	0.49
1:A:1066:HIS:CD2	4:G:1:GLC:H1	2.47	0.49
1:B:284:ASP:HB2	1:B:440:PRO:HA	1.94	0.49
1:A:1097:LYS:HG3	1:A:1150:LEU:HD13	1.94	0.49
1:A:1428:PRO:HB3	1:A:1493:LEU:HD21	1.94	0.49
1:B:380:LEU:HD13	1:B:392:ILE:HG23	1.94	0.49
1:A:430:ARG:O	1:A:438:GLN:HB2	2.13	0.49
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.95	0.48
1:A:287:THR:HB	1:A:290:ASP:H	1.77	0.48
1:B:614:LYS:HB2	1:B:1004:LEU:HD13	1.94	0.48
1:B:1438:ILE:HA	1:B:1441:TYR:HB3	1.95	0.48
1:A:611:GLY:N	1:A:753:GLU:OE1	2.44	0.48
1:B:523:GLU:HB2	1:B:555:VAL:HG21	1.94	0.48
1:B:754:MET:HG2	1:B:755:HIS:N	2.27	0.48
1:A:27:VAL:HG22	1:A:578:GLU:HG3	1.96	0.48
1:B:1221:VAL:HG22	1:B:1228:ILE:HG23	1.96	0.48
1:A:400:LEU:O	1:A:404:ASN:ND2	2.47	0.48
1:B:466:ALA:HB3	1:B:501:LYS:CE	2.43	0.48
1:B:721:SER:HA	1:B:822:ILE:HD11	1.94	0.48
1:B:1196:LYS:HD2	1:B:1218:GLU:HG2	1.95	0.48
1:B:1337:ARG:HB2	1:B:1340:ILE:HD12	1.95	0.48
1:A:142:PRO:HG2	1:A:743:ALA:HB1	1.95	0.47
1:A:611:GLY:HA2	1:A:997:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:LYS:HB3	1:A:1124:TYR:CE2	2.48	0.47
1:A:287:THR:HB	1:A:290:ASP:HB3	1.96	0.47
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.15	0.47
1:B:1170:ASP:HB3	1:B:1172:LYS:HG3	1.95	0.47
1:A:13:ASP:OD2	1:A:1479:ARG:NH2	2.29	0.47
1:A:314:VAL:HG11	1:A:371:ILE:HD13	1.96	0.47
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.49	0.47
1:A:13:ASP:OD2	1:A:1472:TYR:OH	2.32	0.47
1:B:1239:TRP:HE1	1:B:1359:ASN:ND2	2.11	0.47
1:B:1420:LYS:HD3	1:B:1420:LYS:HA	1.63	0.47
1:A:256:SER:HB2	1:A:258:HIS:CE1	2.49	0.47
1:A:312:TYR:CE1	1:A:363:LEU:HD21	2.49	0.47
1:B:238:ASN:HB2	1:B:453:THR:HG21	1.97	0.47
1:B:1211:LYS:H	1:B:1211:LYS:HG2	1.38	0.47
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.50	0.47
1:A:704:ASP:OD1	1:A:704:ASP:N	2.47	0.47
1:A:925:VAL:HG21	1:A:1486:PRO:HB2	1.96	0.47
1:A:1415:ASP:HB3	1:A:1418:THR:OG1	2.15	0.47
1:B:452:PHE:CE1	1:B:466:ALA:HB2	2.49	0.47
1:B:1123:ARG:HE	1:B:1125:ASN:ND2	2.13	0.47
1:B:326:LYS:HB2	1:B:326:LYS:HE2	1.70	0.46
1:B:414:ASP:O	1:B:418:VAL:HG23	2.15	0.46
1:B:695:SER:O	1:B:739:ARG:NH2	2.38	0.46
1:B:1196:LYS:HA	1:B:1218:GLU:HG2	1.98	0.46
1:A:103:VAL:O	1:A:107:TYR:OH	2.20	0.46
1:A:962:TYR:CZ	1:A:966:ARG:HD3	2.50	0.46
1:A:1151:LEU:HD11	1:A:1280:LEU:HD21	1.96	0.46
1:B:1228:ILE:HD11	1:B:1270:LEU:HD22	1.96	0.46
1:B:1435:GLY:HA3	1:B:1514:CYS:HB3	1.96	0.46
1:B:953:LEU:HD13	1:B:999:PRO:HA	1.98	0.46
1:B:1211:LYS:HE2	1:B:1211:LYS:HB3	1.80	0.46
1:A:252:ASN:HB3	1:A:465:LEU:HD23	1.98	0.46
1:B:1131:TRP:CD1	1:B:1266:ILE:HG23	2.50	0.46
1:A:312:TYR:HE1	1:A:363:LEU:HD21	1.80	0.46
1:B:193:TYR:OH	1:B:669:HIS:NE2	2.49	0.46
1:A:213:ALA:HA	1:A:528:ILE:HG23	1.96	0.46
1:B:455:PHE:HE1	1:B:465:LEU:HG	1.81	0.46
1:B:951:ASN:OD1	1:B:954:ARG:NH2	2.49	0.46
1:A:149:GLN:HG2	1:A:170:VAL:HG11	1.98	0.46
1:B:1198:ARG:HE	1:B:1198:ARG:HB2	1.50	0.46
1:A:938:LYS:HE2	1:A:942:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:PHE:CD1	1:B:466:ALA:HB2	2.51	0.46
1:B:53:ILE:HD11	1:B:65:ILE:HD11	1.97	0.46
1:B:1156:THR:CG2	1:B:1174:PHE:HA	2.45	0.46
1:A:312:TYR:HD2	1:A:411:TYR:HB2	1.80	0.46
1:A:426:ILE:HA	1:A:429:LEU:HD23	1.98	0.46
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.15	0.46
1:A:1259:ARG:HH12	1:A:1343:ASP:CG	2.19	0.46
1:B:505:GLY:HA3	1:B:510:ASP:HB2	1.97	0.46
1:B:673:THR:HG21	1:B:707:PHE:O	2.16	0.46
1:A:1131:TRP:CD1	1:A:1266:ILE:HG23	2.51	0.45
1:A:1244:GLY:HA3	1:A:1251:SER:O	2.16	0.45
1:B:13:ASP:OD2	1:B:1472:TYR:OH	2.33	0.45
1:B:149:GLN:HG2	1:B:170:VAL:HG11	1.98	0.45
1:B:917:ASP:O	2:E:2:GLC:O3	2.31	0.45
1:B:870:ILE:HD11	1:B:997:LEU:HD13	1.97	0.45
1:B:1117:ASP:HB3	1:B:1120:ARG:O	2.17	0.45
1:A:1175:SER:HB3	1:A:1176:TYR:H	1.57	0.45
1:A:235:HIS:HB2	1:A:499:CYS:HB3	1.98	0.45
1:A:505:GLY:HA3	1:A:510:ASP:HB2	1.98	0.45
1:A:1254:VAL:HG11	1:A:1416:PHE:HZ	1.82	0.45
1:B:326:LYS:NZ	1:B:329:ASN:HB2	2.32	0.45
1:A:1438:ILE:HA	1:A:1441:TYR:HB3	1.99	0.45
1:B:182:PRO:HG2	1:B:192:PRO:O	2.16	0.45
1:A:905:GLU:OE1	1:A:966:ARG:NH1	2.50	0.45
1:B:1219:VAL:HG22	1:B:1228:ILE:HG22	1.99	0.45
1:A:713:LEU:H	1:A:713:LEU:HD12	1.82	0.45
1:B:1229:HIS:HE1	1:B:1345:TYR:CD2	2.35	0.45
1:A:766:HIS:CE1	1:A:865:THR:HG21	2.50	0.45
1:B:331:LYS:HA	1:B:331:LYS:HD3	1.64	0.45
1:B:1238:THR:OG1	1:B:1259:ARG:HD3	2.17	0.45
1:A:1291:VAL:HG12	1:A:1299:ILE:HB	1.99	0.44
1:A:251:TYR:HB2	1:A:501:LYS:CE	2.47	0.44
1:A:1112:ILE:H	1:A:1130:ALA:HB2	1.82	0.44
1:B:1278:LEU:HD11	1:B:1302:SER:HA	1.99	0.44
1:A:800:THR:HG23	1:A:867:GLN:HA	1.98	0.44
1:B:587:ARG:HG3	1:B:605:HIS:CE1	2.52	0.44
1:B:1351:TYR:O	1:B:1355:GLN:HG3	2.17	0.44
1:B:326:LYS:HE3	1:B:374:ASP:HB3	2.00	0.44
1:B:713:LEU:HD12	1:B:713:LEU:H	1.82	0.44
1:A:357:GLU:HB3	1:A:358:PRO:HD2	2.00	0.44
1:A:452:PHE:CD1	1:A:466:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:TYR:HE2	1:B:491:ARG:HA	1.83	0.44
1:A:1062:ALA:HB3	1:A:1067:PHE:HB3	1.99	0.44
1:B:273:SER:HA	1:B:276:MET:HB2	1.99	0.44
1:B:467:ASN:HB3	1:B:499:CYS:O	2.18	0.44
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.53	0.44
1:B:1405:PRO:HB2	1:B:1496:LYS:HB2	2.00	0.43
1:A:36:PRO:HG2	1:A:44:MET:SD	2.58	0.43
1:B:328:GLY:H	1:B:331:LYS:HE2	1.83	0.43
1:B:252:ASN:HB3	1:B:465:LEU:HD23	1.99	0.43
1:B:375:LYS:HD3	1:B:375:LYS:HA	1.76	0.43
1:A:370:LYS:HD2	1:A:370:LYS:HA	1.40	0.43
1:A:425:ARG:HE	1:A:425:ARG:HB3	1.57	0.43
1:A:467:ASN:HB3	1:A:499:CYS:O	2.18	0.43
1:B:1108:LYS:HG2	1:B:1109:HIS:CD2	2.53	0.43
1:A:1405:PRO:HA	1:A:1428:PRO:HD3	2.01	0.43
1:B:1164:GLU:HB3	1:B:1165:TYR:H	1.54	0.43
1:A:1053:PRO:O	1:A:1120:ARG:NH2	2.50	0.43
1:B:259:LEU:O	1:B:263:ILE:HG13	2.19	0.43
1:B:308:LEU:HD22	1:B:308:LEU:HA	1.78	0.43
1:B:1265:GLU:HG2	1:B:1362:ILE:HD12	2.01	0.43
1:B:1452:CYS:HB3	1:B:1467:LEU:HD22	2.01	0.43
1:B:375:LYS:O	1:B:379:ILE:HG13	2.18	0.43
1:B:800:THR:O	1:B:847:THR:OG1	2.30	0.43
1:A:299:LYS:HE3	1:A:299:LYS:HB3	1.72	0.43
1:A:673:THR:HG21	1:A:707:PHE:O	2.19	0.43
1:A:1061:ALA:HB2	1:A:1073:ARG:CZ	2.49	0.43
1:A:1239:TRP:HE1	1:A:1359:ASN:ND2	2.17	0.43
1:A:1262:ALA:HB1	1:A:1267:ASN:HD21	1.84	0.43
1:B:79:ARG:HA	1:B:79:ARG:HD2	1.90	0.43
1:B:251:TYR:HB2	1:B:501:LYS:CE	2.49	0.43
1:B:1337:ARG:HB2	1:B:1340:ILE:CD1	2.49	0.43
1:A:437:LYS:HA	1:A:437:LYS:HD2	1.50	0.43
1:A:467:ASN:OD1	1:A:467:ASN:N	2.51	0.42
1:A:1122:PRO:HG2	1:A:1124:TYR:CE1	2.54	0.42
1:B:490:ARG:NE	1:B:492:GLU:OE2	2.51	0.42
3:F:1:GLC:H62	3:F:1:GLC:O3	2.19	0.42
1:A:1164:GLU:HB3	1:A:1165:TYR:H	1.68	0.42
1:B:1458:ALA:HB3	1:B:1460:LYS:HE3	2.01	0.42
1:B:1280:LEU:HD12	1:B:1280:LEU:HA	1.88	0.42
1:A:152:VAL:O	1:A:156:MET:HG3	2.20	0.42
1:A:1199:GLU:O	1:A:1202:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:ASP:O	1:B:1120:ARG:HG2	2.19	0.42
1:B:916:TYR:CE2	2:E:2:GLC:H4	2.55	0.42
1:B:1259:ARG:HH12	1:B:1343:ASP:CG	2.23	0.42
4:H:1:GLC:O3	4:H:1:GLC:H61	2.20	0.42
1:B:65:ILE:HB	1:B:85:LYS:HB2	2.00	0.42
1:B:269:LEU:HB3	1:B:448:SER:CB	2.49	0.42
1:A:418:VAL:HG22	1:A:490:ARG:HA	2.00	0.42
1:B:103:VAL:O	1:B:107:TYR:OH	2.20	0.42
1:B:704:ASP:OD1	1:B:704:ASP:N	2.51	0.42
1:B:27:VAL:HG22	1:B:578:GLU:HG3	2.02	0.42
1:B:142:PRO:HG2	1:B:743:ALA:HB1	2.01	0.42
1:B:1061:ALA:HB2	1:B:1073:ARG:CZ	2.50	0.42
1:A:66:TRP:HZ3	1:A:84:LYS:HG2	1.82	0.42
1:A:331:LYS:HA	1:A:331:LYS:HD3	1.77	0.42
1:A:900:ARG:NH2	1:A:904:GLU:O	2.47	0.42
1:B:1192:ALA:HB1	1:B:1223:TRP:HZ2	1.85	0.42
1:A:161:LYS:HD2	1:A:161:LYS:HA	1.69	0.41
1:A:1459:LYS:HA	1:A:1459:LYS:HD2	1.53	0.41
1:B:238:ASN:OD1	1:B:239:ASN:ND2	2.46	0.41
1:A:765:PHE:HE2	1:A:767:ARG:HB2	1.84	0.41
1:A:1133:PHE:CZ	1:A:1137:ILE:HD11	2.55	0.41
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.55	0.41
1:B:35:LEU:HD12	1:B:35:LEU:H	1.85	0.41
1:B:1157:ARG:HG2	1:B:1159:PHE:O	2.21	0.41
1:A:311:PHE:CE2	1:A:366:ARG:HD3	2.55	0.41
1:A:1460:LYS:HB3	1:A:1460:LYS:HE3	1.84	0.41
1:A:1493:LEU:HB3	1:A:1504:SER:HB2	2.03	0.41
1:B:213:ALA:HA	1:B:528:ILE:HG23	2.02	0.41
1:A:66:TRP:CZ3	1:B:1458:ALA:HB2	2.55	0.41
1:A:1158:ARG:HG3	1:A:1173:ALA:HB1	2.02	0.41
1:A:1337:ARG:HD2	1:A:1340:ILE:HD11	2.02	0.41
1:B:188:GLU:H	1:B:239:ASN:HD21	1.68	0.41
1:B:834:THR:HG22	1:B:835:GLY:H	1.86	0.41
1:B:427:LYS:HB3	1:B:427:LYS:HE3	1.76	0.41
1:B:1489:GLY:HA3	1:B:1507:THR:HG23	2.01	0.41
1:B:1493:LEU:HB3	1:B:1504:SER:HB2	2.03	0.41
1:A:831:ARG:NH1	1:A:854:ASP:OD2	2.44	0.41
1:A:1117:ASP:O	1:A:1120:ARG:HG2	2.21	0.41
1:B:235:HIS:HB2	1:B:499:CYS:HB3	2.03	0.41
1:B:264:GLU:O	1:B:268:LYS:HB2	2.20	0.41
1:B:738:MET:HB3	1:B:776:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ALA:HB2	1:A:703:TYR:HE2	1.86	0.41
1:A:402:ASP:HA	1:A:405:LEU:HG	2.03	0.41
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.53	0.41
1:A:1280:LEU:HB3	1:A:1286:PHE:HB2	2.02	0.41
1:A:1417:ALA:O	1:A:1423:ASN:ND2	2.53	0.41
1:A:1439:ARG:HD2	1:A:1521:ASP:OD2	2.21	0.41
1:B:323:LEU:O	1:B:327:TRP:HB2	2.21	0.41
1:B:1151:LEU:HA	1:B:1180:ILE:HB	2.02	0.41
1:B:1260:ASP:OD1	1:B:1260:ASP:N	2.53	0.41
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	2.21	0.41
1:A:338:ILE:HG12	1:A:350:PHE:CZ	2.56	0.41
1:B:675:ASN:HB2	1:B:680:VAL:HG12	2.02	0.41
1:B:1432:TRP:CG	1:B:1510:TRP:CD1	3.10	0.41
1:A:263:ILE:HD13	1:A:464:ALA:HB3	2.02	0.40
1:A:430:ARG:HH12	1:A:445:LEU:HD13	1.87	0.40
1:A:1204:PRO:HB2	1:A:1208:ARG:NH1	2.36	0.40
1:B:310:GLU:HB2	1:B:366:ARG:HD2	2.03	0.40
1:B:315:ASP:O	1:B:319:THR:OG1	2.39	0.40
1:A:757:HIS:HB3	1:A:764:THR:HB	2.02	0.40
1:A:1157:ARG:HG2	1:A:1176:TYR:OH	2.21	0.40
1:A:1334:ILE:H	1:A:1334:ILE:HG13	1.69	0.40
1:B:1312:PHE:CG	1:B:1370:LEU:HD13	2.56	0.40
1:A:281:TYR:H	1:A:282:PRO:CD	2.34	0.40
1:B:1084:ARG:NH2	1:B:1521:ASP:OD1	2.54	0.40
1:A:160:ILE:HG12	1:A:205:VAL:CG1	2.51	0.40
1:B:19:THR:HA	1:B:656:THR:HG23	2.03	0.40
1:B:251:TYR:CE2	1:B:503:ARG:HG3	2.57	0.40
1:A:251:TYR:HB2	1:A:501:LYS:NZ	2.37	0.40
1:A:452:PHE:CE1	1:A:466:ALA:HB2	2.56	0.40
1:A:908:TYR:CE2	1:A:1047:LYS:HE2	2.57	0.40
1:A:1157:ARG:HG2	1:A:1176:TYR:CZ	2.56	0.40
1:B:953:LEU:HB2	1:B:999:PRO:HG3	2.04	0.40
1:B:1270:LEU:HD23	1:B:1308:LEU:HD11	2.03	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%)	1416 (93%)	97 (6%)	11 (1%)	22	61
1	B	1524/1536 (99%)	1405 (92%)	105 (7%)	14 (1%)	17	56
All	All	3048/3072 (99%)	2821 (93%)	202 (7%)	25 (1%)	19	58

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	TYR
1	A	1167	PRO
1	B	282	PRO
1	B	437	LYS
1	A	436	PRO
1	A	432	ASP
1	A	900	ARG
1	A	1296	GLY
1	B	280	GLY
1	B	330	SER
1	B	900	ARG
1	B	1163	ASP
1	B	1164	GLU
1	B	1410	GLY
1	A	332	SER
1	A	1164	GLU
1	B	1296	GLY
1	A	706	VAL
1	B	440	PRO
1	B	501	LYS
1	A	1159	PHE
1	B	1155	VAL
1	B	706	VAL
1	A	431	ILE
1	B	283	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%)	1247 (93%)	96 (7%)	14	47
1	B	1343/1353 (99%)	1228 (91%)	115 (9%)	10	38
All	All	2686/2706 (99%)	2475 (92%)	211 (8%)	12	43

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	185	HIS
1	A	229	THR
1	A	268	LYS
1	A	271	ASP
1	A	277	GLU
1	A	283	VAL
1	A	287	THR
1	A	288	VAL
1	A	290	ASP
1	A	294	VAL
1	A	299	LYS
1	A	300	GLU
1	A	308	LEU
1	A	319	THR
1	A	330	SER
1	A	332	SER
1	A	333	TRP
1	A	334	SER
1	A	337	ASN
1	A	341	LYS
1	A	342	ASP
1	A	344	SER
1	A	374	ASP
1	A	421	GLN
1	A	423	PHE
1	A	425	ARG

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Mol	Chain	Res	Type
1	A	429	LEU
1	A	434	HIS
1	A	437	LYS
1	A	443	LYS
1	A	447	LEU
1	A	449	GLU
1	A	467	ASN
1	A	498	ASP
1	A	543	HIS
1	A	612	SER
1	A	616	VAL
1	A	631	GLU
1	A	664	PHE
1	A	704	ASP
1	A	721	SER
1	A	742	ILE
1	A	751	ASP
1	A	754	MET
1	A	761	GLN
1	A	764	THR
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	1082	SER
1	A	1157	ARG
1	A	1158	ARG
1	A	1161	LEU
1	A	1162	ASP
1	A	1166	ILE
1	A	1172	LYS
1	A	1175	SER
1	A	1177	SER
1	A	1179	THR
1	A	1195	ILE
1	A	1199	GLU
1	A	1213	GLU
1	A	1216	ASN
1	A	1218	GLU
1	A	1219	VAL

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Mol	Chain	Res	Type
1	A	1252	VAL
1	A	1265	GLU
1	A	1287	LYS
1	A	1289	THR
1	A	1291	VAL
1	A	1293	LYS
1	A	1295	ASP
1	A	1298	LYS
1	A	1300	SER
1	A	1320	LYS
1	A	1321	ASN
1	A	1322	LYS
1	A	1323	GLU
1	A	1330	ILE
1	A	1334	ILE
1	A	1335	ILE
1	A	1338	ARG
1	A	1349	LYS
1	A	1356	PHE
1	A	1401	TYR
1	A	1408	ASN
1	A	1414	ASP
1	A	1424	TYR
1	A	1442	HIS
1	A	1454	VAL
1	A	1459	LYS
1	A	1460	LYS
1	B	229	THR
1	B	270	LEU
1	B	274	GLU
1	B	276	MET
1	B	277	GLU
1	B	279	LEU
1	B	283	VAL
1	B	286	LYS
1	B	287	THR
1	B	290	ASP
1	B	293	LYS
1	B	294	VAL
1	B	306	LEU
1	B	308	LEU
1	B	316	VAL

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Mol	Chain	Res	Type
1	B	319	THR
1	B	325	GLU
1	B	330	SER
1	B	333	TRP
1	B	335	ASP
1	B	336	ASP
1	B	341	LYS
1	B	342	ASP
1	B	344	SER
1	B	349	GLN
1	B	371	ILE
1	B	373	ILE
1	B	374	ASP
1	B	383	LEU
1	B	384	HIS
1	B	385	SER
1	B	409	LYS
1	B	415	ILE
1	B	417	GLU
1	B	419	LEU
1	B	421	GLN
1	B	423	PHE
1	B	425	ARG
1	B	441	ILE
1	B	442	THR
1	B	443	LYS
1	B	444	LYS
1	B	447	LEU
1	B	454	ARG
1	B	467	ASN
1	B	498	ASP
1	B	500	VAL
1	B	543	HIS
1	B	583	SER
1	B	585	LEU
1	B	612	SER
1	B	616	VAL
1	B	631	GLU
1	B	664	PHE
1	B	704	ASP
1	B	709	GLN
1	B	742	ILE

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Mol	Chain	Res	Type
1	B	751	ASP
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	1105	LYS
1	B	1116	LEU
1	B	1156	THR
1	B	1157	ARG
1	B	1158	ARG
1	B	1161	LEU
1	B	1162	ASP
1	B	1164	GLU
1	B	1165	TYR
1	B	1166	ILE
1	B	1169	ASP
1	B	1170	ASP
1	B	1172	LYS
1	B	1190	ARG
1	B	1195	ILE
1	B	1198	ARG
1	B	1211	LYS
1	B	1218	GLU
1	B	1228	ILE
1	B	1233	GLN
1	B	1236	CYS
1	B	1243	MET
1	B	1245	GLU
1	B	1247	GLU
1	B	1248	LYS
1	B	1264	VAL
1	B	1282	LYS
1	B	1283	ASP
1	B	1287	LYS
1	B	1289	THR

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Mol	Chain	Res	Type
1	B	1291	VAL
1	B	1293	LYS
1	B	1295	ASP
1	B	1300	SER
1	B	1321	ASN
1	B	1325	ASP
1	B	1330	ILE
1	B	1334	ILE
1	B	1347	SER
1	B	1356	PHE
1	B	1361	THR
1	B	1414	ASP
1	B	1422	ARG
1	B	1424	TYR
1	B	1442	HIS
1	B	1527	GLU

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

Mol	Chain	Res	Type
1	A	766	HIS
1	A	1066	HIS
1	A	1279	GLN
1	A	1359	ASN
1	A	1423	ASN
1	B	1138	GLN
1	B	1229	HIS
1	B	1359	ASN

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 ⓘ

19 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	0.66	0	17,17,17	0.83	1 (5%)
2	GLC	C	2	2	11,11,12	0.52	0	15,15,17	0.90	0
2	GLC	D	1	2	12,12,12	0.65	0	17,17,17	0.85	0
2	GLC	D	2	2	11,11,12	0.84	0	15,15,17	1.12	2 (13%)
2	GLC	E	1	2	12,12,12	0.65	0	17,17,17	0.68	0
2	GLC	E	2	2	11,11,12	0.54	0	15,15,17	0.85	0
3	GLC	F	1	3	12,12,12	1.12	1 (8%)	17,17,17	0.94	1 (5%)
3	GLC	F	2	3	11,11,12	1.25	1 (9%)	15,15,17	1.37	2 (13%)
3	GLC	F	3	3	11,11,12	0.63	0	15,15,17	1.06	0
4	GLC	G	1	4	12,12,12	0.96	1 (8%)	17,17,17	1.19	2 (11%)
4	GLC	G	2	4	11,11,12	0.73	0	15,15,17	1.57	4 (26%)
4	GLC	G	3	4	11,11,12	0.73	0	15,15,17	2.40	3 (20%)
4	GLC	G	4	4	11,11,12	1.14	1 (9%)	15,15,17	1.44	3 (20%)
4	GLC	G	5	4	11,11,12	0.62	0	15,15,17	1.48	4 (26%)
4	GLC	H	1	4	12,12,12	0.86	0	17,17,17	0.91	1 (5%)
4	GLC	H	2	4	11,11,12	0.88	1 (9%)	15,15,17	1.58	2 (13%)
4	GLC	H	3	4	11,11,12	1.03	1 (9%)	15,15,17	1.60	3 (20%)
4	GLC	H	4	4	11,11,12	0.75	0	15,15,17	1.10	1 (6%)
4	GLC	H	5	4	11,11,12	0.62	0	15,15,17	1.20	1 (6%)

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	-	1/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	1/2/19/22	0/1/1/1
2	GLC	E	1	2	-	1/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	2	2	-	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	-	0/2/19/22	0/1/1/1
3	GLC	F	3	3	-	1/2/19/22	0/1/1/1
4	GLC	G	1	4	-	0/2/22/22	0/1/1/1
4	GLC	G	2	4	-	0/2/19/22	0/1/1/1
4	GLC	G	3	4	-	0/2/19/22	0/1/1/1
4	GLC	G	4	4	-	1/2/19/22	0/1/1/1
4	GLC	G	5	4	-	0/2/19/22	0/1/1/1
4	GLC	H	1	4	-	0/2/22/22	0/1/1/1
4	GLC	H	2	4	-	1/2/19/22	0/1/1/1
4	GLC	H	3	4	-	0/2/19/22	0/1/1/1
4	GLC	H	4	4	-	1/2/19/22	0/1/1/1
4	GLC	H	5	4	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	3	GLC	C4-C5	2.97	1.59	1.53
4	G	4	GLC	O4-C4	2.80	1.49	1.43
3	F	2	GLC	O4-C4	2.35	1.48	1.43
4	H	2	GLC	O4-C4	2.19	1.48	1.43
3	F	1	GLC	O4-C4	2.15	1.48	1.43
4	G	1	GLC	O4-C4	2.15	1.48	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	GLC	C1-O5-C5	6.37	120.82	112.19
4	G	3	GLC	O5-C1-C2	-5.42	102.40	110.77
4	H	2	GLC	O4-C4-C3	3.85	119.26	110.35
4	H	5	GLC	O5-C5-C6	3.74	113.07	107.20
4	G	2	GLC	O4-C4-C3	3.70	118.91	110.35
4	G	4	GLC	O4-C4-C3	3.55	118.55	110.35
4	G	5	GLC	C2-C3-C4	-2.88	105.91	110.89
3	F	1	GLC	O3-C3-C4	2.77	116.76	110.35
4	H	3	GLC	O5-C5-C6	2.77	111.55	107.20
4	H	3	GLC	O4-C4-C3	-2.72	104.06	110.35
4	G	5	GLC	O5-C5-C4	-2.70	104.27	110.83
4	H	2	GLC	O5-C1-C2	-2.68	106.64	110.77
4	H	3	GLC	O4-C4-C5	2.68	115.94	109.30
4	G	2	GLC	C2-C3-C4	-2.63	106.34	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	C2-C3-C4	-2.54	106.51	110.89
2	D	2	GLC	O5-C5-C6	2.48	111.10	107.20
3	F	2	GLC	O5-C1-C2	-2.48	106.94	110.77
4	G	1	GLC	C3-C4-C5	-2.46	105.85	110.24
4	H	4	GLC	O4-C4-C3	-2.44	104.71	110.35
4	G	1	GLC	C6-C5-C4	-2.41	107.37	113.00
4	G	3	GLC	O2-C2-C1	2.33	113.93	109.15
4	H	1	GLC	O3-C3-C4	2.30	115.68	110.35
4	G	5	GLC	C1-C2-C3	-2.26	106.89	109.67
4	G	2	GLC	C6-C5-C4	-2.21	107.84	113.00
4	G	5	GLC	C3-C4-C5	2.18	114.13	110.24
2	D	2	GLC	C6-C5-C4	-2.12	108.03	113.00
4	G	4	GLC	O3-C3-C4	2.12	115.25	110.35
4	G	4	GLC	C6-C5-C4	-2.06	108.19	113.00
4	G	2	GLC	O5-C5-C6	-2.05	103.99	107.20
2	C	1	GLC	O5-C5-C6	-2.04	101.36	106.44

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 11 short contacts:

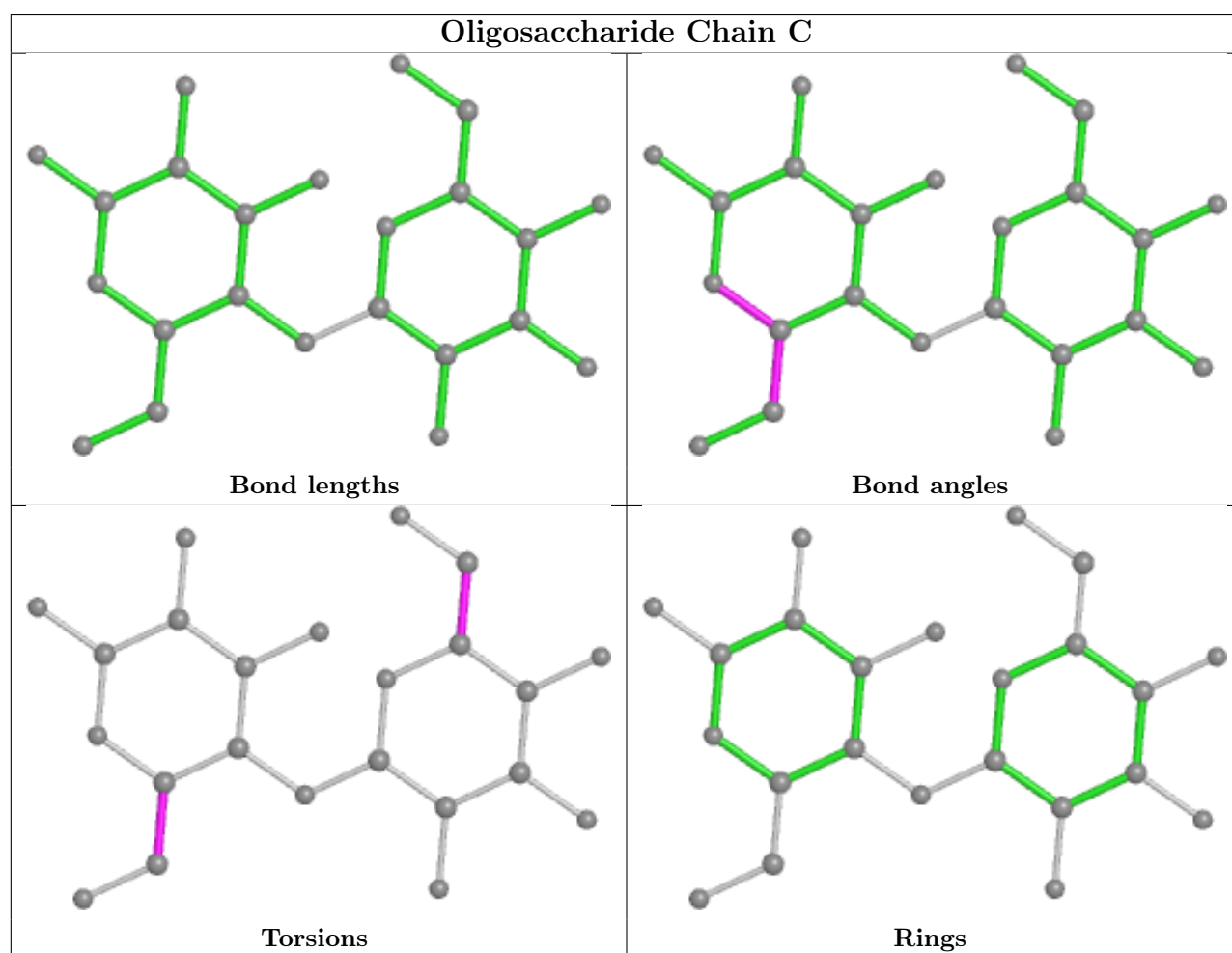
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	GLC	1	0
3	F	3	GLC	1	0

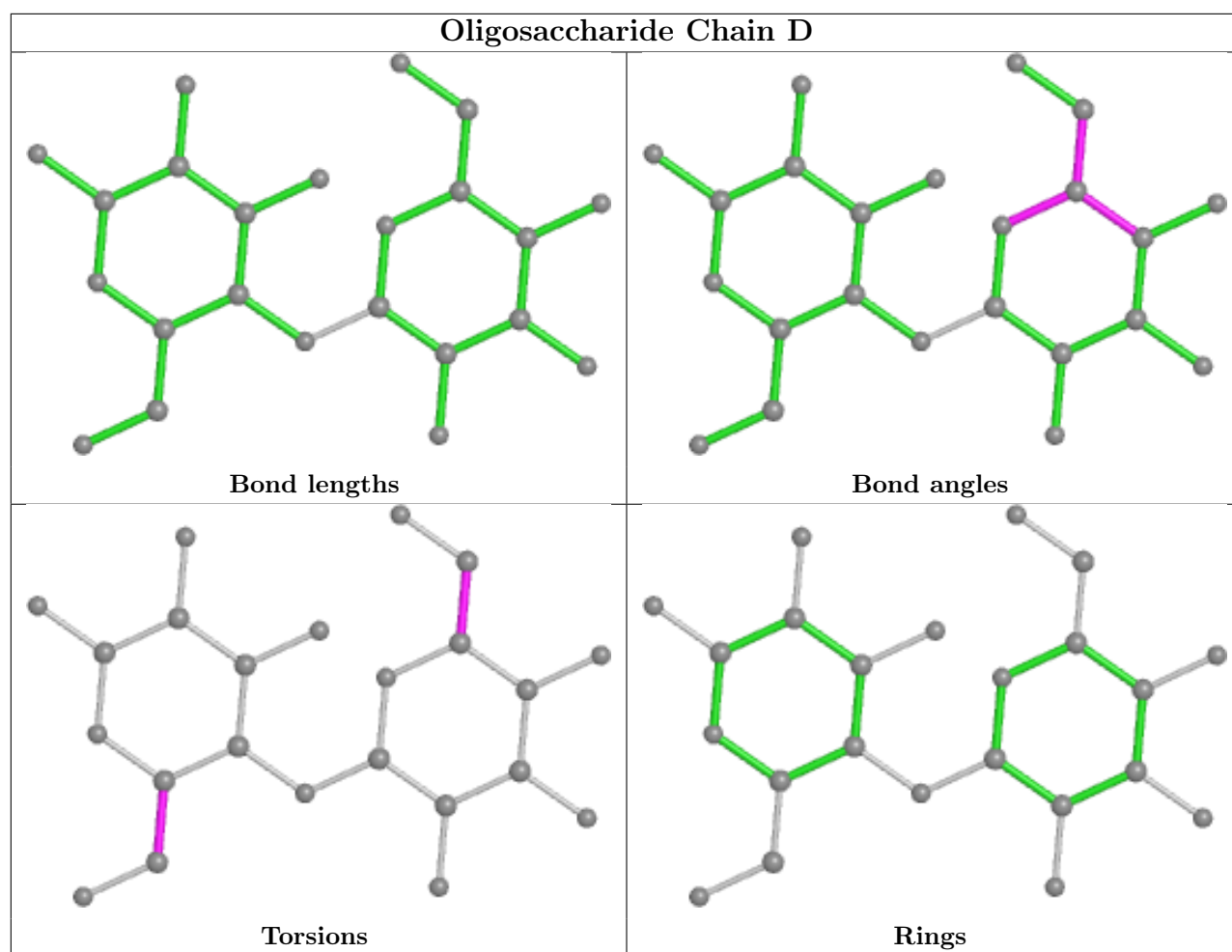
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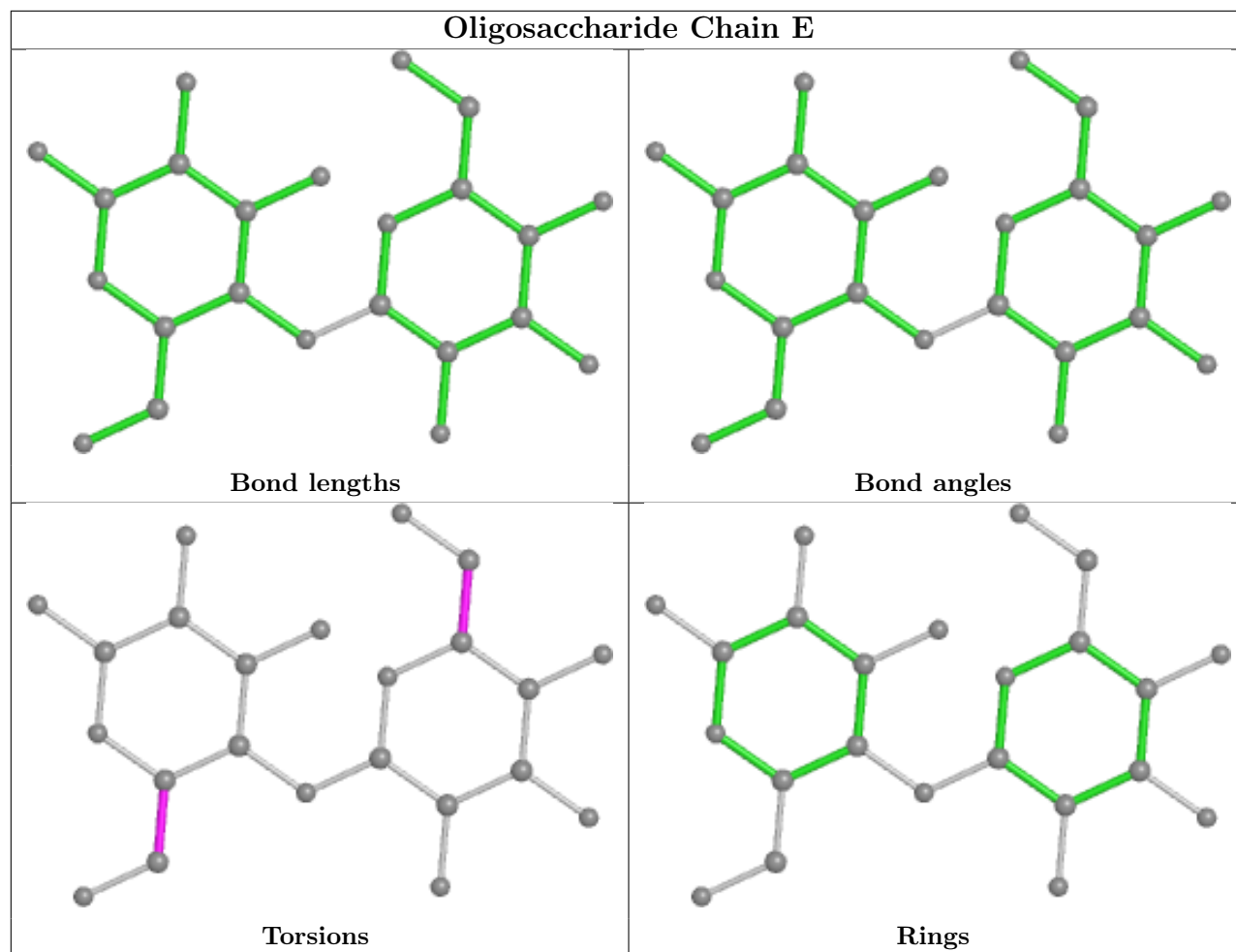
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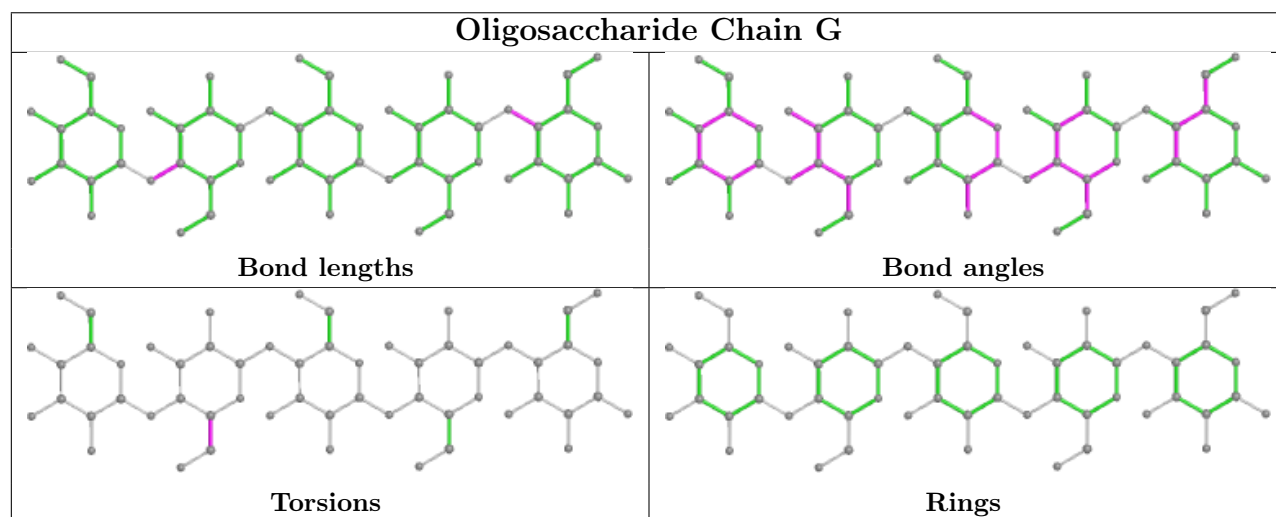
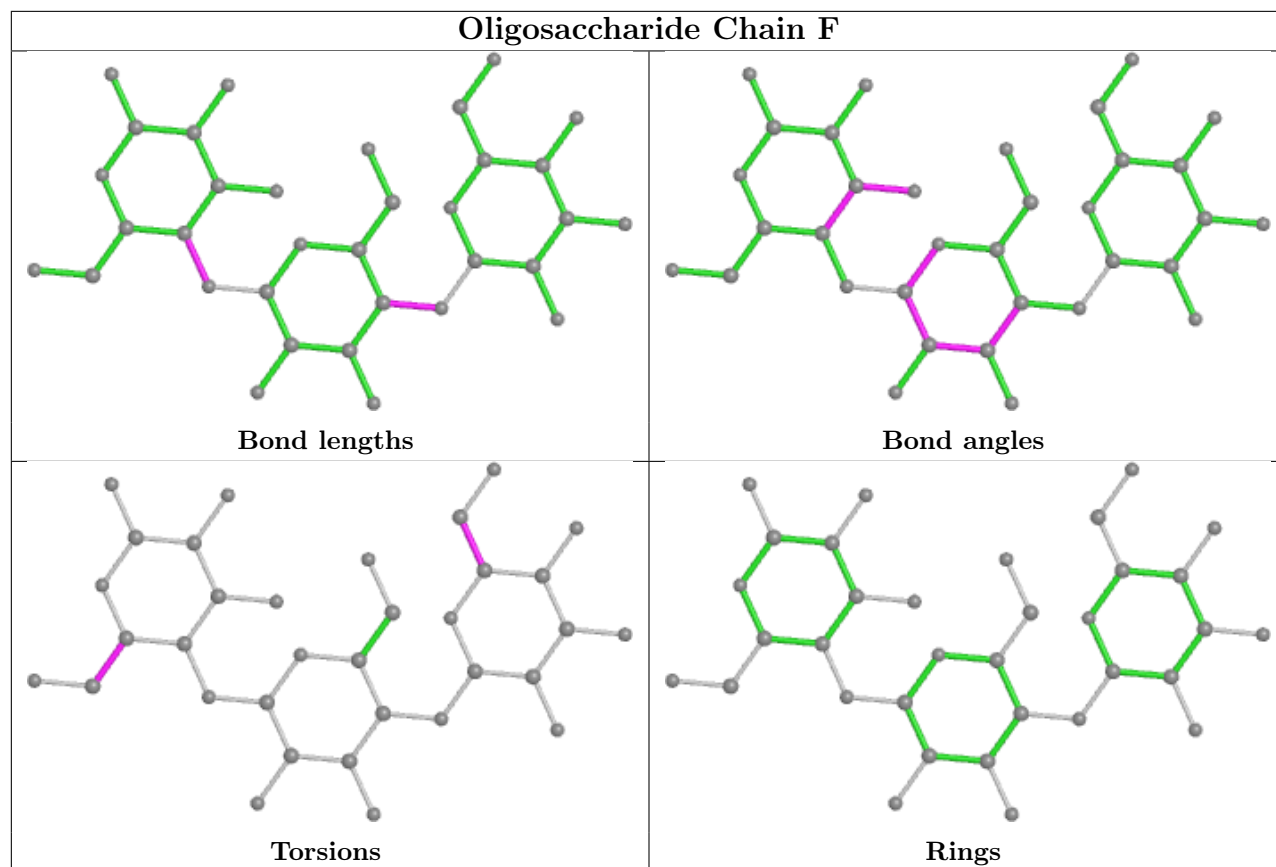
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	4	GLC	1	0
4	H	2	GLC	1	0
4	G	3	GLC	1	0
4	G	1	GLC	2	0
2	E	2	GLC	2	0
4	H	3	GLC	2	0
3	F	1	GLC	1	0
4	G	2	GLC	1	0

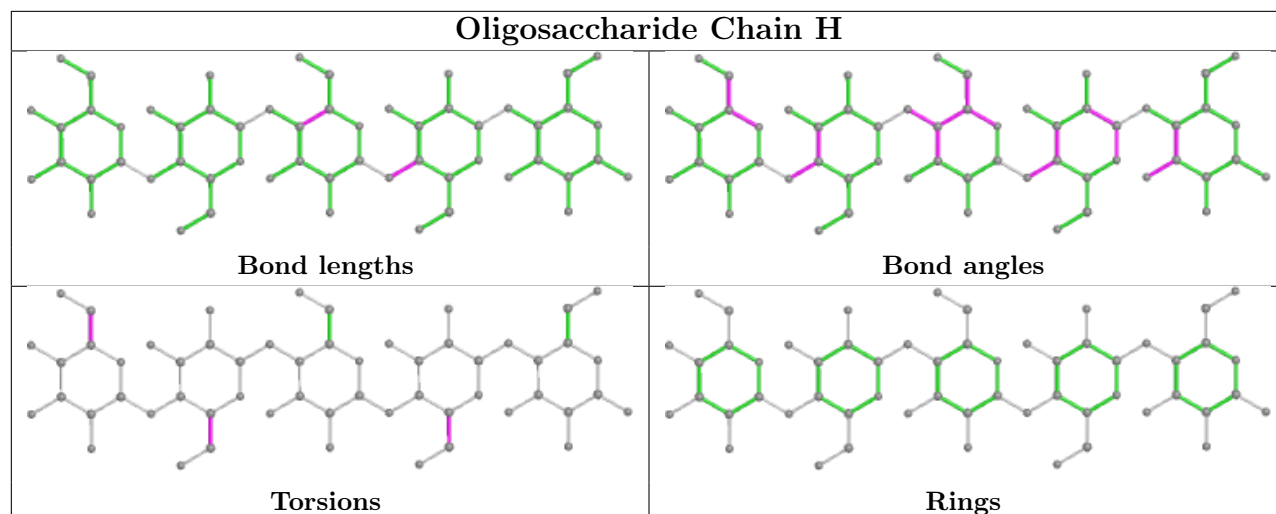
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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

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%)	0.14	57 (3%)	41	26	67, 108, 149, 173	0
1	B	1526/1536 (99%)	0.18	53 (3%)	44	28	66, 109, 169, 213	0
All	All	3052/3072 (99%)	0.16	110 (3%)	42	27	66, 109, 160, 213	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1165	TYR	5.8
1	B	1511	SER	4.7
1	A	1354	TYR	4.5
1	B	309	TRP	4.4
1	A	1457	SER	4.3
1	B	289	ASP	4.2
1	A	1238	THR	4.1
1	B	1238	THR	3.9
1	A	1241	ASP	3.9
1	B	444	LYS	3.8
1	A	1423	ASN	3.8
1	B	1412	ASP	3.5
1	A	281	TYR	3.5
1	B	379	ILE	3.4
1	A	1237	GLY	3.3
1	B	1354	TYR	3.3
1	B	1078	ASP	3.3
1	A	38	GLY	3.2
1	B	1334	ILE	3.2
1	A	1240	MET	3.2
1	A	593	TRP	3.1
1	B	1209	VAL	3.1
1	B	1128	ASP	3.0
1	B	1433	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	377	ALA	3.0
1	B	636	TYR	3.0
1	B	288	VAL	3.0
1	B	376	PHE	2.9
1	A	389	ASN	2.9
1	A	1078	ASP	2.9
1	A	1128	ASP	2.9
1	B	241	GLN	2.9
1	B	1510	TRP	2.9
1	B	593	TRP	2.9
1	B	341	LYS	2.9
1	B	1458	ALA	2.8
1	B	1236	CYS	2.8
1	A	376	PHE	2.7
1	B	1204	PRO	2.7
1	B	1239	TRP	2.7
1	A	1511	SER	2.7
1	B	287	THR	2.7
1	A	1236	CYS	2.7
1	A	241	GLN	2.7
1	B	1514	CYS	2.6
1	B	1080	PHE	2.6
1	A	1165	TYR	2.6
1	B	1237	GLY	2.6
1	A	1359	ASN	2.6
1	A	1321	ASN	2.6
1	B	1259	ARG	2.6
1	A	1239	TRP	2.6
1	B	1075	TRP	2.6
1	A	455	PHE	2.6
1	A	1456	GLY	2.6
1	B	1432	TRP	2.6
1	A	1234	PHE	2.5
1	A	1460	LYS	2.5
1	B	1512	THR	2.5
1	B	1401	TYR	2.5
1	A	1199	GLU	2.5
1	A	348	ALA	2.5
1	B	330	SER	2.4
1	A	1338	ARG	2.4
1	B	281	TYR	2.4
1	A	347	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	394	GLU	2.4
1	A	354	ASN	2.4
1	B	1513	GLY	2.4
1	A	535	ASP	2.3
1	A	1458	ALA	2.3
1	B	285	LEU	2.3
1	A	434	HIS	2.3
1	B	1180	ILE	2.3
1	A	912	ARG	2.3
1	A	1433	CYS	2.3
1	A	1485	SER	2.3
1	A	1077	ARG	2.3
1	B	1240	MET	2.3
1	B	1509	ALA	2.3
1	A	1455	GLU	2.2
1	B	399	ILE	2.2
1	B	1321	ASN	2.2
1	A	1510	TRP	2.2
1	A	1343	ASP	2.2
1	B	371	ILE	2.2
1	B	1071	TYR	2.2
1	A	1257	THR	2.2
1	A	260	ILE	2.2
1	A	1246	SER	2.2
1	B	1082	SER	2.2
1	A	1412	ASP	2.2
1	A	1065	PRO	2.2
1	A	1259	ARG	2.1
1	B	1267	ASN	2.1
1	A	1263	ALA	2.1
1	A	1242	LYS	2.1
1	A	1528	GLU	2.1
1	A	351	VAL	2.1
1	A	1122	PRO	2.0
1	A	325	GLU	2.0
1	B	403	ILE	2.0
1	A	568	GLY	2.0
1	A	1432	TRP	2.0
1	B	1261	GLY	2.0
1	B	44	MET	2.0
1	B	1528	GLU	2.0
1	B	1160	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	745	GLU	2.0
1	A	380	LEU	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](#)

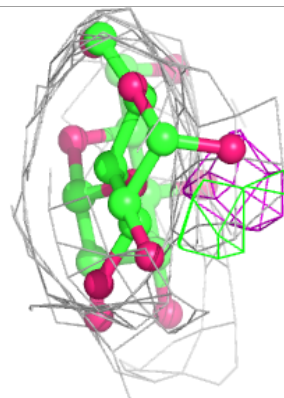
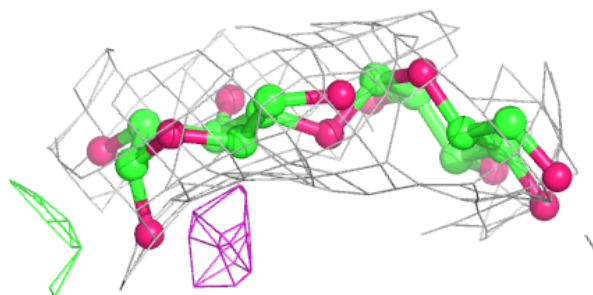
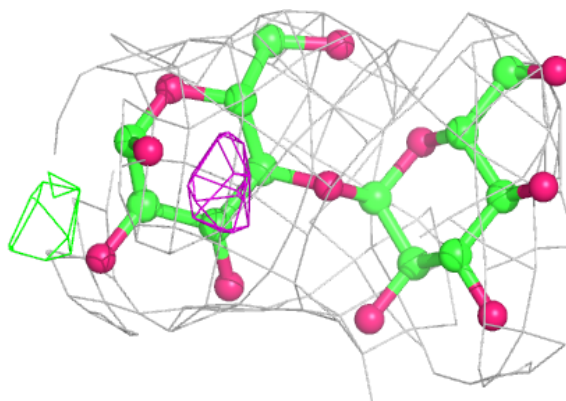
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	1	12/12	0.73	0.26	132,136,139,141	0
2	GLC	D	2	11/12	0.75	0.17	133,139,143,144	0
2	GLC	E	1	12/12	0.76	0.33	107,110,112,112	0
2	GLC	E	2	11/12	0.77	0.28	99,105,107,108	0
2	GLC	D	1	12/12	0.78	0.24	147,154,155,155	0
3	GLC	F	1	12/12	0.78	0.29	117,123,125,125	0
4	GLC	H	5	11/12	0.78	0.28	146,147,148,149	0
4	GLC	G	2	11/12	0.80	0.32	120,122,123,124	0
4	GLC	G	5	11/12	0.81	0.23	120,122,123,123	0
4	GLC	H	3	11/12	0.82	0.21	131,132,135,138	0
2	GLC	C	2	11/12	0.82	0.30	138,140,141,141	0
4	GLC	H	1	12/12	0.86	0.24	116,124,127,128	0
4	GLC	G	3	11/12	0.88	0.26	117,119,120,122	0
3	GLC	F	2	11/12	0.89	0.17	99,106,109,111	0
4	GLC	H	4	11/12	0.89	0.24	142,145,147,148	0
4	GLC	H	2	11/12	0.89	0.20	127,130,133,134	0
3	GLC	F	3	11/12	0.90	0.15	92,96,97,98	0
4	GLC	G	4	11/12	0.90	0.20	123,125,128,128	0
4	GLC	G	1	12/12	0.91	0.23	117,122,123,125	0

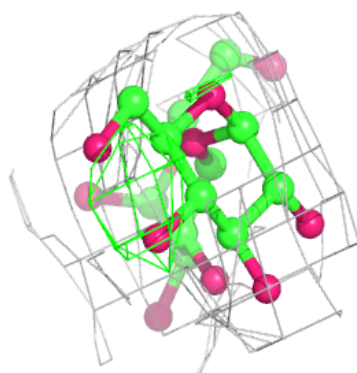
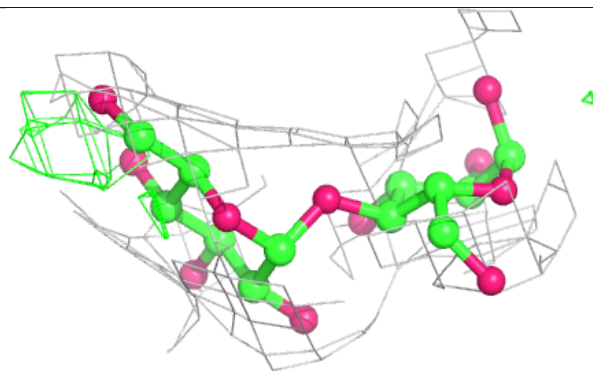
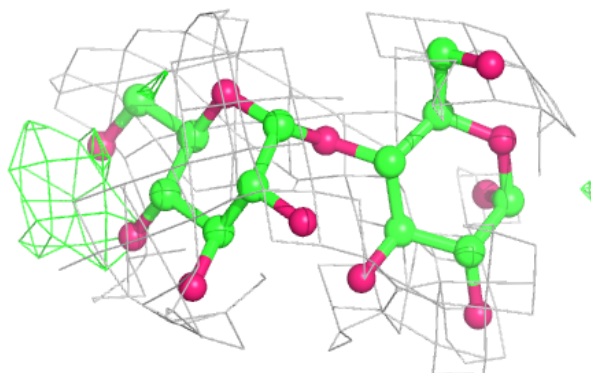
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

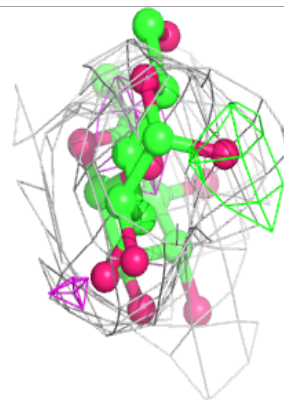
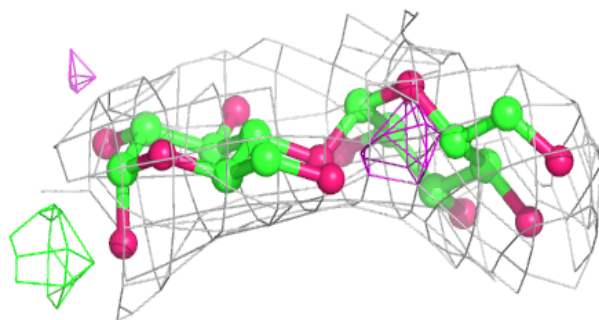
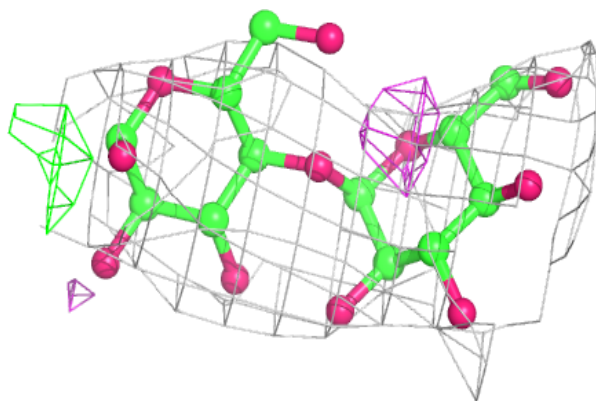
**Electron density around Chain D:**

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

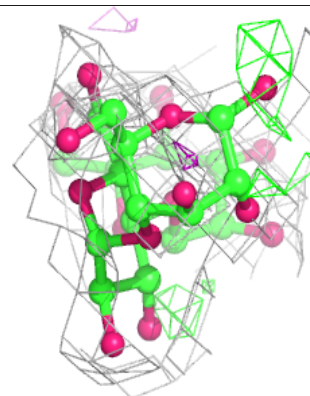
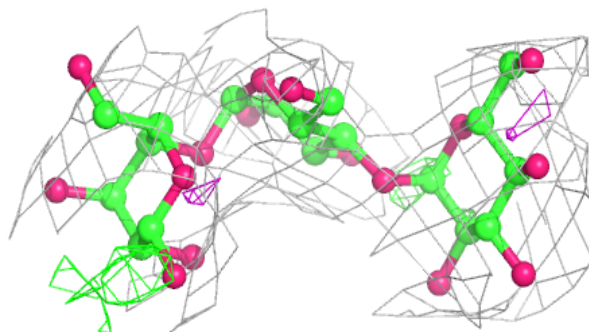
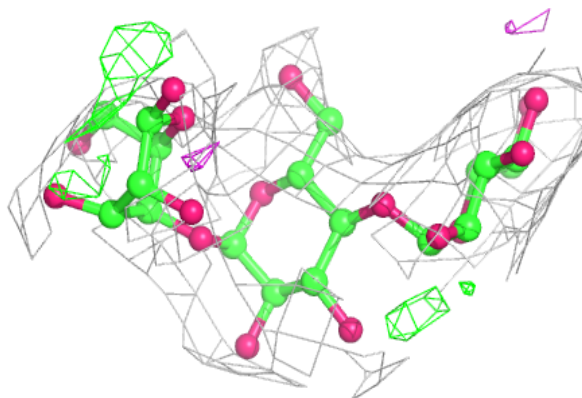


Electron density around Chain E:

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

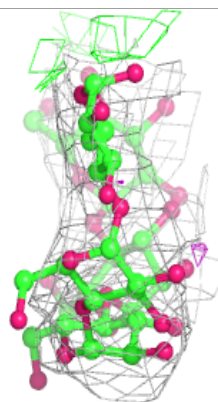
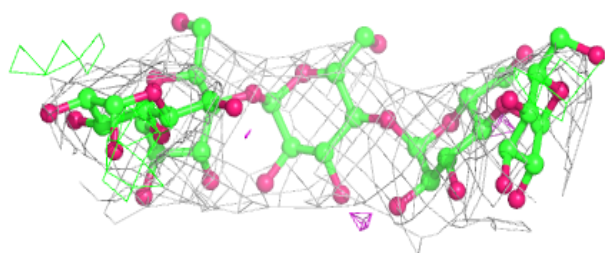
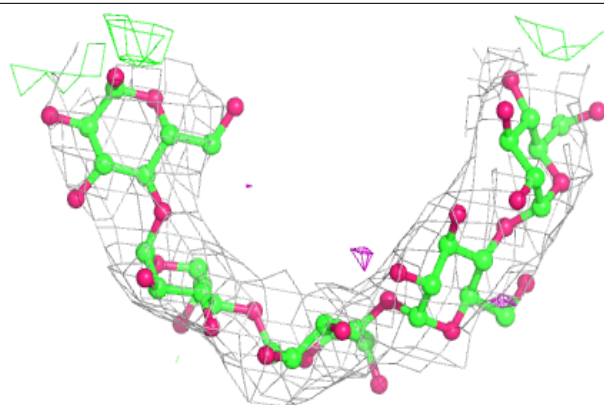
**Electron density around Chain F:**

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

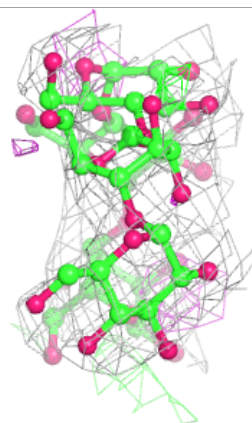
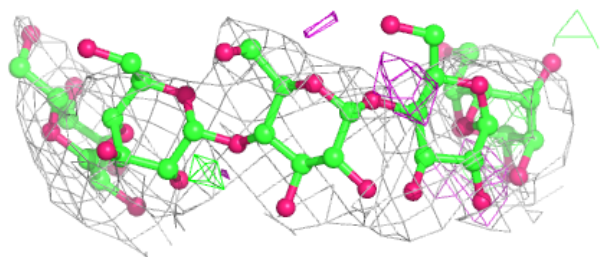
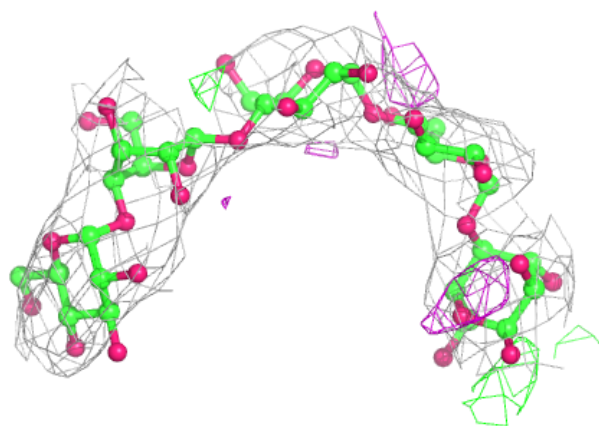


Electron density around Chain G:

$2mF_o-DF_c$ (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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.