



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:51 AM UTC

PDB ID : 7EJP / pdb_00007ejp
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (W470A) in complex with maltohexaose
Authors : Shen, M.; Xiang, S.
Deposited on : 2021-04-02
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

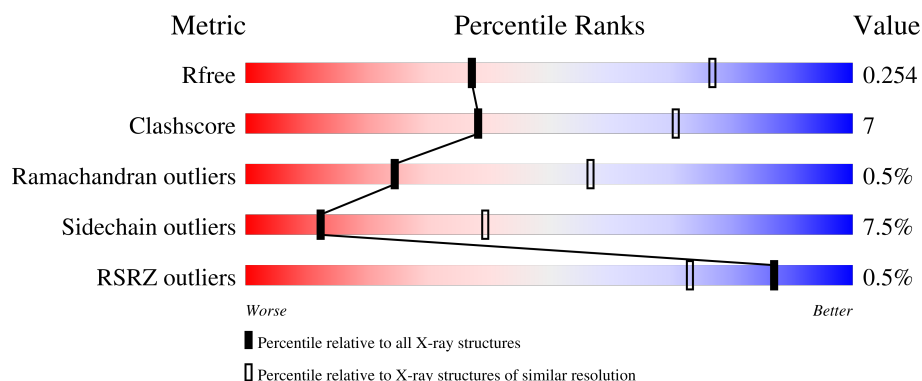
1 Overall quality at a glance

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.



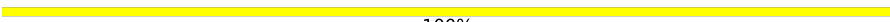
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	76% 21% ..
1	B	1536	% 78% 20% ..
2	C	2	100%
2	D	2	100%
3	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	F	3	 100%
4	G	5	 100%
4	H	5	 40% 60%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24762 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:

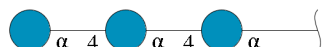
Chain	Residue	Modelled	Actual	Comment	Reference
A	470	ALA	TRP	engineered mutation	UNP Q6FSK0
A	1529	LEU	-	expression tag	UNP Q6FSK0
A	1530	GLU	-	expression tag	UNP Q6FSK0
A	1531	HIS	-	expression tag	UNP Q6FSK0
A	1532	HIS	-	expression tag	UNP Q6FSK0
A	1533	HIS	-	expression tag	UNP Q6FSK0
A	1534	HIS	-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



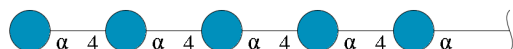
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- 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	E	3	Total	C	O	0	0	0
			33	18	15			
3	F	3	Total	C	O	0	0	0
			33	18	15			

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

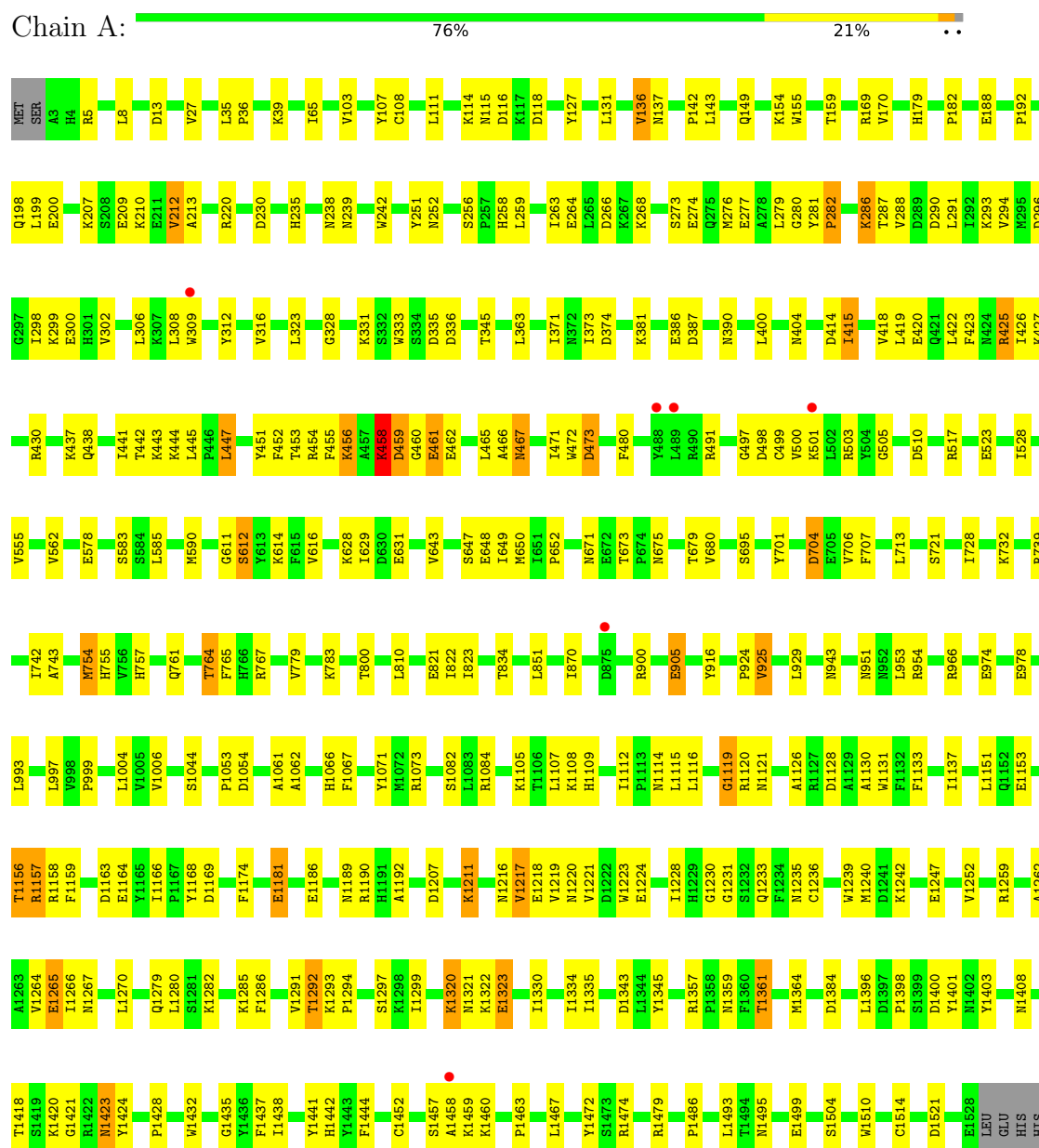


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	5	Total	C	O	0	0	0
			56	30	26			
4	H	5	Total	C	O	0	0	0
			56	30	26			

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.

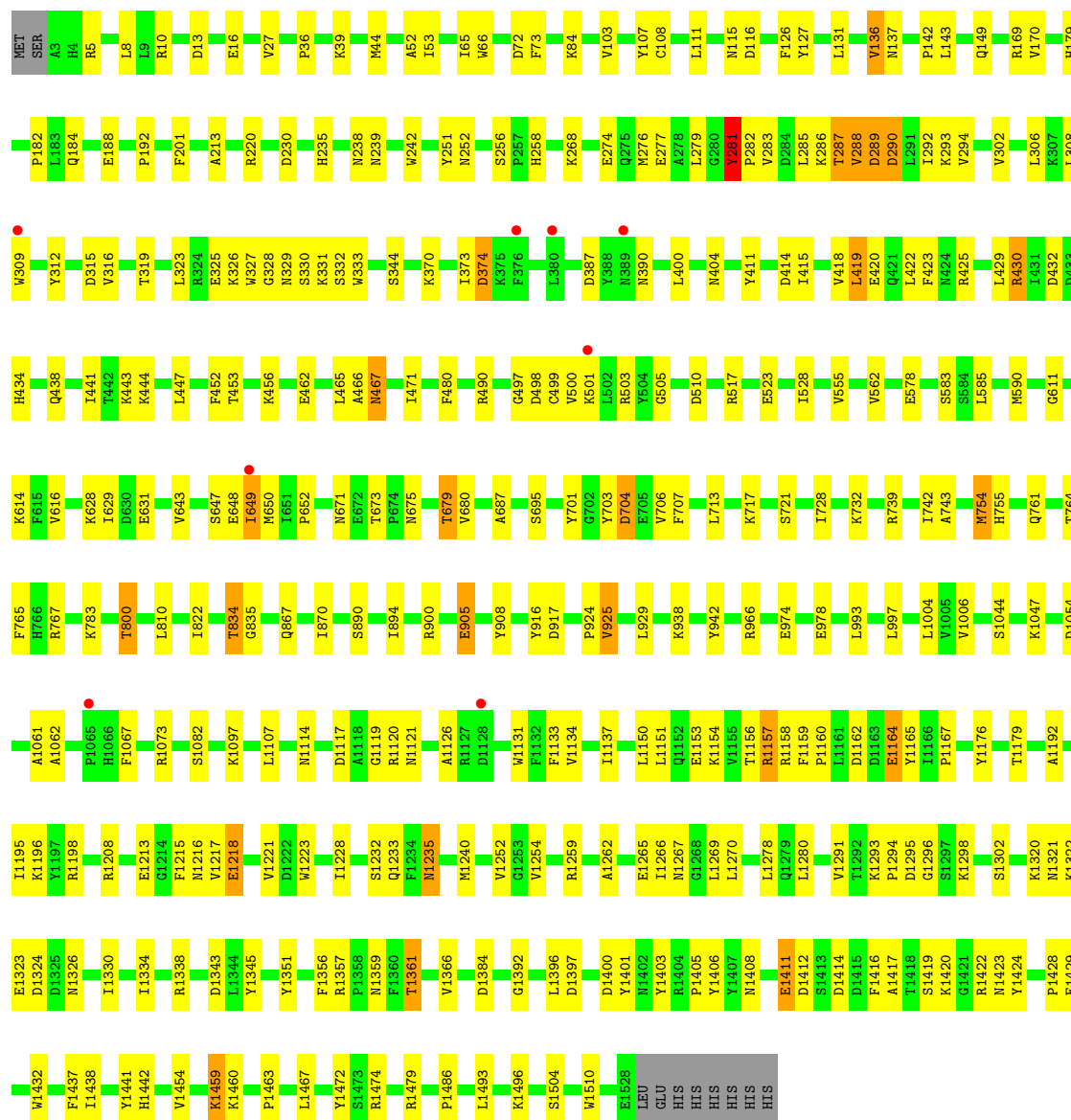
- Molecule 1: 4-alpha-glucanotransferase



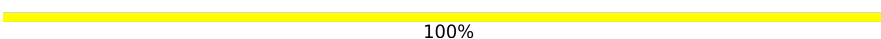
HIS
HIS
HIS
HIS

• Molecule 1: 4-alpha-glucanotransferase

Chain B:  78% 20% ..



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

Chain C:  100%

GLC1
GLC2

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

Chain D:  100%

GLC1
GLC2

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

Chain E:  67% 33%

GLC1
GLC2
GLC3

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

Chain F:  100%

GLC1
GLC2
GLC3

- 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

Chain G:  100%

GLC1
GLC2
GLC3
GLC4
GLC5

- 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

Chain H:  40% 60%

GLC1
GLC2
GLC3
GLC4
GLC5

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.54Å 199.83Å 133.88Å 90.00° 100.78° 90.00°	Depositor
Resolution (Å)	38.44 – 3.10 38.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.44-3.10) 99.8 (38.44-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.236 , 0.256 0.235 , 0.254	Depositor DCC
R_{free} test set	3844 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24762	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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	0.12	0/12578	0.33	0/17055
1	B	0.12	0/12578	0.33	0/17055
All	All	0.12	0/25156	0.33	0/34110

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12269	0	11955	167	0
1	B	12269	0	11955	167	0
2	C	23	0	21	1	0
2	D	23	0	21	3	0
3	E	33	0	28	1	0
3	F	33	0	28	4	0
4	G	56	0	48	0	0
4	H	56	0	48	2	0
All	All	24762	0	24104	339	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 (339) 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:458:LYS:O	1:A:460:GLY:N	2.13	0.81
1:B:182:PRO:HD3	1:B:230:ASP:HB2	1.64	0.80
1:A:182:PRO:HD3	1:A:230:ASP:HB2	1.66	0.78
1:A:169:ARG:NH1	1:A:721:SER:O	2.17	0.77
1:B:1107:LEU:O	1:B:1157:ARG:NH1	2.19	0.76
1:A:452:PHE:HA	1:A:466:ALA:HA	1.66	0.76
1:B:1361:THR:HG21	1:B:1437:PHE:HA	1.66	0.76
1:B:466:ALA:H	1:B:501:LYS:HD2	1.52	0.75
1:A:331:LYS:HB3	1:A:381:LYS:HD2	1.68	0.74
1:A:286:LYS:HD3	1:A:438:GLN:HE22	1.53	0.73
1:B:8:LEU:HB2	1:B:652:PRO:HG2	1.69	0.73
1:A:266:ASP:HB3	1:A:454:ARG:HH22	1.54	0.73
1:A:466:ALA:H	1:A:501:LYS:HD2	1.54	0.73
1:A:8:LEU:HB2	1:A:652:PRO:HG2	1.73	0.71
1:A:1221:VAL:HG22	1:A:1228:ILE:HG12	1.71	0.71
1:A:1361:THR:HG21	1:A:1437:PHE:HA	1.71	0.71
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.73	0.69
1:B:169:ARG:NH1	1:B:721:SER:O	2.25	0.69
1:B:1384:ASP:OD1	1:B:1474:ARG:NH1	2.26	0.69
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.27	0.68
1:B:1221:VAL:HG22	1:B:1228:ILE:HG12	1.76	0.68
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.27	0.68
1:A:1053:PRO:HB2	1:A:1168:TYR:HE1	1.59	0.67
1:B:242:TRP:CG	1:B:517:ARG:HH12	2.14	0.66
1:A:400:LEU:O	1:A:404:ASN:ND2	2.30	0.64
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.78	0.64
1:A:1384:ASP:OD1	1:A:1474:ARG:NH1	2.31	0.63
3:F:1:GLC:H5	3:F:2:GLC:H2	1.79	0.63
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.81	0.63
1:B:695:SER:O	1:B:739:ARG:NH2	2.29	0.63
1:B:1262:ALA:HB1	1:B:1267:ASN:HD21	1.64	0.63
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.32	0.62
1:B:456:LYS:HG3	1:B:462:GLU:HG2	1.82	0.62
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.33	0.61
1:B:179:HIS:NE2	1:B:230:ASP:OD1	2.32	0.61
1:A:453:THR:N	1:A:465:LEU:O	2.33	0.61
1:B:929:LEU:HD22	1:B:1006:VAL:HG13	1.82	0.61
1:A:238:ASN:ND2	1:A:497:GLY:O	2.34	0.61
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.83	0.60
1:A:131:LEU:HD13	1:A:143:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:MET:HE1	1:B:1357:ARG:HD3	1.83	0.60
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.83	0.60
1:B:400:LEU:O	1:B:404:ASN:ND2	2.35	0.60
1:B:1293:LYS:HD2	1:B:1294:PRO:HD2	1.83	0.59
1:A:282:PRO:HG3	1:A:293:LYS:HB2	1.84	0.59
1:B:115:ASN:OD1	1:B:116:ASP:N	2.35	0.59
1:B:1196:LYS:HD2	1:B:1218:GLU:HG2	1.85	0.59
1:A:13:ASP:OD2	1:A:1479:ARG:NH2	2.26	0.59
1:A:312:TYR:HE1	1:A:363:LEU:HD21	1.68	0.59
1:B:452:PHE:HA	1:B:466:ALA:HA	1.85	0.58
1:B:590:MET:HB2	1:B:671:ASN:HD22	1.66	0.58
1:A:728:ILE:HD11	1:A:810:LEU:HD22	1.85	0.58
1:A:115:ASN:OD1	1:A:116:ASP:N	2.36	0.58
1:B:27:VAL:HG22	1:B:578:GLU:HG3	1.85	0.58
1:B:268:LYS:HG3	1:B:302:VAL:HG12	1.86	0.58
3:F:2:GLC:H4	3:F:3:GLC:O2	2.04	0.58
1:A:1458:ALA:HB3	1:A:1460:LYS:HE3	1.86	0.57
1:A:1105:LYS:HE2	1:A:1156:THR:H	1.68	0.57
1:B:142:PRO:HG2	1:B:743:ALA:HB1	1.86	0.57
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.86	0.57
1:B:374:ASP:OD1	1:B:374:ASP:N	2.19	0.57
1:B:306:LEU:HD13	1:B:309:TRP:HZ2	1.68	0.56
1:A:328:GLY:H	1:A:331:LYS:HE2	1.69	0.56
1:A:242:TRP:CG	1:A:517:ARG:HH12	2.24	0.56
1:B:1405:PRO:HB2	1:B:1496:LYS:HB2	1.87	0.56
1:B:1441:TYR:OH	1:B:1474:ARG:NH2	2.40	0.55
1:A:306:LEU:HD13	1:A:309:TRP:HZ2	1.70	0.55
1:A:466:ALA:HB3	1:A:501:LYS:HE3	1.88	0.55
1:B:870:ILE:HD11	1:B:997:LEU:HD13	1.89	0.55
1:A:188:GLU:H	1:A:239:ASN:HD21	1.53	0.55
1:B:315:ASP:O	1:B:319:THR:OG1	2.22	0.55
1:A:695:SER:O	1:A:739:ARG:NH2	2.33	0.55
1:A:721:SER:HA	1:A:822:ILE:HD11	1.88	0.55
1:B:306:LEU:HD13	1:B:309:TRP:CZ2	2.42	0.55
1:B:1165:TYR:C	1:B:1167:PRO:HD3	2.32	0.55
1:A:590:MET:HB2	1:A:671:ASN:HD22	1.71	0.54
1:B:328:GLY:H	1:B:331:LYS:HE2	1.72	0.54
1:A:430:ARG:HB3	1:A:438:GLN:HG3	1.88	0.54
1:B:1228:ILE:HG13	1:B:1270:LEU:HD22	1.89	0.54
1:B:238:ASN:ND2	1:B:497:GLY:O	2.40	0.54
1:A:721:SER:OG	1:A:823:ILE:O	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:TYR:O	1:A:924:PRO:HD2	2.07	0.53
1:B:429:LEU:HG	1:B:430:ARG:HD3	1.90	0.53
1:B:13:ASP:OD2	1:B:1472:TYR:OH	2.26	0.53
1:A:611:GLY:HA2	1:A:997:LEU:HD23	1.90	0.53
1:A:36:PRO:HB2	1:A:39:LYS:HG3	1.89	0.53
1:B:188:GLU:H	1:B:239:ASN:HD21	1.55	0.53
1:B:453:THR:N	1:B:465:LEU:O	2.38	0.53
1:A:870:ILE:HG12	1:A:993:LEU:HD22	1.91	0.53
1:B:1160:PRO:HG2	1:B:1164:GLU:HG3	1.89	0.53
1:A:452:PHE:CD1	1:A:466:ALA:HB2	2.43	0.52
1:B:5:ARG:HA	1:B:643:VAL:HG12	1.90	0.52
1:A:1053:PRO:HB3	1:A:1119:GLY:HA3	1.90	0.52
1:B:13:ASP:OD2	1:B:1479:ARG:NH2	2.26	0.52
1:B:131:LEU:HD13	1:B:143:LEU:HD13	1.90	0.52
1:B:1097:LYS:HG3	1:B:1150:LEU:HD13	1.91	0.52
1:A:466:ALA:HB3	1:A:501:LYS:CE	2.40	0.52
1:B:53:ILE:HD11	1:B:65:ILE:HD11	1.91	0.52
1:A:209:GLU:HG2	1:A:528:ILE:HD11	1.92	0.52
1:A:1228:ILE:H	1:A:1267:ASN:ND2	2.07	0.52
1:B:36:PRO:HB2	1:B:39:LYS:HG3	1.92	0.52
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.91	0.52
1:A:13:ASP:OD2	1:A:1472:TYR:OH	2.28	0.52
1:B:721:SER:HA	1:B:822:ILE:HD11	1.91	0.51
1:B:925:VAL:HG21	1:B:1486:PRO:HB2	1.92	0.51
1:B:1411:GLU:HB3	1:B:1419:SER:HA	1.93	0.51
1:A:1259:ARG:NH1	1:A:1343:ASP:OD2	2.43	0.51
1:B:252:ASN:HB3	1:B:465:LEU:HD23	1.93	0.51
1:B:1396:LEU:HD21	1:B:1400:ASP:HB3	1.92	0.51
1:A:757:HIS:HB3	1:A:764:THR:HB	1.92	0.51
1:B:938:LYS:HE2	1:B:942:TYR:HE2	1.74	0.51
1:A:306:LEU:HD13	1:A:309:TRP:CZ2	2.45	0.51
1:A:1293:LYS:HB2	1:A:1294:PRO:HD2	1.93	0.51
1:B:387:ASP:HB3	1:B:390:ASN:OD1	2.11	0.51
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.92	0.50
1:A:951:ASN:OD1	1:A:954:ARG:NH2	2.43	0.50
1:B:289:ASP:O	1:B:293:LYS:HD2	2.10	0.50
1:A:136:VAL:HG13	1:A:137:ASN:H	1.76	0.50
1:A:1186:GLU:O	1:A:1190:ARG:HB2	2.12	0.50
1:A:1435:GLY:HA3	1:A:1514:CYS:HB3	1.93	0.50
1:A:5:ARG:HA	1:A:643:VAL:HG12	1.93	0.50
1:B:466:ALA:HB3	1:B:501:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:HB3	1:A:465:LEU:HD23	1.92	0.50
1:B:103:VAL:O	1:B:107:TYR:OH	2.23	0.50
1:A:27:VAL:HG22	1:A:578:GLU:HG3	1.94	0.49
1:B:136:VAL:HG13	1:B:137:ASN:H	1.76	0.49
1:A:458:LYS:C	1:A:460:GLY:H	2.21	0.49
1:A:614:LYS:HB2	1:A:1004:LEU:HD13	1.94	0.49
1:A:1239:TRP:HE1	1:A:1359:ASN:HD21	1.61	0.49
1:A:198:GLN:HG2	1:A:517:ARG:HH21	1.77	0.49
1:B:1192:ALA:HB1	1:B:1223:TRP:HZ2	1.78	0.49
1:B:916:TYR:O	1:B:924:PRO:HD2	2.13	0.49
1:A:456:LYS:H	1:A:456:LYS:HD2	1.78	0.49
1:A:925:VAL:HG21	1:A:1486:PRO:HB2	1.93	0.49
1:B:647:SER:OG	1:B:648:GLU:N	2.46	0.49
1:B:1351:TYR:HB2	2:D:1:GLC:O1	2.13	0.49
1:B:1259:ARG:HH12	1:B:1343:ASP:CG	2.20	0.49
1:B:1432:TRP:CG	1:B:1510:TRP:HD1	2.31	0.49
1:A:1131:TRP:CD1	1:A:1266:ILE:HG23	2.48	0.49
1:B:256:SER:HB2	1:B:258:HIS:CE1	2.48	0.49
1:B:1278:LEU:HD11	1:B:1302:SER:HA	1.95	0.49
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.48	0.49
1:A:754:MET:HG2	1:A:755:HIS:N	2.27	0.48
1:B:800:THR:HG23	1:B:867:GLN:HA	1.95	0.48
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.94	0.48
1:B:611:GLY:HA2	1:B:997:LEU:HD23	1.96	0.48
1:B:916:TYR:CE2	3:F:3:GLC:H2	2.48	0.48
2:D:1:GLC:O6	2:D:2:GLC:O5	2.22	0.48
1:A:870:ILE:HD11	1:A:997:LEU:HD13	1.95	0.48
1:A:929:LEU:HD22	1:A:1006:VAL:HG13	1.95	0.48
1:A:425:ARG:HH22	1:A:491:ARG:HB3	1.78	0.48
1:A:1181:GLU:HG2	1:A:1286:PHE:CD1	2.49	0.48
1:B:1295:ASP:OD1	1:B:1296:GLY:N	2.46	0.48
1:B:182:PRO:HG2	1:B:192:PRO:O	2.14	0.48
1:B:213:ALA:HA	1:B:528:ILE:HG23	1.95	0.48
1:B:452:PHE:CD1	1:B:466:ALA:HB2	2.47	0.48
1:B:1356:PHE:HB3	1:B:1397:ASP:HB2	1.96	0.48
1:A:1054:ASP:OD1	1:A:1054:ASP:N	2.43	0.48
1:B:1417:ALA:O	1:B:1422:ARG:HB2	2.13	0.48
1:A:1240:MET:HE1	1:A:1357:ARG:HD3	1.94	0.47
1:A:268:LYS:HG3	1:A:302:VAL:HG12	1.96	0.47
1:B:754:MET:HG2	1:B:755:HIS:N	2.29	0.47
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:ARG:HH12	1:A:1343:ASP:CG	2.23	0.47
1:A:256:SER:HB2	1:A:258:HIS:CE1	2.49	0.47
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.15	0.47
1:B:1320:LYS:HA	1:B:1338:ARG:HB2	1.97	0.47
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.14	0.47
1:A:1323:GLU:H	1:A:1323:GLU:HG3	1.45	0.47
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.49	0.47
1:B:418:VAL:HG22	1:B:490:ARG:HA	1.97	0.47
1:B:1198:ARG:HE	1:B:1215:PHE:HB2	1.79	0.47
1:A:387:ASP:HB3	1:A:390:ASN:OD1	2.15	0.46
1:A:679:THR:OG1	1:A:783:LYS:HG2	2.15	0.46
1:A:298:ILE:HD13	1:A:422:LEU:HD13	1.98	0.46
1:B:917:ASP:O	3:F:3:GLC:O2	2.32	0.46
1:A:114:LYS:NZ	1:A:118:ASP:OD1	2.49	0.46
1:B:466:ALA:HB3	1:B:501:LYS:CE	2.46	0.46
1:B:467:ASN:OD1	1:B:467:ASN:N	2.48	0.46
1:B:614:LYS:HB2	1:B:1004:LEU:HD13	1.97	0.46
1:A:213:ALA:HA	1:A:528:ILE:HG23	1.97	0.46
1:A:1219:VAL:HG22	1:A:1230:GLY:HA3	1.97	0.46
1:A:1259:ARG:NH2	1:A:1265:GLU:OE2	2.49	0.46
1:A:647:SER:OG	1:A:648:GLU:N	2.47	0.46
1:B:1493:LEU:HB3	1:B:1504:SER:HB2	1.98	0.46
1:B:235:HIS:HB2	1:B:499:CYS:HB3	1.98	0.46
4:H:2:GLC:H61	4:H:3:GLC:O5	2.16	0.46
1:A:1438:ILE:HA	1:A:1441:TYR:HB3	1.98	0.45
1:B:467:ASN:HB3	1:B:499:CYS:O	2.16	0.45
1:A:1108:LYS:HE2	1:A:1109:HIS:CE1	2.51	0.45
1:A:472:TRP:HD1	1:A:473:ASP:OD1	2.00	0.45
1:A:612:SER:OG	1:A:943:ASN:ND2	2.49	0.45
1:B:66:TRP:CZ3	1:B:84:LYS:HG2	2.51	0.45
1:B:72:ASP:OD1	1:B:73:PHE:N	2.45	0.45
1:B:679:THR:OG1	1:B:783:LYS:HG2	2.17	0.45
1:A:182:PRO:HG2	1:A:192:PRO:O	2.17	0.45
1:A:451:TYR:HE2	1:A:491:ARG:HA	1.81	0.45
1:A:1428:PRO:HB3	1:A:1493:LEU:HD21	1.98	0.45
1:B:287:THR:HB	1:B:290:ASP:H	1.82	0.45
1:B:905:GLU:OE1	1:B:966:ARG:NH1	2.49	0.45
1:B:1232:SER:H	1:B:1235:ASN:HB2	1.82	0.45
1:B:713:LEU:HD12	1:B:713:LEU:H	1.81	0.45
1:B:1351:TYR:HB2	2:D:1:GLC:HO1	1.81	0.45
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:ALA:HB3	1:A:1067:PHE:HB3	1.99	0.45
1:B:765:PHE:HE2	1:B:767:ARG:HB2	1.82	0.45
1:B:1151:LEU:HD11	1:B:1280:LEU:HD21	1.99	0.45
1:A:381:LYS:HD3	1:A:386:GLU:HG2	2.00	0.44
1:A:425:ARG:HE	1:A:425:ARG:HB3	1.50	0.44
1:A:471:ILE:HD11	1:A:480:PHE:HB3	1.98	0.44
1:A:713:LEU:H	1:A:713:LEU:HD12	1.82	0.44
1:B:370:LYS:HD2	1:B:370:LYS:HA	1.50	0.44
1:A:1071:TYR:HB2	1:A:1115:LEU:HD11	1.99	0.44
1:B:149:GLN:HG2	1:B:170:VAL:HG11	2.00	0.44
1:B:323:LEU:HD23	1:B:373:ILE:HG23	1.98	0.44
1:B:505:GLY:HA3	1:B:510:ASP:HB2	1.98	0.44
1:A:1192:ALA:HB1	1:A:1223:TRP:HZ2	1.81	0.44
1:A:1280:LEU:HB3	1:A:1286:PHE:HB2	1.99	0.44
1:B:1061:ALA:HB2	1:B:1073:ARG:CZ	2.48	0.44
1:B:1254:VAL:HG11	1:B:1416:PHE:HZ	1.82	0.44
1:A:1432:TRP:CG	1:A:1510:TRP:HD1	2.35	0.44
1:B:870:ILE:HG12	1:B:993:LEU:HD22	1.99	0.44
1:A:1066:HIS:CD2	4:H:1:GLC:H1	2.53	0.44
1:A:1420:LYS:HA	1:A:1420:LYS:HD3	1.87	0.44
1:A:505:GLY:HA3	1:A:510:ASP:HB2	2.00	0.44
1:A:953:LEU:HD13	1:A:999:PRO:HA	2.00	0.44
1:A:1457:SER:O	1:A:1460:LYS:HG2	2.18	0.44
1:B:1131:TRP:CD1	1:B:1266:ILE:HG23	2.53	0.44
1:B:1438:ILE:HA	1:B:1441:TYR:HB3	2.00	0.44
1:B:1459:LYS:HD2	1:B:1459:LYS:HA	1.65	0.44
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.53	0.43
1:A:1495:ASN:HB2	1:A:1499:GLU:HB3	1.99	0.43
1:A:212:VAL:HG22	1:A:528:ILE:HD13	2.00	0.43
1:A:673:THR:HG21	1:A:707:PHE:O	2.18	0.43
1:A:1151:LEU:HD11	1:A:1280:LEU:HD21	1.99	0.43
1:A:1418:THR:HA	1:A:1423:ASN:HD21	1.83	0.43
1:B:281:TYR:HD2	1:B:282:PRO:HD3	1.83	0.43
1:B:471:ILE:HD11	1:B:480:PHE:HB3	1.99	0.43
1:B:1062:ALA:HB3	1:B:1067:PHE:HB3	1.99	0.43
1:B:1240:MET:HE3	1:B:1359:ASN:HD21	1.82	0.43
1:B:288:VAL:O	1:B:292:ILE:HG13	2.18	0.43
1:B:523:GLU:HB2	1:B:555:VAL:HG21	2.00	0.43
1:B:282:PRO:HG2	1:B:294:VAL:HG23	2.00	0.43
1:A:142:PRO:HG2	1:A:743:ALA:HB1	1.99	0.43
1:A:420:GLU:HA	1:A:423:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:TYR:HD2	1:B:411:TYR:HB2	1.83	0.43
1:A:103:VAL:O	1:A:107:TYR:OH	2.21	0.43
1:B:10:ARG:HA	1:B:52:ALA:HB3	2.00	0.43
1:B:251:TYR:HB2	1:B:501:LYS:NZ	2.34	0.43
1:B:704:ASP:OD1	1:B:704:ASP:N	2.50	0.43
1:B:649:ILE:H	1:B:649:ILE:HG13	1.47	0.43
1:B:242:TRP:NE1	1:B:517:ARG:HH22	2.17	0.43
1:B:1160:PRO:HA	1:B:1176:TYR:HE2	1.84	0.43
1:A:235:HIS:HB2	1:A:499:CYS:HB3	2.01	0.42
1:A:296:ASP:O	1:A:300:GLU:HG2	2.19	0.42
1:A:415:ILE:HD13	1:A:415:ILE:HA	1.94	0.42
1:A:1112:ILE:H	1:A:1130:ALA:HB2	1.84	0.42
1:B:1324:ASP:C	1:B:1326:ASN:H	2.27	0.42
1:B:1460:LYS:HB3	1:B:1460:LYS:HE3	1.77	0.42
1:A:273:SER:HB2	1:A:447:LEU:HD23	2.00	0.42
1:A:1320:LYS:HB3	1:A:1320:LYS:HE2	1.77	0.42
1:A:414:ASP:O	1:A:418:VAL:HG23	2.20	0.42
1:B:717:LYS:HD3	1:B:717:LYS:HA	1.90	0.42
1:B:1164:GLU:HB3	1:B:1165:TYR:H	1.55	0.42
1:A:312:TYR:CE1	1:A:363:LEU:HD21	2.52	0.42
1:A:323:LEU:HD23	1:A:373:ILE:HG23	2.01	0.42
1:A:1228:ILE:HG13	1:A:1270:LEU:HD22	2.01	0.42
1:B:430:ARG:HD2	1:B:430:ARG:HA	1.58	0.42
1:A:675:ASN:HB2	1:A:680:VAL:HG12	2.01	0.42
1:A:779:VAL:HG11	1:A:851:LEU:HD11	2.01	0.42
1:A:1452:CYS:HB3	1:A:1467:LEU:HD22	2.01	0.42
1:B:323:LEU:O	1:B:327:TRP:HB2	2.19	0.42
1:A:1158:ARG:HA	1:A:1158:ARG:HD3	1.74	0.42
1:B:430:ARG:O	1:B:438:GLN:HB2	2.18	0.42
1:A:523:GLU:HB2	1:A:555:VAL:HG21	2.01	0.42
1:A:905:GLU:OE1	1:A:966:ARG:NH1	2.53	0.42
1:B:1392:GLY:C	1:B:1429:GLU:HB3	2.44	0.42
1:B:1403:TYR:CZ	1:B:1405:PRO:HB3	2.55	0.42
1:B:251:TYR:CE2	1:B:503:ARG:HG3	2.55	0.42
1:B:687:ALA:HB2	1:B:703:TYR:HE2	1.85	0.42
1:B:1054:ASP:OD1	1:B:1054:ASP:N	2.45	0.42
1:A:1061:ALA:HB2	1:A:1073:ARG:CZ	2.50	0.41
1:A:1242:LYS:HE3	1:A:1421:GLY:O	2.20	0.41
1:A:1280:LEU:HG	1:A:1285:LYS:HB2	2.02	0.41
1:B:1117:ASP:C	1:B:1119:GLY:H	2.28	0.41
1:B:1420:LYS:HA	1:B:1420:LYS:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1131:TRP:HA	1:B:1134:VAL:HG12	2.03	0.41
1:B:1196:LYS:HD2	1:B:1196:LYS:HA	1.65	0.41
1:A:455:PHE:HE1	1:A:465:LEU:HG	1.85	0.41
1:B:628:LYS:O	1:B:650:MET:HB2	2.20	0.41
1:B:675:ASN:HB2	1:B:680:VAL:HG12	2.01	0.41
1:A:1189:ASN:HD21	1:A:1292:THR:HG23	1.84	0.41
1:B:420:GLU:HA	1:B:423:PHE:CE2	2.55	0.41
1:B:687:ALA:HB1	1:B:732:LYS:HE3	2.02	0.41
1:A:1493:LEU:HB3	1:A:1504:SER:HB2	2.03	0.41
1:B:16:GLU:HG2	1:B:126:PHE:HZ	1.86	0.41
1:B:1269:LEU:HD23	1:B:1366:VAL:HG21	2.03	0.41
1:A:149:GLN:HG2	1:A:170:VAL:HG11	2.02	0.41
1:A:1157:ARG:NH2	1:A:1186:GLU:OE2	2.53	0.41
1:B:414:ASP:O	1:B:418:VAL:HG23	2.20	0.41
1:B:419:LEU:HA	1:B:422:LEU:HB2	2.03	0.41
1:B:466:ALA:N	1:B:501:LYS:HD2	2.28	0.41
3:E:2:GLC:H61	3:E:2:GLC:O3	2.21	0.41
1:A:35:LEU:H	1:A:35:LEU:HD12	1.86	0.41
1:B:281:TYR:CD2	1:B:282:PRO:HD3	2.55	0.41
1:B:452:PHE:CE1	1:B:466:ALA:HB2	2.55	0.41
1:A:259:LEU:O	1:A:263:ILE:HG13	2.21	0.41
1:A:461:GLU:H	1:A:461:GLU:HG2	1.39	0.41
1:A:467:ASN:HB3	1:A:499:CYS:O	2.20	0.41
1:A:1084:ARG:NH2	1:A:1521:ASP:OD1	2.53	0.41
1:A:1211:LYS:H	1:A:1211:LYS:HG2	1.48	0.41
1:A:1217:VAL:HG23	1:A:1231:GLY:HA2	2.03	0.41
1:A:1293:LYS:CD	1:A:1297:SER:HB2	2.51	0.41
1:A:1364:MET:HB3	1:A:1444:PHE:HE2	1.86	0.41
1:B:36:PRO:HG2	1:B:44:MET:SD	2.61	0.41
1:B:673:THR:HG21	1:B:707:PHE:O	2.21	0.41
1:B:1133:PHE:CZ	1:B:1137:ILE:HD11	2.55	0.41
1:B:1157:ARG:HG2	1:B:1159:PHE:O	2.21	0.41
1:B:1291:VAL:O	1:B:1298:LYS:HA	2.21	0.41
1:A:154:LYS:HG3	1:A:155:TRP:CD1	2.56	0.41
1:A:423:PHE:O	1:A:427:LYS:HB2	2.21	0.41
1:A:628:LYS:O	1:A:650:MET:HB2	2.20	0.41
1:A:765:PHE:HE2	1:A:767:ARG:HB2	1.85	0.41
1:A:1335:ILE:O	2:C:1:GLC:O3	2.39	0.41
1:B:834:THR:HG22	1:B:835:GLY:H	1.85	0.41
1:B:908:TYR:CE2	1:B:1047:LYS:HE2	2.56	0.41
1:A:1133:PHE:CZ	1:A:1137:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:TYR:HB2	1:B:501:LYS:CE	2.51	0.40
1:B:329:ASN:H	1:B:331:LYS:HZ3	1.69	0.40
1:A:264:GLU:O	1:A:268:LYS:HB2	2.21	0.40
1:A:1211:LYS:HB3	1:A:1211:LYS:HE2	1.88	0.40
1:B:890:SER:O	1:B:894:ILE:HG13	2.21	0.40
1:A:242:TRP:NE1	1:A:517:ARG:HH22	2.20	0.40
1:B:184:GLN:HA	1:B:201:PHE:HA	2.03	0.40
1:A:251:TYR:HB2	1:A:501:LYS:CE	2.51	0.40
1:A:251:TYR:CE2	1:A:503:ARG:HG3	2.57	0.40
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.88	0.40
1:A:1400:ASP:OD1	1:A:1401:TYR:N	2.55	0.40
1:B:1406:TYR:O	1:B:1423:ASN:ND2	2.55	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%)	1413 (93%)	102 (7%)	9 (1%)	21	52
1	B	1524/1536 (99%)	1418 (93%)	100 (7%)	6 (0%)	30	61
All	All	3048/3072 (99%)	2831 (93%)	202 (7%)	15 (0%)	24	57

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	PRO
1	A	459	ASP
1	A	280	GLY
1	A	1163	ASP
1	B	281	TYR
1	A	458	LYS

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Mol	Chain	Res	Type
1	A	900	ARG
1	B	332	SER
1	B	900	ARG
1	B	432	ASP
1	A	1121	ASN
1	B	1121	ASN
1	B	706	VAL
1	A	706	VAL
1	A	1119	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1343/1353 (99%)	1230 (92%)	113 (8%)	10	35
1	B	1343/1353 (99%)	1254 (93%)	89 (7%)	15	43
All	All	2686/2706 (99%)	2484 (92%)	202 (8%)	12	39

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	159	THR
1	A	199	LEU
1	A	200	GLU
1	A	207	LYS
1	A	210	LYS
1	A	212	VAL
1	A	220	ARG
1	A	274	GLU
1	A	276	MET
1	A	277	GLU
1	A	279	LEU
1	A	281	TYR
1	A	286	LYS

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Mol	Chain	Res	Type
1	A	287	THR
1	A	288	VAL
1	A	290	ASP
1	A	291	LEU
1	A	294	VAL
1	A	299	LYS
1	A	308	LEU
1	A	316	VAL
1	A	333	TRP
1	A	335	ASP
1	A	336	ASP
1	A	345	THR
1	A	371	ILE
1	A	374	ASP
1	A	415	ILE
1	A	419	LEU
1	A	425	ARG
1	A	426	ILE
1	A	437	LYS
1	A	441	ILE
1	A	442	THR
1	A	443	LYS
1	A	444	LYS
1	A	445	LEU
1	A	447	LEU
1	A	456	LYS
1	A	458	LYS
1	A	459	ASP
1	A	461	GLU
1	A	462	GLU
1	A	467	ASN
1	A	473	ASP
1	A	498	ASP
1	A	500	VAL
1	A	562	VAL
1	A	583	SER
1	A	585	LEU
1	A	612	SER
1	A	616	VAL
1	A	629	ILE
1	A	631	GLU
1	A	649	ILE

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Mol	Chain	Res	Type
1	A	704	ASP
1	A	742	ILE
1	A	754	MET
1	A	761	GLN
1	A	764	THR
1	A	800	THR
1	A	821	GLU
1	A	834	THR
1	A	905	GLU
1	A	925	VAL
1	A	974	GLU
1	A	978	GLU
1	A	1044	SER
1	A	1082	SER
1	A	1116	LEU
1	A	1120	ARG
1	A	1128	ASP
1	A	1153	GLU
1	A	1156	THR
1	A	1157	ARG
1	A	1159	PHE
1	A	1164	GLU
1	A	1166	ILE
1	A	1169	ASP
1	A	1174	PHE
1	A	1181	GLU
1	A	1207	ASP
1	A	1211	LYS
1	A	1216	ASN
1	A	1217	VAL
1	A	1218	GLU
1	A	1220	ASN
1	A	1224	GLU
1	A	1233	GLN
1	A	1235	ASN
1	A	1236	CYS
1	A	1247	GLU
1	A	1252	VAL
1	A	1264	VAL
1	A	1265	GLU
1	A	1279	GLN
1	A	1282	LYS

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Mol	Chain	Res	Type
1	A	1291	VAL
1	A	1292	THR
1	A	1299	ILE
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	1361	THR
1	A	1408	ASN
1	A	1423	ASN
1	A	1424	TYR
1	A	1442	HIS
1	A	1459	LYS
1	B	136	VAL
1	B	220	ARG
1	B	274	GLU
1	B	276	MET
1	B	277	GLU
1	B	279	LEU
1	B	281	TYR
1	B	283	VAL
1	B	285	LEU
1	B	286	LYS
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	325	GLU
1	B	326	LYS
1	B	330	SER
1	B	333	TRP
1	B	344	SER
1	B	374	ASP
1	B	415	ILE
1	B	419	LEU
1	B	425	ARG
1	B	430	ARG
1	B	434	HIS

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Mol	Chain	Res	Type
1	B	441	ILE
1	B	443	LYS
1	B	444	LYS
1	B	447	LEU
1	B	467	ASN
1	B	498	ASP
1	B	500	VAL
1	B	562	VAL
1	B	583	SER
1	B	585	LEU
1	B	616	VAL
1	B	629	ILE
1	B	631	GLU
1	B	649	ILE
1	B	679	THR
1	B	704	ASP
1	B	742	ILE
1	B	754	MET
1	B	761	GLN
1	B	764	THR
1	B	800	THR
1	B	834	THR
1	B	905	GLU
1	B	925	VAL
1	B	974	GLU
1	B	978	GLU
1	B	1044	SER
1	B	1082	SER
1	B	1120	ARG
1	B	1153	GLU
1	B	1154	LYS
1	B	1156	THR
1	B	1157	ARG
1	B	1158	ARG
1	B	1162	ASP
1	B	1164	GLU
1	B	1179	THR
1	B	1195	ILE
1	B	1208	ARG
1	B	1213	GLU
1	B	1216	ASN
1	B	1217	VAL

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Mol	Chain	Res	Type
1	B	1218	GLU
1	B	1233	GLN
1	B	1235	ASN
1	B	1252	VAL
1	B	1265	GLU
1	B	1321	ASN
1	B	1322	LYS
1	B	1323	GLU
1	B	1330	ILE
1	B	1334	ILE
1	B	1361	THR
1	B	1401	TYR
1	B	1408	ASN
1	B	1411	GLU
1	B	1412	ASP
1	B	1414	ASP
1	B	1424	TYR
1	B	1442	HIS
1	B	1454	VAL
1	B	1459	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	184	GLN
1	A	223	HIS
1	A	235	HIS
1	A	239	ASN
1	A	253	HIS
1	A	438	GLN
1	A	468	ASN
1	A	525	ASN
1	A	1066	HIS
1	A	1201	ASN
1	A	1409	ASN
1	A	1425	HIS
1	A	1445	ASN
1	B	37	GLN
1	B	92	HIS
1	B	184	GLN
1	B	198	GLN

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Mol	Chain	Res	Type
1	B	224	ASN
1	B	239	ASN
1	B	246	HIS
1	B	329	ASN
1	B	525	ASN
1	B	1121	ASN
1	B	1201	ASN
1	B	1309	GLN
1	B	1402	ASN
1	B	1425	HIS
1	B	1445	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 ⓘ

20 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	0.60	0	17,17,17	0.66	0
2	GLC	C	2	2	11,11,12	0.49	0	15,15,17	1.34	3 (20%)
2	GLC	D	1	2	12,12,12	0.60	0	17,17,17	1.24	1 (5%)
2	GLC	D	2	2	11,11,12	0.93	1 (9%)	15,15,17	1.31	2 (13%)
3	GLC	E	1	3	11,11,12	0.78	1 (9%)	15,15,17	1.09	2 (13%)
3	GLC	E	2	3	11,11,12	0.81	0	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	E	3	3	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
3	GLC	F	1	3	11,11,12	1.19	1 (9%)	15,15,17	1.33	3 (20%)
3	GLC	F	2	3	11,11,12	1.25	2 (18%)	15,15,17	1.48	4 (26%)
3	GLC	F	3	3	11,11,12	1.01	1 (9%)	15,15,17	1.46	4 (26%)
4	GLC	G	1	4	12,12,12	0.85	0	17,17,17	1.11	2 (11%)
4	GLC	G	2	4	11,11,12	1.31	2 (18%)	15,15,17	1.42	3 (20%)
4	GLC	G	3	4	11,11,12	1.31	1 (9%)	15,15,17	1.55	3 (20%)
4	GLC	G	4	4	11,11,12	0.72	0	15,15,17	1.21	2 (13%)
4	GLC	G	5	4	11,11,12	0.61	0	15,15,17	1.38	3 (20%)
4	GLC	H	1	4	12,12,12	0.99	0	17,17,17	1.15	2 (11%)
4	GLC	H	2	4	11,11,12	1.62	3 (27%)	15,15,17	1.42	2 (13%)
4	GLC	H	3	4	11,11,12	1.29	3 (27%)	15,15,17	1.49	3 (20%)
4	GLC	H	4	4	11,11,12	1.29	1 (9%)	15,15,17	1.24	1 (6%)
4	GLC	H	5	4	11,11,12	0.56	0	15,15,17	1.09	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	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
3	GLC	E	1	3	-	0/2/19/22	0/1/1/1
3	GLC	E	2	3	-	0/2/19/22	0/1/1/1
3	GLC	E	3	3	-	1/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/19/22	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	-	1/2/19/22	0/1/1/1
4	GLC	H	1	4	-	0/2/22/22	0/1/1/1
4	GLC	H	2	4	-	0/2/19/22	0/1/1/1
4	GLC	H	3	4	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	GLC	C4-C5	3.86	1.61	1.53
3	F	1	GLC	O4-C4	3.22	1.50	1.43
3	F	3	GLC	C1-C2	3.02	1.59	1.52
4	H	4	GLC	O4-C4	3.01	1.50	1.43
3	F	2	GLC	O5-C5	2.92	1.49	1.43
4	G	3	GLC	O4-C4	2.88	1.50	1.43
4	G	2	GLC	C4-C5	2.72	1.58	1.53
4	H	2	GLC	O4-C4	2.40	1.48	1.43
4	G	2	GLC	O5-C5	2.34	1.48	1.43
2	D	2	GLC	O5-C1	2.28	1.47	1.43
4	H	3	GLC	O4-C4	2.24	1.48	1.43
4	H	3	GLC	C4-C3	2.13	1.57	1.52
4	H	2	GLC	O5-C5	2.09	1.47	1.43
4	H	3	GLC	C2-C3	-2.06	1.49	1.52
3	F	2	GLC	O5-C1	2.06	1.47	1.43
3	E	1	GLC	O4-C4	2.03	1.48	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	GLC	O4-C4-C5	3.67	118.36	109.32
2	D	1	GLC	C1-O5-C5	-3.57	106.74	113.65
2	D	2	GLC	O5-C5-C6	3.49	114.47	107.66
2	C	2	GLC	O5-C5-C6	3.26	114.00	107.66
4	H	3	GLC	C1-O5-C5	-3.14	107.98	112.19
4	G	2	GLC	O4-C4-C5	3.09	116.94	109.32
4	H	4	GLC	O4-C4-C3	3.06	117.58	110.38
3	F	3	GLC	O5-C5-C6	-3.03	101.77	107.66
3	F	1	GLC	O5-C5-C6	2.95	113.41	107.66
4	G	3	GLC	C1-O5-C5	-2.90	108.30	112.19
4	G	3	GLC	C2-C3-C4	-2.78	105.96	110.86
4	G	2	GLC	C1-O5-C5	-2.78	108.46	112.19
3	F	1	GLC	O4-C4-C5	2.77	116.16	109.32
3	F	2	GLC	O4-C4-C3	-2.71	103.99	110.38
4	G	5	GLC	O5-C5-C6	-2.60	102.61	107.66
3	F	2	GLC	O5-C1-C2	-2.57	104.67	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	GLC	O4-C4-C3	2.55	116.39	110.38
4	G	2	GLC	O4-C4-C3	-2.54	104.40	110.38
3	F	3	GLC	C2-C3-C4	-2.54	106.40	110.86
3	E	1	GLC	O3-C3-C2	-2.48	105.00	110.05
2	C	2	GLC	C1-O5-C5	2.45	115.48	112.19
4	G	5	GLC	C2-C3-C4	-2.42	106.61	110.86
3	F	3	GLC	C6-C5-C4	-2.33	107.31	113.02
4	H	3	GLC	C2-C3-C4	-2.33	106.77	110.86
4	G	5	GLC	C1-C2-C3	-2.32	106.27	109.64
2	C	2	GLC	C2-C3-C4	-2.31	106.80	110.86
4	H	3	GLC	O3-C3-C4	2.31	115.82	110.38
3	F	2	GLC	O6-C6-C5	2.20	118.84	111.33
4	G	4	GLC	C1-O5-C5	2.18	115.10	112.19
4	H	5	GLC	C2-C3-C4	-2.15	107.07	110.86
2	D	2	GLC	C1-C2-C3	-2.15	106.51	109.64
3	F	2	GLC	C1-O5-C5	2.15	115.07	112.19
3	E	1	GLC	O4-C4-C3	2.14	115.42	110.38
4	H	1	GLC	C3-C4-C5	-2.14	106.36	110.23
4	G	1	GLC	C3-C4-C5	-2.11	106.41	110.23
4	G	1	GLC	C6-C5-C4	-2.10	107.86	113.02
4	H	1	GLC	O3-C3-C4	2.10	115.32	110.38
4	G	4	GLC	C2-C3-C4	-2.09	107.19	110.86
4	H	2	GLC	C1-O5-C5	-2.08	109.40	112.19
3	F	3	GLC	C1-C2-C3	-2.07	106.63	109.64
3	E	3	GLC	O5-C5-C6	2.04	111.64	107.66
3	E	2	GLC	O3-C3-C4	2.03	115.16	110.38
3	F	1	GLC	C6-C5-C4	-2.01	108.09	113.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

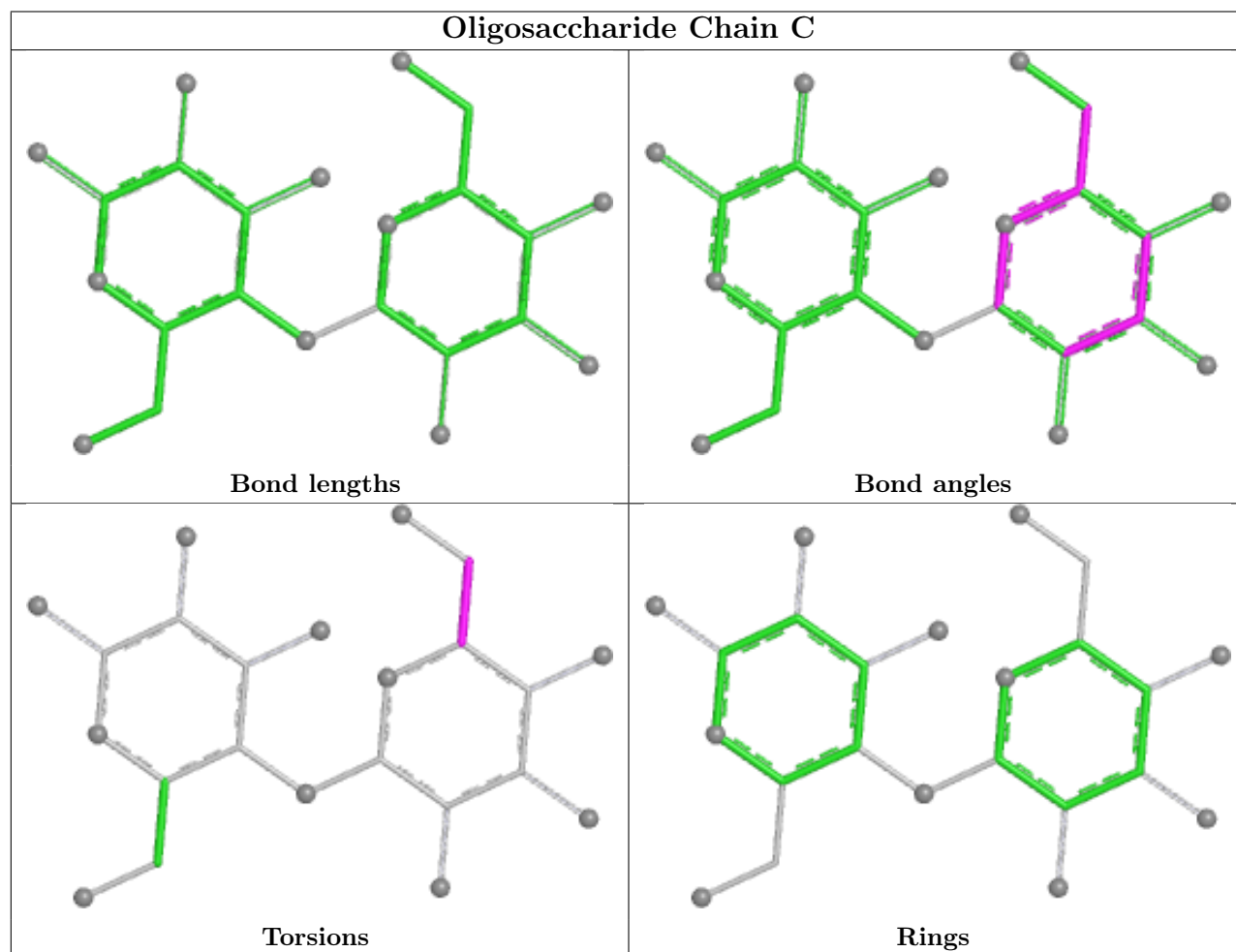
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6
3	E	3	GLC	O5-C5-C6-O6
4	G	4	GLC	O5-C5-C6-O6
4	H	4	GLC	O5-C5-C6-O6
4	H	5	GLC	O5-C5-C6-O6
3	F	3	GLC	O5-C5-C6-O6
4	G	5	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6

There are no ring outliers.

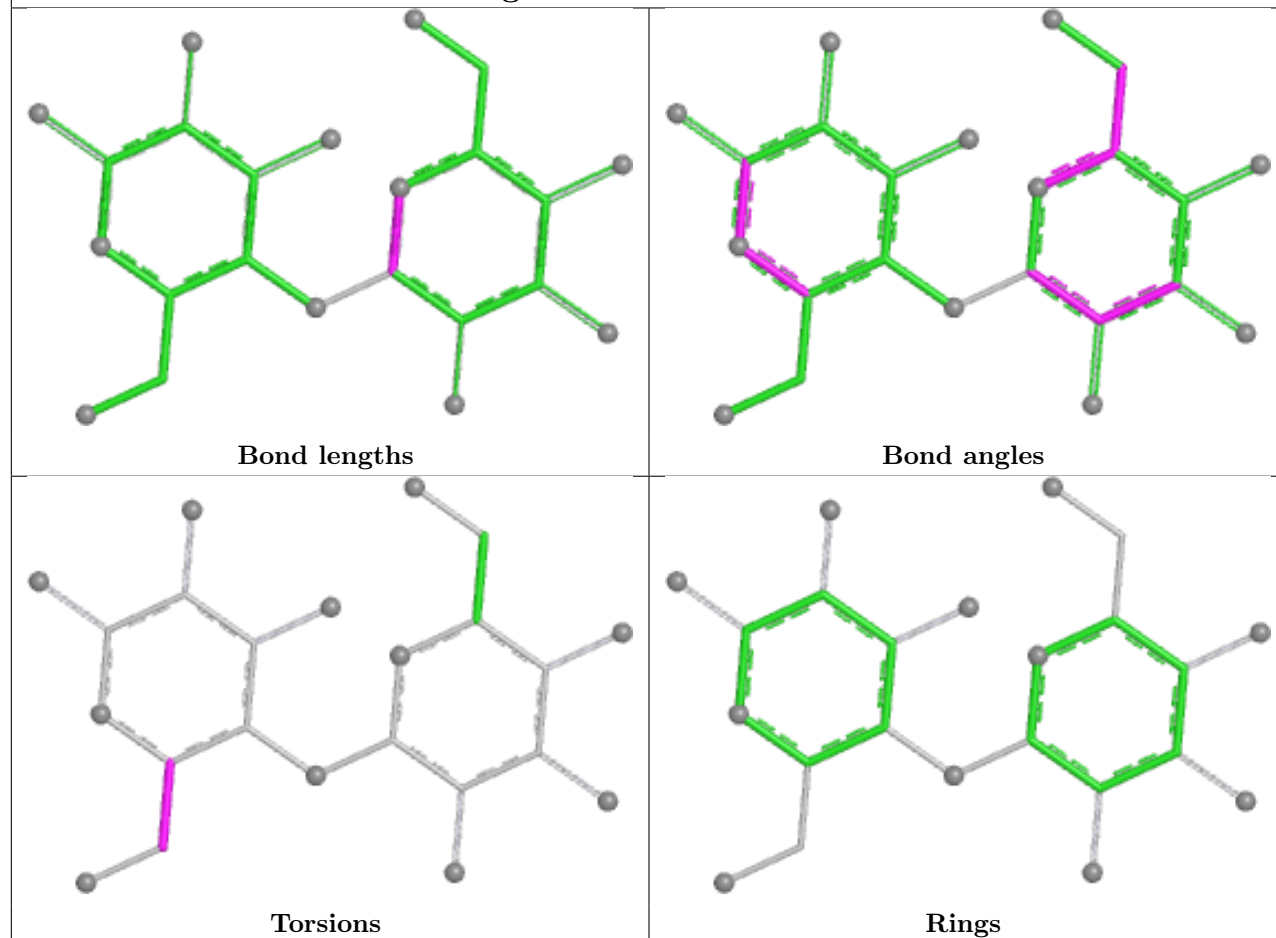
10 monomers are involved in 11 short contacts:

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

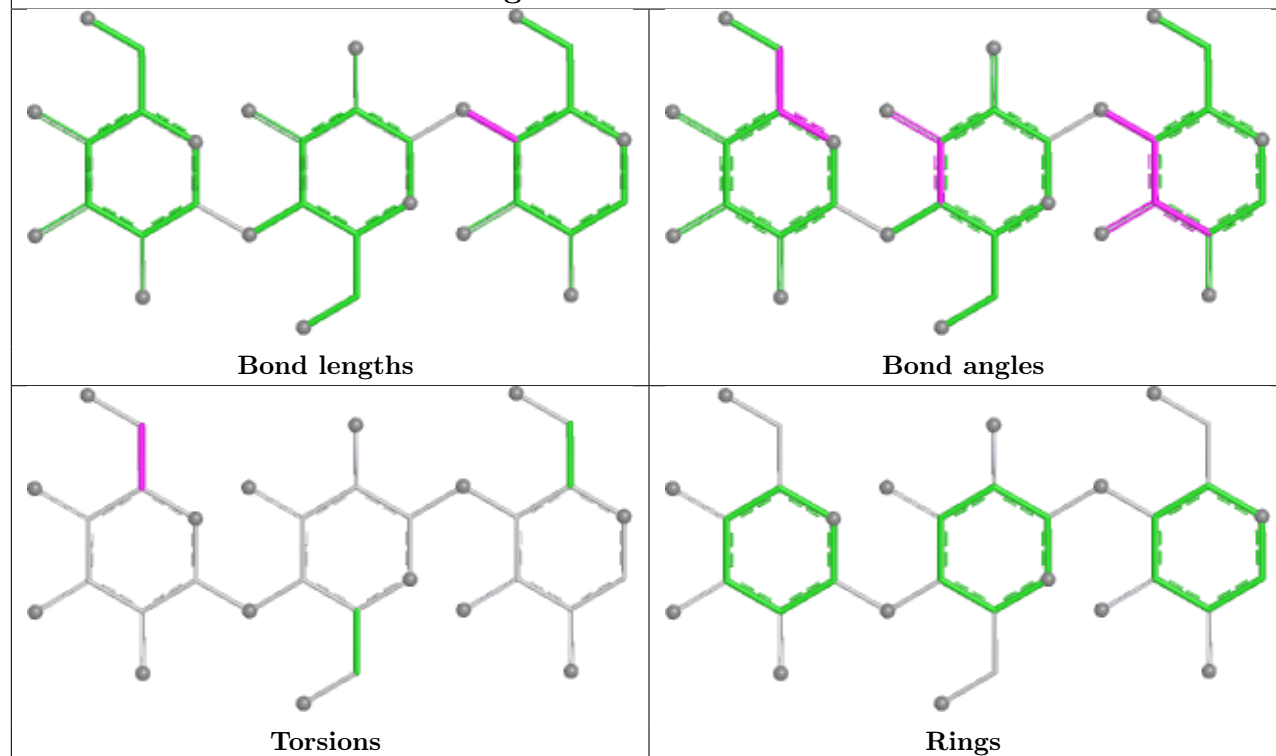
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

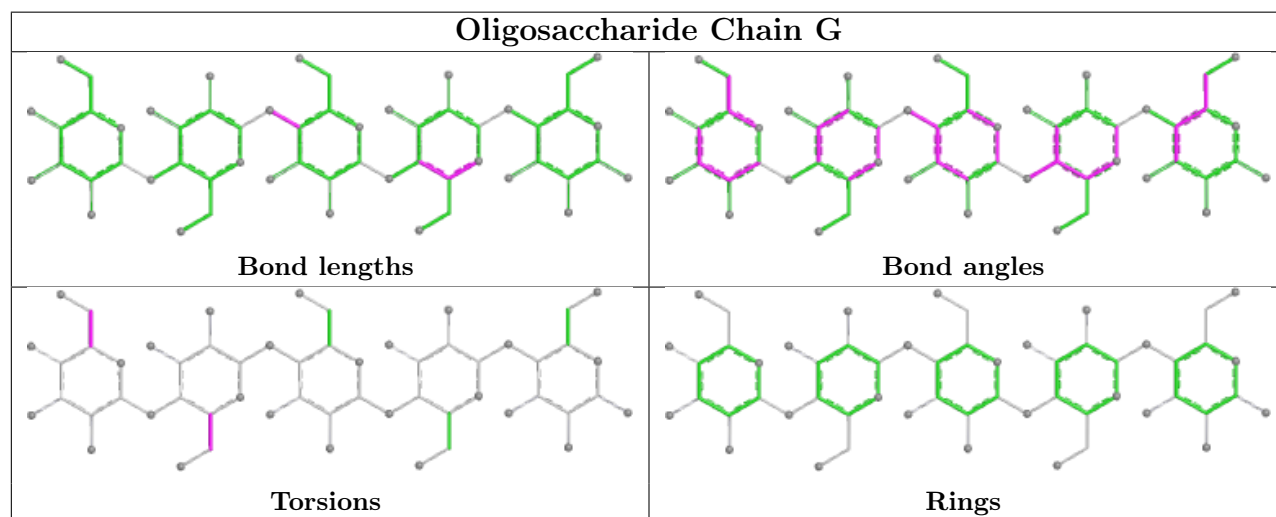
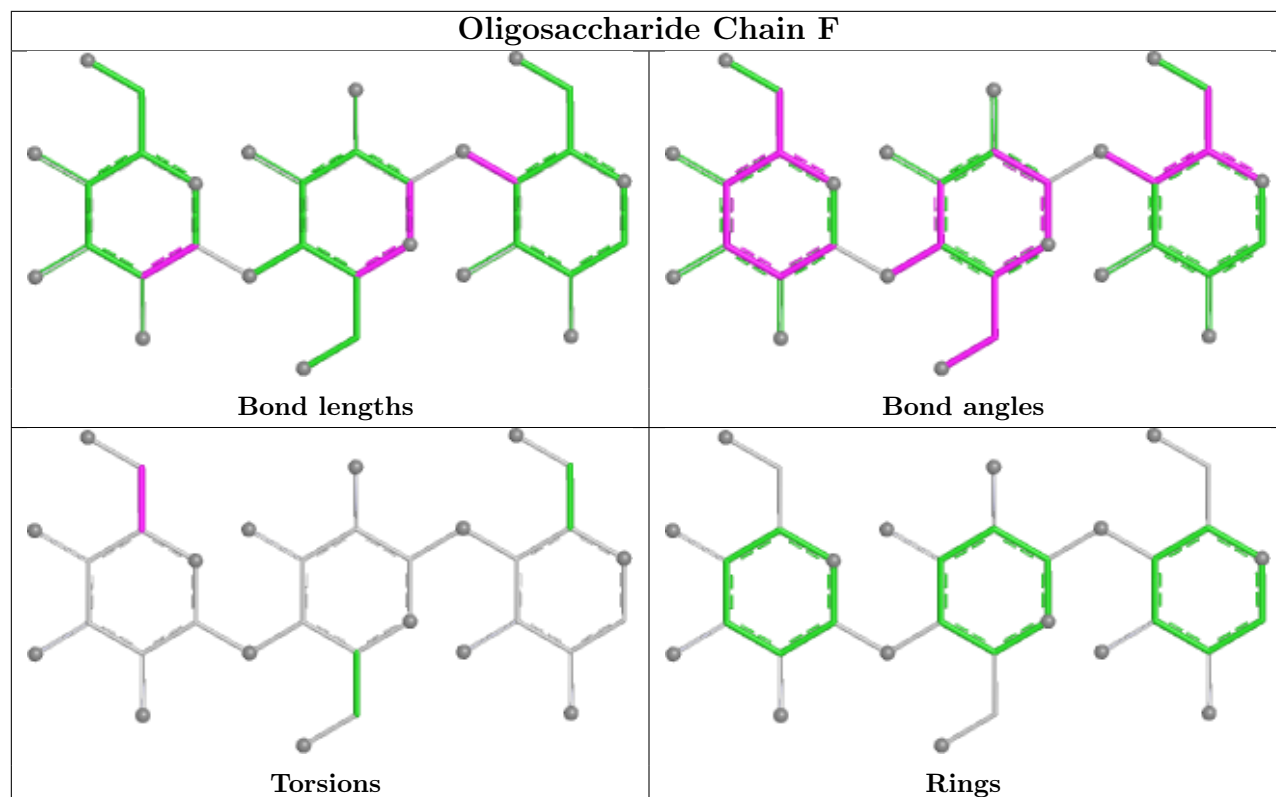


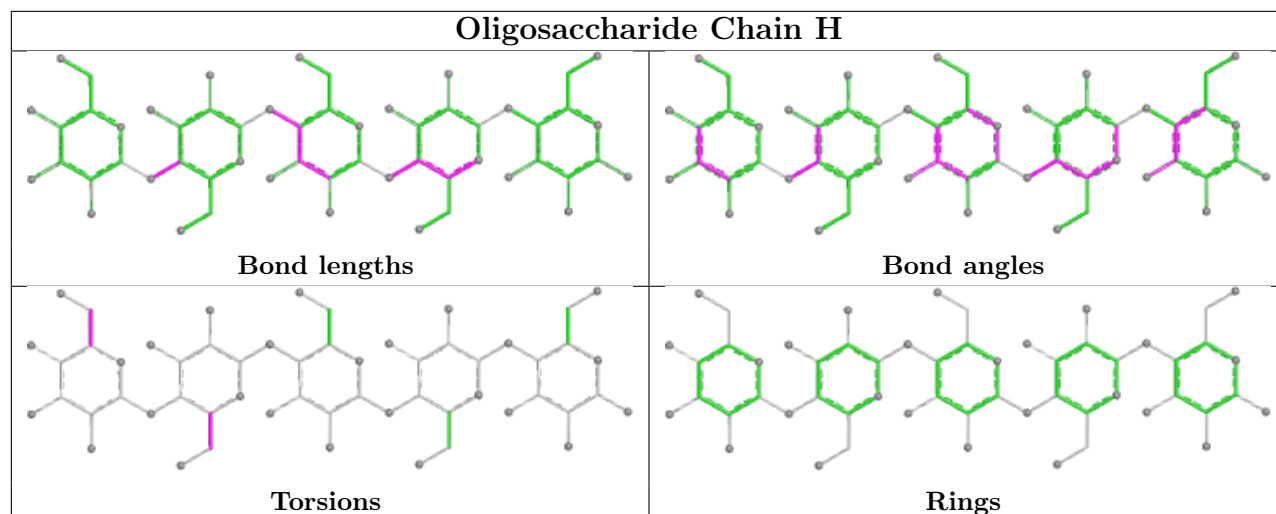
Oligosaccharide Chain D



Oligosaccharide Chain E







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%)	-0.28	6 (0%) 88 76	56, 106, 170, 207	0
1	B	1526/1536 (99%)	-0.28	8 (0%) 87 73	58, 104, 154, 173	0
All	All	3052/3072 (99%)	-0.28	14 (0%) 87 73	56, 105, 162, 207	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LYS	3.4
1	A	309	TRP	3.0
1	B	389	ASN	2.9
1	B	501	LYS	2.9
1	B	380	LEU	2.5
1	B	1128	ASP	2.5
1	A	488	TYR	2.4
1	B	309	TRP	2.4
1	A	1458	ALA	2.3
1	B	376	PHE	2.1
1	B	649	ILE	2.1
1	A	489	LEU	2.1
1	B	1065	PRO	2.1
1	A	875	ASP	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,

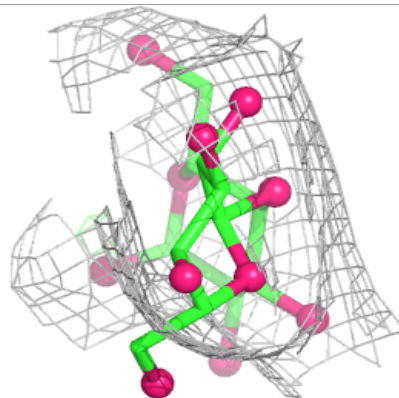
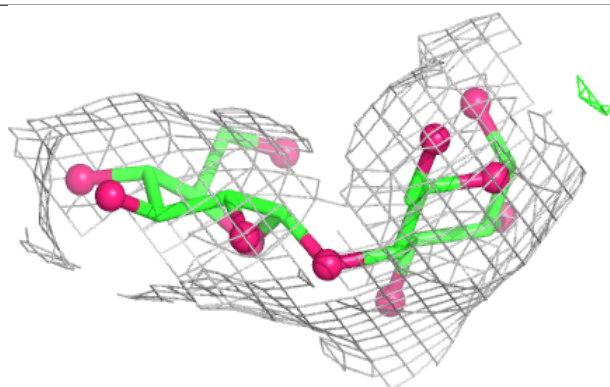
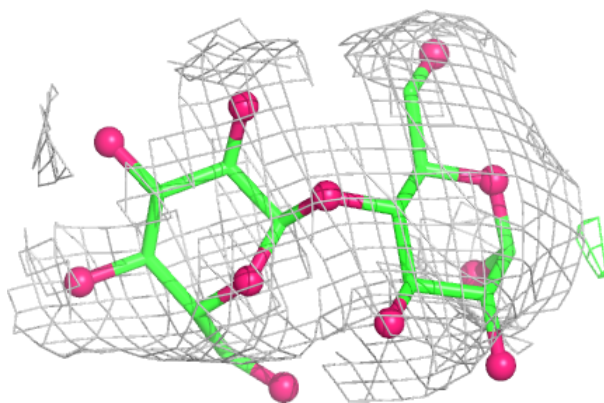
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	H	5	11/12	0.34	0.12	131,148,156,157	0
4	GLC	G	5	11/12	0.43	0.10	128,135,142,150	0
3	GLC	F	2	11/12	0.49	0.17	116,127,146,151	0
3	GLC	F	1	11/12	0.52	0.10	114,130,140,145	0
3	GLC	E	1	11/12	0.52	0.09	121,131,142,152	0
2	GLC	C	1	12/12	0.54	0.08	120,141,151,151	0
2	GLC	D	2	11/12	0.60	0.08	138,148,159,161	0
3	GLC	E	3	11/12	0.66	0.11	81,109,130,140	0
3	GLC	E	2	11/12	0.69	0.10	118,130,133,141	0
4	GLC	H	1	12/12	0.69	0.11	113,121,132,134	0
4	GLC	G	1	12/12	0.69	0.14	104,119,127,130	0
2	GLC	D	1	12/12	0.70	0.08	133,146,150,150	0
3	GLC	F	3	11/12	0.73	0.13	85,94,106,117	0
2	GLC	C	2	11/12	0.77	0.09	121,130,138,148	0
4	GLC	H	2	11/12	0.79	0.11	119,127,135,137	0
4	GLC	H	3	11/12	0.84	0.12	115,127,135,147	0
4	GLC	H	4	11/12	0.87	0.08	127,138,146,150	0
4	GLC	G	4	11/12	0.87	0.09	125,138,146,150	0
4	GLC	G	3	11/12	0.89	0.07	106,121,132,133	0
4	GLC	G	2	11/12	0.90	0.07	106,122,131,141	0

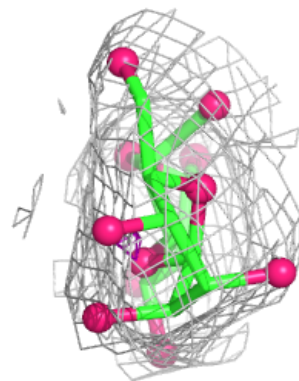
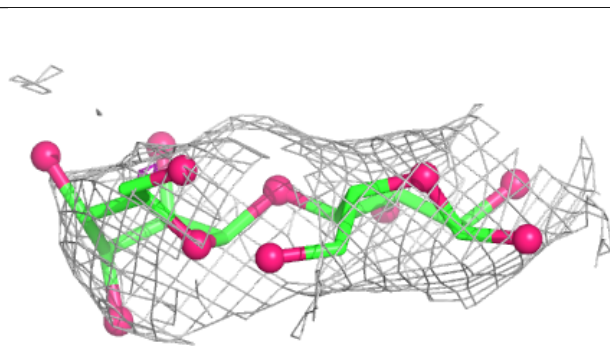
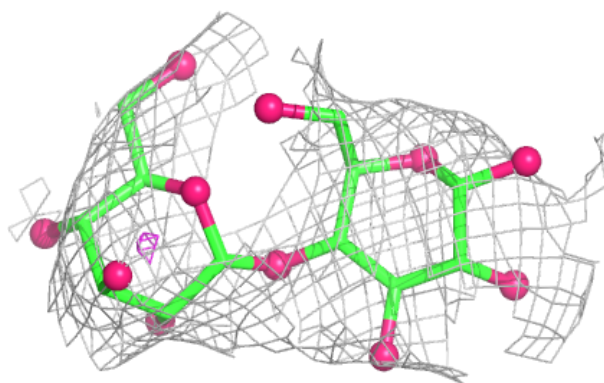
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

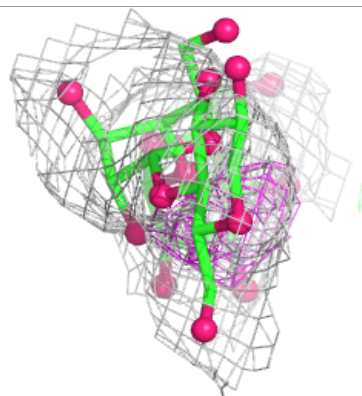
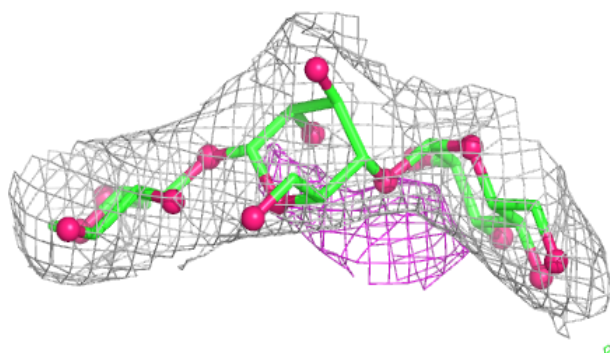
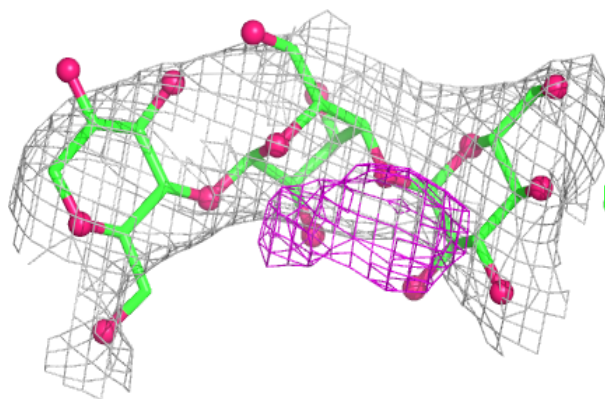
**Electron density around Chain D:**

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

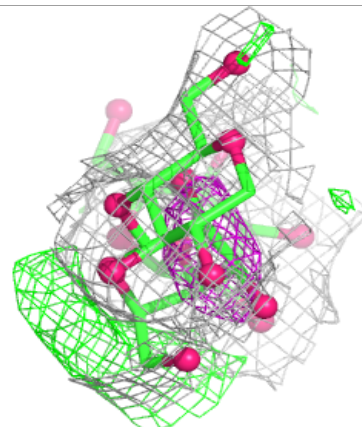
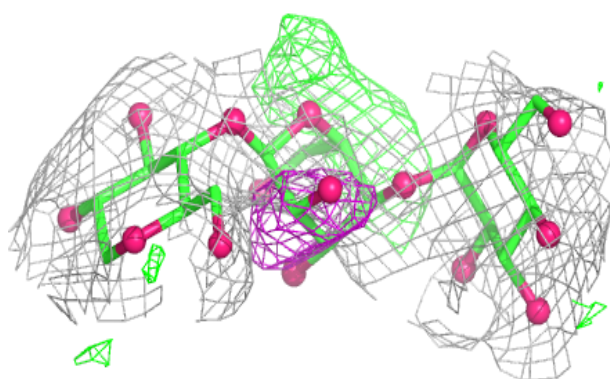
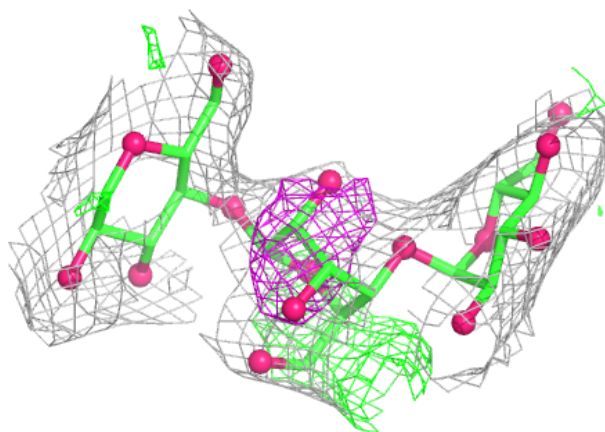


Electron density around Chain E:

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

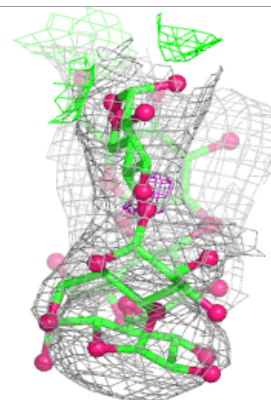
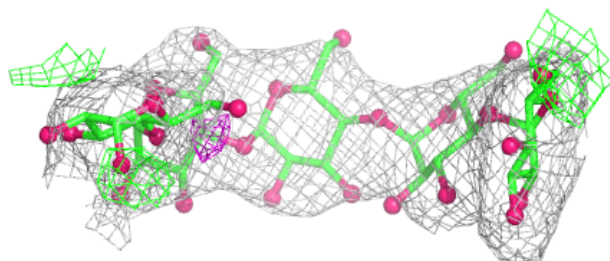
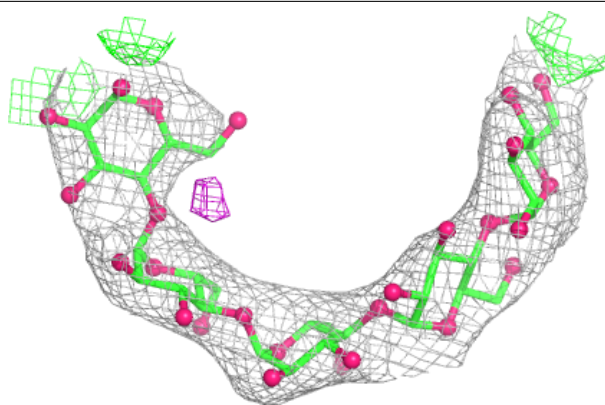
**Electron density around Chain F:**

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

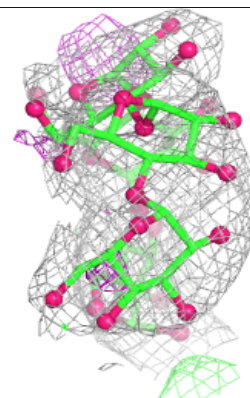
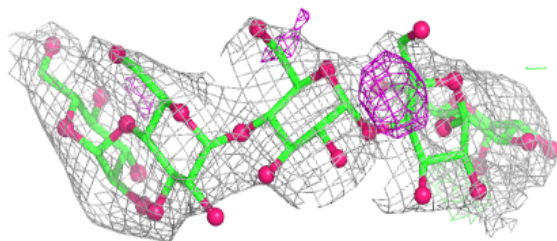
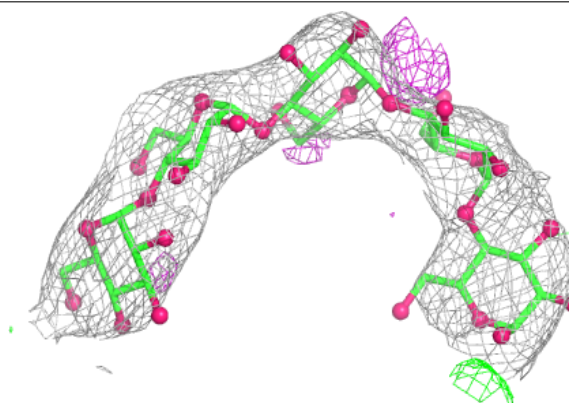


Electron density around Chain G:

$2mF_o-DF_c$ (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.