



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:09 PM BST

PDB ID : 2Z1K  
Title : Crystal Structure of Ttha1563 from *Thermus thermophilus* HB8  
Authors : Niwa, H.; Shimada, A.; Matsunaga, E.; Kuramitsu, S.; Yokoyama, S.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-05-08  
Resolution : 2.30 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

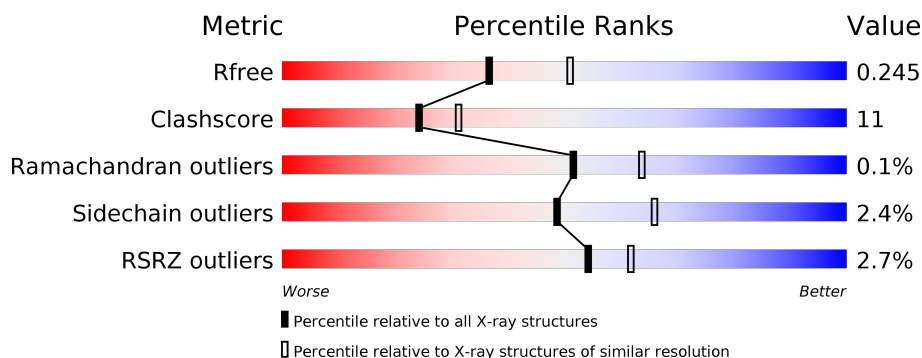
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.







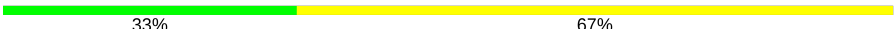

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	475	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>22%</div> </div> </div>
1	B	475	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>21%</div> </div> </div>
1	C	475	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>21%</div> </div> </div>
1	D	475	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>26%</div> </div> </div>
2	E	7	<div> <div></div> <div> <div></div> <div>57%</div> <div>43%</div> </div> </div>
2	G	7	<div> <div></div> <div> <div></div> <div>57%</div> <div>43%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	7	 57% 43%
2	K	7	 29% 57% 14%
3	F	3	 67% 33%
3	H	3	 67% 33%
3	J	3	 33% 67%
3	L	3	 67% 33%

## 2 Entry composition [i](#)

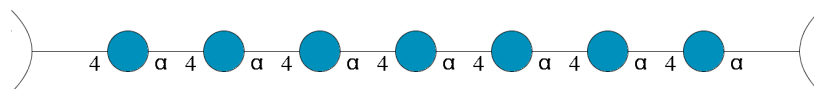
There are 5 unique types of molecules in this entry. The entry contains 16422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (Neo)pullulanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	Se	0	0	0
			3803	2464	675	655	2	7			
1	B	474	Total	C	N	O	S	Se	0	1	0
			3801	2462	672	658	2	7			
1	C	474	Total	C	N	O	S	Se	0	0	0
			3789	2456	670	654	2	7			
1	D	474	Total	C	N	O	S	Se	0	0	0
			3803	2464	675	655	2	7			

- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



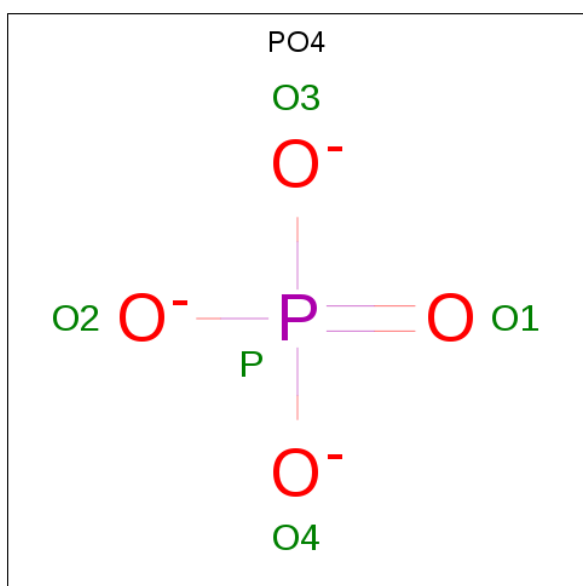
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	7	Total	C	O	0	0	0
			77	42	35			
2	G	7	Total	C	O	0	0	0
			77	42	35			
2	I	7	Total	C	O	0	0	0
			77	42	35			
2	K	7	Total	C	O	0	0	0
			77	42	35			

- 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
			33	18	15			
3	H	3	Total	C	O	0	0	0
			33	18	15			
3	J	3	Total	C	O	0	0	0
			33	18	15			
3	L	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		

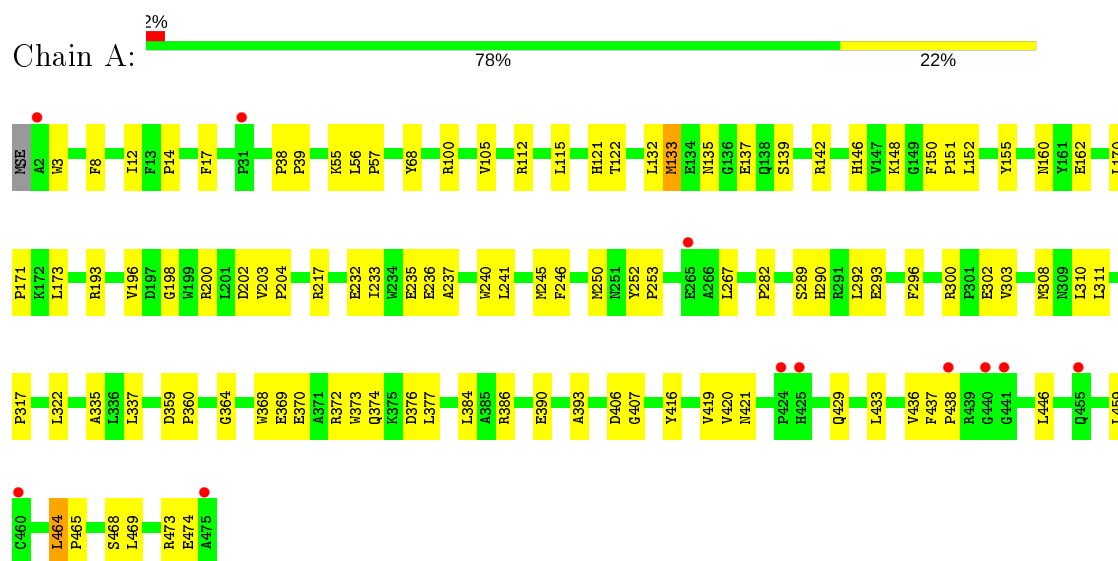
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total	O	0	0
			166	166		
5	B	227	Total	O	0	0
			227	227		
5	C	197	Total	O	0	0
			197	197		
5	D	191	Total	O	0	0
			191	191		

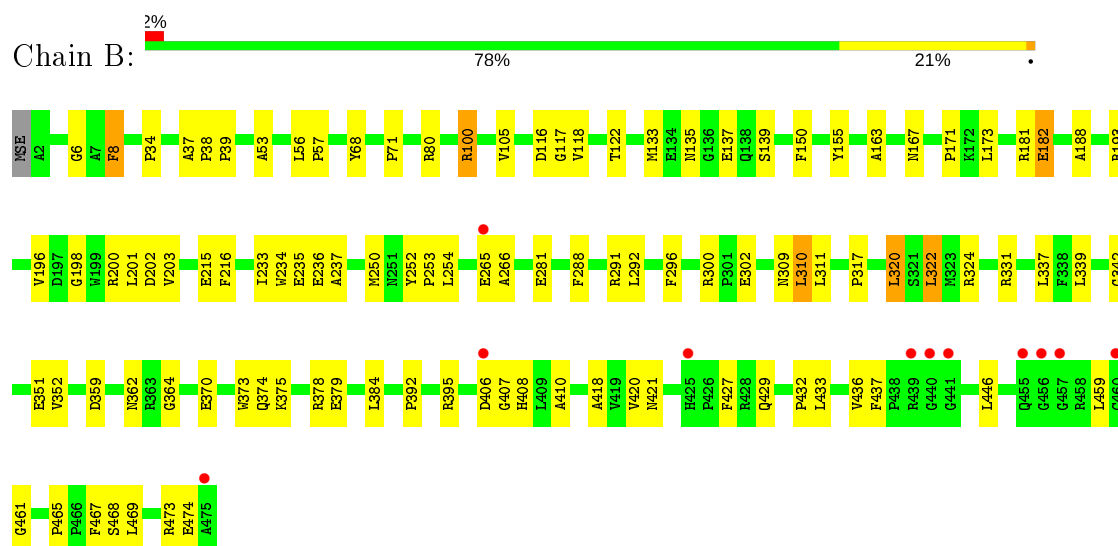
### 3 Residue-property plots [i](#)

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

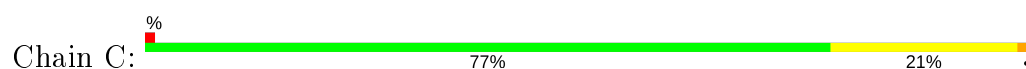
#### • Molecule 1: (Neo)pullulanase

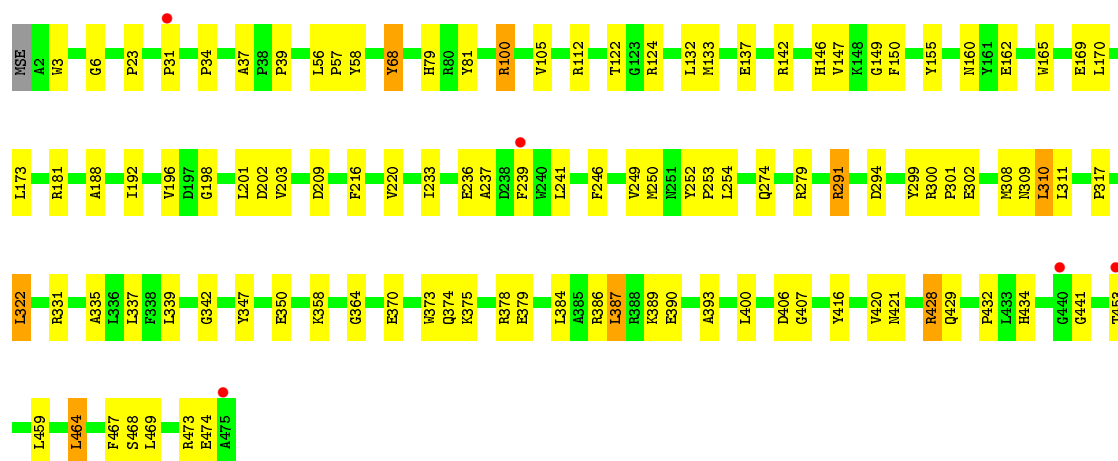


#### • Molecule 1: (Neo)pullulanase

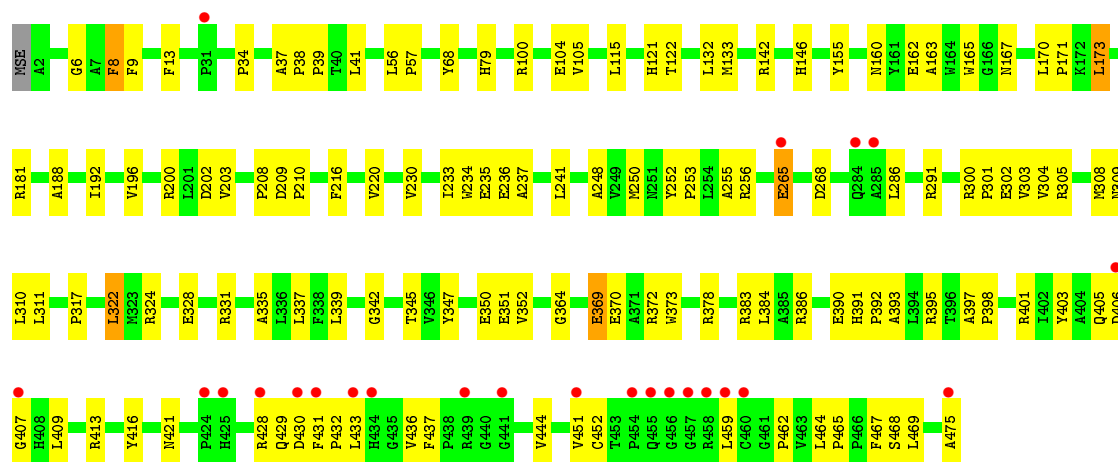
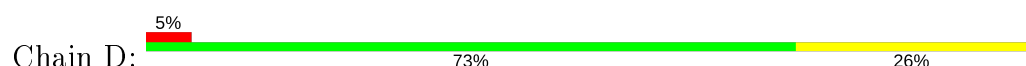


#### • Molecule 1: (Neo)pullulanase





• Molecule 1: (Neo)pullulanase



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



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

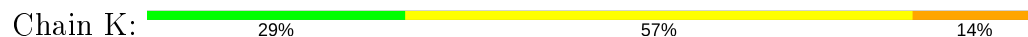


• Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)





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



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



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



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.14Å 95.90Å 140.60Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	46.66 – 2.30 46.66 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.66-2.30) 99.5 (46.66-2.29)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.32 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.236 0.198 , 0.245	Depositor DCC
$R_{free}$ test set	3980 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16422	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6636e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: PO4, 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	0.34	0/3926	0.58	0/5339
1	B	0.35	0/3924	0.59	0/5339
1	C	0.34	0/3912	0.59	0/5323
1	D	0.33	0/3926	0.57	0/5339
All	All	0.34	0/15688	0.58	0/21340

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 [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	3803	0	3682	82	0
1	B	3801	0	3663	76	0
1	C	3789	0	3654	82	0
1	D	3803	0	3682	96	0
2	E	77	0	63	1	0
2	G	77	0	63	3	0
2	I	77	0	63	1	0
2	K	77	0	63	3	0
3	F	33	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	33	0	28	1	0
3	J	33	0	28	2	0
3	L	33	0	28	1	0
4	D	5	0	0	0	0
5	A	166	0	0	3	0
5	B	227	0	0	8	0
5	C	197	0	0	7	0
5	D	191	0	0	5	0
All	All	16422	0	15045	337	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 11.

All (337) 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:C:406:ASP:CG	1:C:407:GLY:H	1.63	0.99
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.28	0.98
1:D:406:ASP:CG	1:D:407:GLY:H	1.69	0.95
1:D:311:LEU:HG	1:D:337:LEU:HD11	1.49	0.92
1:D:429:GLN:HB3	1:D:459:LEU:HD23	1.54	0.90
1:A:406:ASP:CG	1:A:407:GLY:H	1.74	0.90
1:B:406:ASP:CG	1:B:407:GLY:H	1.75	0.85
1:C:100:ARG:HH11	1:C:100:ARG:HG2	1.46	0.80
1:C:311:LEU:HG	1:C:337:LEU:HD11	1.65	0.79
1:B:34:PRO:HG2	1:B:37:ALA:HB2	1.64	0.78
1:C:406:ASP:CG	1:C:407:GLY:N	2.35	0.77
1:A:406:ASP:CG	1:A:407:GLY:N	2.39	0.76
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.49	0.76
1:B:465:PRO:HG2	1:B:468:SER:OG	1.86	0.75
1:D:406:ASP:CG	1:D:407:GLY:N	2.39	0.74
1:B:406:ASP:CG	1:B:407:GLY:N	2.41	0.73
1:B:118:VAL:HG22	1:B:202[B]:ASP:OD2	1.88	0.72
1:B:235:GLU:HG2	1:C:301:PRO:HG3	1.73	0.71
1:D:202:ASP:OD1	3:L:1:GLC:C1	2.39	0.70
1:A:429:GLN:HB3	1:A:459:LEU:HD23	1.74	0.70
1:A:56:LEU:HD22	1:A:105:VAL:HG12	1.74	0.70
1:D:132:LEU:HD21	1:D:142:ARG:HA	1.74	0.69
1:D:465:PRO:HG2	1:D:468:SER:OG	1.92	0.69
1:B:200:ARG:NH1	1:B:202[B]:ASP:OD1	2.26	0.68
1:C:233:ILE:HG21	1:C:237:ALA:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ARG:HH11	1:D:100:ARG:HG2	1.59	0.67
1:B:311:LEU:HG	1:B:337:LEU:HD11	1.76	0.67
1:B:433:LEU:O	1:B:436:VAL:HG23	1.96	0.66
1:A:393:ALA:HB3	1:A:416:TYR:HE2	1.61	0.66
1:C:429:GLN:HB3	1:C:459:LEU:HD23	1.77	0.66
1:A:133:MSE:HE1	1:A:155:TYR:HE2	1.61	0.66
1:C:317:PRO:HB2	1:C:322:LEU:HD13	1.76	0.65
1:D:339:LEU:HD11	1:D:469:LEU:HD21	1.77	0.65
1:C:300:ARG:HB3	1:C:302:GLU:OE2	1.97	0.64
1:A:282:PRO:HG3	5:A:658:HOH:O	1.96	0.64
1:A:122:THR:O	1:A:171:PRO:HD2	1.98	0.64
1:A:464:LEU:CD2	1:A:468:SER:HB2	2.28	0.64
1:C:241:LEU:HD21	1:C:249:VAL:HG13	1.79	0.64
1:B:100:ARG:NH1	1:B:100:ARG:HG2	2.07	0.63
1:B:370:GLU:HG2	1:B:373:TRP:CH2	2.34	0.63
1:A:132:LEU:HD21	1:A:142:ARG:HA	1.80	0.63
1:A:289:SER:O	1:A:293:GLU:HG3	1.98	0.62
1:A:386:ARG:O	1:A:390:GLU:HG3	1.99	0.62
1:B:202[A]:ASP:OD1	3:H:1:GLC:C1	2.47	0.62
1:C:132:LEU:HD21	1:C:142:ARG:HA	1.80	0.62
1:A:446:LEU:HD21	1:A:473:ARG:HD3	1.82	0.62
1:B:302:GLU:H	1:B:302:GLU:CD	2.03	0.61
1:C:370:GLU:HG2	1:C:373:TRP:CZ3	2.35	0.61
1:C:464:LEU:HD22	1:C:468:SER:HB2	1.83	0.61
1:C:339:LEU:HD11	1:C:469:LEU:HD21	1.83	0.61
1:C:56:LEU:N	1:C:57:PRO:HD2	2.16	0.61
1:B:56:LEU:HD22	1:B:105:VAL:HG12	1.83	0.60
1:D:433:LEU:O	1:D:436:VAL:HG23	2.02	0.59
1:C:389:LYS:HE3	5:C:617:HOH:O	2.02	0.59
1:A:311:LEU:HG	1:A:337:LEU:HD11	1.84	0.59
1:B:122:THR:O	1:B:171:PRO:HD2	2.02	0.59
1:B:317:PRO:HB2	1:B:322:LEU:HD13	1.84	0.58
1:D:392:PRO:HA	1:D:395:ARG:NH1	2.18	0.58
1:A:56:LEU:N	1:A:57:PRO:HD2	2.18	0.58
1:C:56:LEU:HD23	1:C:105:VAL:HG12	1.84	0.58
1:D:208:PRO:O	1:D:210:PRO:HD3	2.03	0.58
1:D:369:GLU:HG2	1:D:372:ARG:HG3	1.84	0.58
1:C:375:LYS:O	1:C:379:GLU:HG3	2.03	0.58
1:A:317:PRO:HB2	1:A:322:LEU:HD13	1.85	0.57
1:B:100:ARG:CG	1:B:100:ARG:HH11	2.07	0.57
1:C:146:HIS:HB2	1:C:162:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:HG2	1:A:373:TRP:CZ3	2.40	0.57
1:B:432:PRO:HG2	5:B:718:HOH:O	2.03	0.57
1:C:39:PRO:HG3	1:C:364:GLY:HA2	1.87	0.57
1:A:146:HIS:HB2	1:A:162:GLU:HB2	1.86	0.57
1:D:122:THR:O	1:D:171:PRO:HD2	2.05	0.57
1:A:290:HIS:HA	1:A:293:GLU:OE1	2.04	0.57
1:B:292:LEU:HB3	1:B:296:PHE:CE2	2.39	0.57
1:A:121:HIS:CD2	1:A:170:LEU:HD23	2.40	0.56
1:A:121:HIS:NE2	1:A:170:LEU:HD23	2.20	0.56
1:D:34:PRO:HG2	1:D:37:ALA:HB2	1.86	0.56
5:B:784:HOH:O	1:C:434:HIS:HD2	1.87	0.56
1:C:56:LEU:CD2	1:C:105:VAL:HG12	2.36	0.56
1:A:421:ASN:HB2	1:A:464:LEU:HD13	1.88	0.56
1:D:309:ASN:ND2	1:D:342:GLY:HA3	2.21	0.55
1:B:429:GLN:HB3	1:B:459:LEU:HD23	1.88	0.55
1:A:202:ASP:OD1	3:F:1:GLC:C1	2.54	0.55
1:C:441:GLY:O	1:C:453:THR:HG23	2.07	0.55
1:D:328:GLU:HG2	5:D:920:HOH:O	2.05	0.55
1:B:56:LEU:CD2	1:B:105:VAL:HG12	2.37	0.55
1:D:250:MSE:HE2	1:D:310:LEU:HD13	1.89	0.55
1:C:188:ALA:HB2	1:C:216:PHE:CE1	2.42	0.55
1:D:56:LEU:CD2	1:D:105:VAL:HG12	2.35	0.55
1:D:317:PRO:HB2	1:D:322:LEU:HD13	1.88	0.55
1:A:465:PRO:HG2	1:A:468:SER:OG	2.06	0.55
1:D:236:GLU:CD	1:D:236:GLU:H	2.10	0.54
1:C:170:LEU:HD12	1:C:170:LEU:N	2.22	0.54
1:C:370:GLU:HG2	1:C:373:TRP:CH2	2.43	0.54
1:A:137:GLU:HG2	1:A:150:PHE:CE2	2.43	0.54
1:C:420:VAL:HG22	1:C:469:LEU:CD1	2.36	0.54
1:D:146:HIS:HB2	1:D:162:GLU:HB2	1.88	0.54
1:C:122:THR:HG23	1:C:173:LEU:HD13	1.88	0.54
1:D:317:PRO:HB2	1:D:322:LEU:CD1	2.38	0.54
1:C:6:GLY:HA2	1:C:342:GLY:O	2.08	0.54
1:D:310:LEU:H	1:D:310:LEU:HD23	1.72	0.54
1:C:100:ARG:HH11	1:C:100:ARG:CG	2.19	0.54
1:C:309:ASN:ND2	1:C:342:GLY:HA3	2.23	0.54
1:D:234:TRP:CE2	2:K:1:GLC:H2	2.43	0.53
1:B:351:GLU:HG2	1:B:352:VAL:HG13	1.91	0.53
1:B:56:LEU:N	1:B:57:PRO:HD2	2.23	0.53
1:C:241:LEU:HD12	1:C:299:TYR:CE1	2.43	0.53
1:B:181:ARG:NH1	1:B:215:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ASN:O	1:B:467:PHE:HA	2.08	0.53
1:D:339:LEU:CD1	1:D:469:LEU:HD21	2.39	0.53
1:C:34:PRO:HG2	1:C:37:ALA:HB2	1.91	0.53
1:D:133:MSE:HE1	1:D:155:TYR:HE2	1.73	0.53
1:D:39:PRO:HG3	1:D:364:GLY:HA2	1.90	0.53
1:C:3:TRP:CE3	1:C:112:ARG:HG3	2.43	0.53
1:C:147:VAL:HG12	1:C:149:GLY:H	1.72	0.53
1:D:192:ILE:HG13	1:D:220:VAL:HG13	1.91	0.53
1:A:302:GLU:H	1:A:302:GLU:CD	2.12	0.53
1:A:203:VAL:HG23	1:A:203:VAL:O	2.10	0.52
1:A:236:GLU:CD	1:A:236:GLU:H	2.10	0.52
1:D:265:GLU:CD	1:D:265:GLU:H	2.13	0.52
1:A:100:ARG:CG	1:A:100:ARG:HH11	2.22	0.52
1:A:3:TRP:CE3	1:A:112:ARG:HG3	2.44	0.52
1:A:39:PRO:HG3	1:A:364:GLY:HA2	1.91	0.52
1:C:302:GLU:H	1:C:302:GLU:CD	2.12	0.52
1:B:196:VAL:HG12	1:B:198:GLY:H	1.75	0.52
1:B:39:PRO:HG3	1:B:364:GLY:HA2	1.91	0.52
1:D:6:GLY:HA3	1:D:395:ARG:HD2	1.92	0.52
1:C:331:ARG:NH1	5:C:659:HOH:O	2.42	0.51
1:D:309:ASN:HD21	1:D:342:GLY:HA3	1.73	0.51
1:D:421:ASN:O	1:D:467:PHE:HA	2.10	0.51
1:D:56:LEU:HD22	1:D:105:VAL:HG12	1.91	0.51
1:A:437:PHE:CD1	1:A:474:GLU:HG3	2.44	0.51
1:C:31:PRO:HA	5:C:763:HOH:O	2.09	0.51
1:C:100:ARG:HG2	1:C:100:ARG:NH1	2.22	0.51
1:C:254:LEU:HD23	1:C:309:ASN:OD1	2.11	0.51
1:A:133:MSE:HE1	1:A:155:TYR:CE2	2.44	0.51
1:D:444:VAL:HG12	1:D:475:ALA:HB2	1.91	0.51
1:A:56:LEU:CD2	1:A:105:VAL:HG12	2.39	0.51
1:B:100:ARG:CG	1:B:100:ARG:NH1	2.71	0.51
1:C:335:ALA:HB1	1:C:384:LEU:HD22	1.92	0.51
1:D:370:GLU:HG2	1:D:373:TRP:CZ3	2.45	0.51
1:D:252:TYR:N	1:D:253:PRO:CD	2.74	0.51
1:D:429:GLN:HB3	1:D:459:LEU:CD2	2.35	0.50
1:C:181:ARG:NH2	1:C:209:ASP:OD1	2.44	0.50
1:B:233:ILE:HG21	1:B:237:ALA:HB2	1.93	0.50
2:E:3:GLC:H61	2:E:4:GLC:O5	2.11	0.50
1:B:116:ASP:OD2	1:B:202[B]:ASP:OD1	2.29	0.50
1:D:203:VAL:HG23	1:D:203:VAL:O	2.11	0.50
1:B:6:GLY:HA2	1:B:342:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:GLN:HE21	1:C:358:LYS:HD3	1.77	0.50
1:A:100:ARG:NH1	1:A:100:ARG:HG2	2.24	0.49
1:A:39:PRO:CG	1:A:364:GLY:HA2	2.43	0.49
1:B:310:LEU:HD23	1:B:310:LEU:H	1.78	0.49
1:B:375:LYS:O	1:B:379:GLU:HG3	2.12	0.49
1:C:192:ILE:HG13	1:C:220:VAL:HG13	1.95	0.49
1:B:410:ALA:HA	1:B:418:ALA:O	2.13	0.49
1:C:23:PRO:HB3	5:C:777:HOH:O	2.12	0.49
1:C:58:TYR:CE1	1:C:378:ARG:NH2	2.81	0.49
1:A:335:ALA:HA	1:A:384:LEU:HD22	1.95	0.49
1:B:234:TRP:CE2	2:G:1:GLC:H2	2.48	0.49
1:D:268:ASP:HA	1:D:324:ARG:NH2	2.28	0.49
5:C:723:HOH:O	1:D:301:PRO:HG2	2.12	0.49
1:C:165:TRP:HZ3	2:I:3:GLC:H5	1.77	0.48
1:C:201:LEU:HD12	1:C:246:PHE:CE1	2.48	0.48
1:C:473:ARG:HG2	1:C:473:ARG:HH11	1.78	0.48
1:A:235:GLU:HB3	1:A:236:GLU:OE2	2.14	0.48
1:B:266:ALA:O	1:B:324:ARG:HD2	2.13	0.48
1:C:252:TYR:N	1:C:253:PRO:CD	2.77	0.48
1:D:122:THR:HG23	1:D:173:LEU:HD13	1.95	0.48
1:D:405:GLN:O	1:D:406:ASP:HB3	2.12	0.48
1:A:233:ILE:HG21	1:A:237:ALA:HB2	1.96	0.48
1:B:34:PRO:HG2	1:B:37:ALA:CB	2.41	0.48
1:D:369:GLU:HB3	1:D:372:ARG:HD3	1.94	0.48
1:D:378:ARG:HG2	1:D:378:ARG:HH11	1.79	0.48
1:D:393:ALA:HB3	1:D:416:TYR:HE2	1.79	0.48
1:A:12:ILE:O	1:A:14:PRO:HD3	2.14	0.47
1:A:250:MSE:HE2	1:A:310:LEU:HD13	1.96	0.47
1:A:300:ARG:HB3	1:A:302:GLU:OE2	2.14	0.47
1:B:331:ARG:HG2	1:B:331:ARG:HH11	1.79	0.47
1:D:100:ARG:O	1:D:104:GLU:HG3	2.15	0.47
1:D:121:HIS:CD2	1:D:170:LEU:HD23	2.49	0.47
1:D:235:GLU:HB3	1:D:236:GLU:OE2	2.13	0.47
1:D:56:LEU:N	1:D:57:PRO:HD2	2.30	0.47
1:C:279:ARG:HH11	1:C:279:ARG:HG2	1.79	0.47
1:D:403:TYR:O	1:D:409:LEU:HD12	2.15	0.47
1:B:71:PRO:HB2	1:B:80:ARG:HB3	1.96	0.47
1:A:193:ARG:HD3	5:A:737:HOH:O	2.14	0.47
1:A:433:LEU:O	1:A:436:VAL:HG23	2.15	0.47
1:D:115:LEU:HD11	1:D:196:VAL:HG21	1.96	0.47
1:D:335:ALA:HA	1:D:384:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:VAL:O	1:D:452:CYS:HB3	2.15	0.47
1:C:202:ASP:OD1	3:J:1:GLC:C1	2.63	0.47
1:A:252:TYR:N	1:A:253:PRO:CD	2.78	0.47
1:B:420:VAL:HG22	1:B:469:LEU:CD1	2.46	0.46
1:C:137:GLU:HG2	1:C:150:PHE:CE2	2.50	0.46
1:D:13:PHE:CZ	1:D:79:HIS:HA	2.50	0.46
1:B:408:HIS:HB3	1:B:427:PHE:CZ	2.51	0.46
1:B:252:TYR:N	1:B:253:PRO:CD	2.78	0.46
1:B:39:PRO:HD2	5:B:740:HOH:O	2.15	0.46
1:A:420:VAL:HG22	1:A:469:LEU:CD1	2.45	0.46
1:B:201:LEU:HD21	1:B:216:PHE:CZ	2.51	0.46
1:B:300:ARG:HB3	1:B:302:GLU:OE2	2.16	0.46
2:G:4:GLC:H61	2:G:5:GLC:O5	2.16	0.46
1:A:135:ASN:HB2	1:A:139:SER:HB2	1.97	0.45
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.79	0.45
1:B:281:GLU:HG2	5:B:798:HOH:O	2.15	0.45
1:B:437:PHE:HB3	1:B:474:GLU:OE2	2.16	0.45
1:D:331:ARG:HG2	1:D:331:ARG:HH11	1.80	0.45
1:A:55:LYS:HE3	1:A:368:TRP:CE2	2.52	0.45
1:B:163:ALA:HB1	1:B:167:ASN:O	2.16	0.45
1:C:68:TYR:C	1:C:68:TYR:CD1	2.89	0.45
1:D:300:ARG:O	1:D:304:VAL:HG23	2.16	0.45
1:A:115:LEU:HD11	1:A:196:VAL:HG21	1.99	0.45
1:A:369:GLU:HB3	1:A:372:ARG:HD3	1.98	0.45
1:B:310:LEU:H	1:B:310:LEU:CD2	2.29	0.45
1:D:431:PHE:HB2	1:D:432:PRO:HD2	1.99	0.45
1:A:310:LEU:HD23	1:A:310:LEU:H	1.80	0.45
1:C:386:ARG:O	1:C:390:GLU:HG3	2.16	0.45
1:A:374:GLN:HG3	1:A:377:LEU:H	1.82	0.45
1:B:182:GLU:HG2	5:B:796:HOH:O	2.17	0.45
5:C:723:HOH:O	1:D:302:GLU:HG3	2.16	0.45
1:D:230:VAL:HA	1:D:248:ALA:O	2.17	0.45
1:D:241:LEU:HD13	1:D:303:VAL:HG11	1.99	0.45
1:C:233:ILE:CG2	1:C:237:ALA:HB2	2.45	0.44
1:C:347:TYR:O	1:C:350:GLU:HG2	2.17	0.44
1:D:286:LEU:HD11	1:D:401:ARG:NH1	2.31	0.44
1:D:163:ALA:HB1	1:D:167:ASN:O	2.17	0.44
1:C:202:ASP:O	1:C:203:VAL:C	2.55	0.44
1:A:200:ARG:C	1:A:200:ARG:HD3	2.38	0.44
1:A:335:ALA:CA	1:A:384:LEU:HD22	2.48	0.44
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:HIS:CE1	1:C:81:TYR:HB2	2.53	0.44
1:D:370:GLU:HG2	1:D:373:TRP:CH2	2.53	0.44
1:D:428:ARG:HD2	1:D:430:ASP:OD2	2.18	0.44
1:A:17:PHE:HB3	5:A:608:HOH:O	2.18	0.44
1:C:100:ARG:NH1	1:C:100:ARG:CG	2.79	0.44
1:C:428:ARG:CD	1:C:428:ARG:H	2.29	0.44
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.81	0.44
1:A:38:PRO:HA	1:A:39:PRO:HD3	1.92	0.44
1:B:446:LEU:HD21	1:B:473:ARG:HD2	2.00	0.44
1:C:387:LEU:HD12	1:C:387:LEU:HA	1.86	0.44
1:D:100:ARG:HG2	1:D:100:ARG:NH1	2.30	0.44
1:A:420:VAL:HG22	1:A:469:LEU:HD11	2.00	0.44
1:B:291:ARG:HD2	5:B:787:HOH:O	2.18	0.44
1:C:124:ARG:NH2	1:C:169:GLU:HG2	2.33	0.44
1:C:203:VAL:O	1:C:203:VAL:HG23	2.18	0.44
1:B:133:MSE:HE1	1:B:155:TYR:HE2	1.83	0.43
1:D:200:ARG:C	1:D:200:ARG:HD3	2.38	0.43
1:D:8:PHE:C	1:D:8:PHE:CD1	2.90	0.43
1:A:359:ASP:OD1	1:A:360:PRO:HA	2.17	0.43
1:D:165:TRP:HZ3	2:K:3:GLC:H5	1.84	0.43
1:B:203:VAL:O	1:B:203:VAL:HG23	2.18	0.43
1:D:369:GLU:HG2	1:D:372:ARG:CD	2.49	0.43
1:B:202[B]:ASP:O	1:B:203:VAL:C	2.56	0.43
1:D:209:ASP:HB2	5:D:926:HOH:O	2.17	0.43
1:A:240:TRP:HB3	1:A:246:PHE:CD2	2.54	0.43
1:B:370:GLU:HG2	1:B:373:TRP:CZ3	2.54	0.43
1:A:250:MSE:HE3	1:A:308:MSE:SE	2.69	0.43
1:A:393:ALA:HB3	1:A:416:TYR:CE2	2.47	0.43
1:A:419:VAL:HG12	1:A:464:LEU:HD12	2.00	0.43
1:A:465:PRO:HG2	1:A:468:SER:CB	2.49	0.43
1:A:217:ARG:HD2	1:A:245:MSE:O	2.18	0.43
1:C:133:MSE:HE1	1:C:155:TYR:HE2	1.84	0.43
1:B:236:GLU:CD	1:B:236:GLU:H	2.21	0.43
1:C:56:LEU:N	1:C:57:PRO:CD	2.81	0.43
1:B:200:ARG:HE	1:B:250:MSE:SE	2.52	0.42
1:B:38:PRO:HA	1:B:39:PRO:HD3	1.92	0.42
1:A:370:GLU:HG2	1:A:373:TRP:CH2	2.53	0.42
1:C:331:ARG:HH11	1:C:331:ARG:HG2	1.84	0.42
1:C:250:MSE:HA	1:C:308:MSE:HB3	2.01	0.42
1:C:335:ALA:CA	1:C:384:LEU:HD22	2.49	0.42
1:D:433:LEU:HD13	1:D:437:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:HB2	1:B:216:PHE:CE1	2.54	0.42
1:D:301:PRO:O	1:D:305:ARG:HG3	2.20	0.42
1:D:391:HIS:HA	1:D:392:PRO:HD2	1.86	0.42
1:A:292:LEU:HB3	1:A:296:PHE:CE2	2.55	0.42
1:A:267:LEU:HD12	1:A:322:LEU:O	2.19	0.42
1:A:446:LEU:HD21	1:A:473:ARG:CD	2.49	0.42
1:C:393:ALA:HB3	1:C:416:TYR:HE2	1.84	0.42
1:C:416:TYR:CE1	1:C:473:ARG:HD3	2.54	0.42
1:D:347:TYR:O	1:D:350:GLU:HG2	2.20	0.42
1:A:232:GLU:O	1:A:232:GLU:HG2	2.20	0.42
1:A:137:GLU:HG2	1:A:150:PHE:CD2	2.54	0.42
1:D:188:ALA:HB2	1:D:216:PHE:CE1	2.54	0.42
1:A:150:PHE:HA	1:A:151:PRO:C	2.40	0.42
1:B:117:GLY:HA2	5:B:614:HOH:O	2.19	0.42
1:B:137:GLU:HG2	1:B:150:PHE:CD2	2.54	0.42
1:B:288:PHE:CE2	1:B:292:LEU:HD11	2.55	0.42
1:D:252:TYR:O	1:D:256:ARG:HG3	2.20	0.42
1:D:305:ARG:NH2	5:D:917:HOH:O	2.53	0.42
1:D:383:ARG:HH11	1:D:383:ARG:HG2	1.85	0.42
1:D:250:MSE:HA	1:D:308:MSE:HB3	2.02	0.41
1:D:351:GLU:HG2	1:D:352:VAL:HG13	2.02	0.41
1:D:115:LEU:CD1	1:D:196:VAL:HG21	2.50	0.41
1:A:204:PRO:HG2	1:A:233:ILE:HD11	2.02	0.41
1:A:241:LEU:HD13	1:A:303:VAL:HG11	2.02	0.41
1:B:352:VAL:HG12	1:B:378:ARG:HD2	2.02	0.41
1:C:310:LEU:H	1:C:310:LEU:HD23	1.85	0.41
1:C:473:ARG:NH1	1:C:474:GLU:O	2.53	0.41
1:D:39:PRO:CG	1:D:364:GLY:HA2	2.49	0.41
1:D:444:VAL:CG1	1:D:475:ALA:HB2	2.50	0.41
1:A:133:MSE:HG2	1:A:152:LEU:HD12	2.01	0.41
1:C:236:GLU:OE1	1:D:301:PRO:HG2	2.20	0.41
1:D:386:ARG:O	1:D:390:GLU:HG3	2.20	0.41
1:D:397:ALA:HA	1:D:398:PRO:HD3	1.90	0.41
1:D:57:PRO:HG2	5:D:921:HOH:O	2.19	0.41
1:A:250:MSE:HA	1:A:308:MSE:HB3	2.03	0.41
1:B:254:LEU:HD23	1:B:309:ASN:OD1	2.21	0.41
1:D:133:MSE:HE2	5:D:823:HOH:O	2.20	0.41
1:A:148:LYS:HB2	1:A:160:ASN:OD1	2.21	0.41
1:B:53:ALA:HB3	5:B:715:HOH:O	2.20	0.41
1:C:196:VAL:HG12	1:C:198:GLY:H	1.85	0.41
1:C:239:PHE:C	1:C:239:PHE:CD1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ALA:CB	1:C:384:LEU:HD22	2.50	0.41
1:D:233:ILE:HG21	1:D:237:ALA:HB2	2.03	0.41
1:B:234:TRP:CD2	2:G:1:GLC:H2	2.55	0.41
1:A:374:GLN:OE1	1:A:376:ASP:HB3	2.21	0.41
1:A:436:VAL:C	1:A:438:PRO:HD3	2.41	0.41
1:D:335:ALA:CA	1:D:384:LEU:HD22	2.51	0.41
2:K:5:GLC:H61	2:K:6:GLC:O5	2.21	0.41
1:B:193:ARG:HG2	1:B:193:ARG:NH1	2.36	0.41
1:C:149:GLY:N	1:C:160:ASN:OD1	2.54	0.41
1:D:255:ALA:HB2	1:D:310:LEU:O	2.21	0.41
1:C:79:HIS:CD2	3:J:2:GLC:H2	2.56	0.41
1:B:8:PHE:CD1	1:B:8:PHE:C	2.95	0.41
1:D:181:ARG:NH2	1:D:209:ASP:OD2	2.54	0.41
1:B:359:ASP:HA	1:B:362:ASN:OD1	2.21	0.40
1:D:38:PRO:HA	1:D:39:PRO:HD3	1.92	0.40
1:A:196:VAL:HG12	1:A:198:GLY:H	1.85	0.40
1:B:392:PRO:HA	1:B:395:ARG:NH1	2.37	0.40
1:C:291:ARG:NH1	1:C:294:ASP:OD2	2.54	0.40
1:B:339:LEU:HD11	1:B:469:LEU:HD21	2.03	0.40
1:D:9:PHE:HB3	1:D:345:THR:HG23	2.01	0.40
1:D:413:ARG:HH11	1:D:413:ARG:HG3	1.86	0.40
1:A:202:ASP:O	1:A:203:VAL:C	2.59	0.40
1:C:421:ASN:O	1:C:467:PHE:HA	2.22	0.40
1:C:432:PRO:HG2	5:C:653:HOH:O	2.21	0.40
1:B:135:ASN:HB2	1:B:139:SER:HB2	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	472/475 (99%)	446 (94%)	26 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	473/475 (100%)	451 (95%)	21 (4%)	1 (0%)	47	58
1	C	472/475 (99%)	450 (95%)	22 (5%)	0	100	100
1	D	472/475 (99%)	444 (94%)	27 (6%)	1 (0%)	47	58
All	All	1889/1900 (99%)	1791 (95%)	96 (5%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	461	GLY
1	D	462	PRO

### 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	379/373 (102%)	374 (99%)	5 (1%)	69	82
1	B	378/373 (101%)	367 (97%)	11 (3%)	42	58
1	C	376/373 (101%)	366 (97%)	10 (3%)	44	61
1	D	379/373 (102%)	369 (97%)	10 (3%)	46	63
All	All	1512/1492 (101%)	1476 (98%)	36 (2%)	49	66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	68	TYR
1	A	133	MSE
1	A	173	LEU
1	A	464	LEU
1	B	8	PHE
1	B	68	TYR
1	B	100	ARG
1	B	173	LEU

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Mol	Chain	Res	Type
1	B	182	GLU
1	B	265	GLU
1	B	310	LEU
1	B	320	LEU
1	B	322	LEU
1	B	374	GLN
1	B	384	LEU
1	C	68	TYR
1	C	100	ARG
1	C	291	ARG
1	C	310	LEU
1	C	322	LEU
1	C	374	GLN
1	C	387	LEU
1	C	400	LEU
1	C	428	ARG
1	C	464	LEU
1	D	8	PHE
1	D	41	LEU
1	D	68	TYR
1	D	160	ASN
1	D	173	LEU
1	D	265	GLU
1	D	291	ARG
1	D	322	LEU
1	D	369	GLU
1	D	464	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	GLN
1	A	274	GLN
1	B	11	GLN
1	B	70	ASN
1	B	88	GLN
1	B	274	GLN
1	B	434	HIS
1	C	11	GLN
1	C	70	ASN
1	C	88	GLN

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Mol	Chain	Res	Type
1	C	274	GLN
1	C	434	HIS
1	D	11	GLN
1	D	70	ASN
1	D	88	GLN
1	D	274	GLN
1	D	455	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

40 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	E	1	2	11,11,12	0.53	0	15,15,17	0.58	0
2	GLC	E	2	2	11,11,12	0.62	0	15,15,17	0.63	0
2	GLC	E	3	2	11,11,12	0.62	0	15,15,17	0.65	0
2	GLC	E	4	2	11,11,12	0.59	0	15,15,17	0.61	0
2	GLC	E	5	2	11,11,12	0.53	0	15,15,17	0.58	1 (6%)
2	GLC	E	6	2	11,11,12	0.61	0	15,15,17	0.58	0
2	GLC	E	7	2	11,11,12	0.62	0	15,15,17	0.75	0
3	GLC	F	1	3	11,11,12	0.46	0	15,15,17	0.60	0
3	GLC	F	2	3	11,11,12	0.56	0	15,15,17	0.54	0
3	GLC	F	3	3	11,11,12	0.47	0	15,15,17	0.51	0
2	GLC	G	1	2	11,11,12	0.53	0	15,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	G	2	2	11,11,12	0.56	0	15,15,17	0.57	0
2	GLC	G	3	2	11,11,12	0.54	0	15,15,17	0.70	0
2	GLC	G	4	2	11,11,12	0.42	0	15,15,17	0.55	0
2	GLC	G	5	2	11,11,12	0.54	0	15,15,17	0.52	0
2	GLC	G	6	2	11,11,12	0.55	0	15,15,17	0.70	0
2	GLC	G	7	2	11,11,12	0.63	0	15,15,17	0.58	0
3	GLC	H	1	3	11,11,12	0.49	0	15,15,17	0.89	1 (6%)
3	GLC	H	2	3	11,11,12	0.61	0	15,15,17	0.50	0
3	GLC	H	3	3	11,11,12	0.52	0	15,15,17	0.47	0
2	GLC	I	1	2	11,11,12	0.57	0	15,15,17	0.54	0
2	GLC	I	2	2	11,11,12	0.62	0	15,15,17	0.72	1 (6%)
2	GLC	I	3	2	11,11,12	0.64	0	15,15,17	0.60	0
2	GLC	I	4	2	11,11,12	0.53	0	15,15,17	0.57	0
2	GLC	I	5	2	11,11,12	0.55	0	15,15,17	0.56	0
2	GLC	I	6	2	11,11,12	0.55	0	15,15,17	0.60	1 (6%)
2	GLC	I	7	2	11,11,12	0.68	0	15,15,17	0.82	0
3	GLC	J	1	3	11,11,12	0.48	0	15,15,17	0.56	0
3	GLC	J	2	3	11,11,12	0.55	0	15,15,17	0.54	0
3	GLC	J	3	3	11,11,12	0.55	0	15,15,17	0.47	0
2	GLC	K	1	2	11,11,12	0.53	0	15,15,17	0.68	0
2	GLC	K	2	2	11,11,12	0.62	0	15,15,17	0.67	1 (6%)
2	GLC	K	3	2	11,11,12	0.58	0	15,15,17	0.59	0
2	GLC	K	4	2	11,11,12	0.56	0	15,15,17	0.57	0
2	GLC	K	5	2	11,11,12	0.52	0	15,15,17	0.61	1 (6%)
2	GLC	K	6	2	11,11,12	0.61	0	15,15,17	0.60	0
2	GLC	K	7	2	11,11,12	0.70	0	15,15,17	0.70	0
3	GLC	L	1	3	11,11,12	0.42	0	15,15,17	0.70	0
3	GLC	L	2	3	11,11,12	0.56	0	15,15,17	0.55	0
3	GLC	L	3	3	11,11,12	0.60	0	15,15,17	0.53	0

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	E	1	2	-	0/2/19/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	6	2	-	2/2/19/22	0/1/1/1
2	GLC	E	7	2	-	2/2/19/22	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
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	2/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	G	6	2	-	0/2/19/22	0/1/1/1
2	GLC	G	7	2	-	0/2/19/22	0/1/1/1
3	GLC	H	1	3	-	0/2/19/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
3	GLC	H	3	3	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	2/2/19/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	1/2/19/22	0/1/1/1
2	GLC	I	5	2	-	0/2/19/22	0/1/1/1
2	GLC	I	6	2	-	2/2/19/22	0/1/1/1
2	GLC	I	7	2	-	2/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/19/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	3	3	-	1/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	0/2/19/22	0/1/1/1
2	GLC	K	5	2	-	2/2/19/22	0/1/1/1
2	GLC	K	6	2	-	0/2/19/22	0/1/1/1
2	GLC	K	7	2	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/19/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	GLC	C2-C3-C4	-2.24	107.03	110.89
2	I	2	GLC	C1-O5-C5	2.17	115.13	112.19
2	K	5	GLC	C1-O5-C5	2.09	115.03	112.19
2	K	2	GLC	C1-O5-C5	2.06	114.98	112.19
2	I	6	GLC	C1-O5-C5	2.03	114.94	112.19
2	E	5	GLC	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	6	GLC	O5-C5-C6-O6
2	I	6	GLC	C4-C5-C6-O6
2	E	6	GLC	C4-C5-C6-O6
2	K	5	GLC	O5-C5-C6-O6
2	E	7	GLC	C4-C5-C6-O6
2	K	5	GLC	C4-C5-C6-O6
2	E	6	GLC	O5-C5-C6-O6
2	I	7	GLC	C4-C5-C6-O6
2	E	7	GLC	O5-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
3	J	3	GLC	O5-C5-C6-O6
2	I	7	GLC	O5-C5-C6-O6
2	G	4	GLC	C4-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	G	4	GLC	O5-C5-C6-O6
2	I	4	GLC	C4-C5-C6-O6
3	F	3	GLC	O5-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	GLC	2	0
2	I	3	GLC	1	0
2	K	6	GLC	1	0
3	J	1	GLC	1	0
2	K	3	GLC	1	0
3	H	1	GLC	1	0

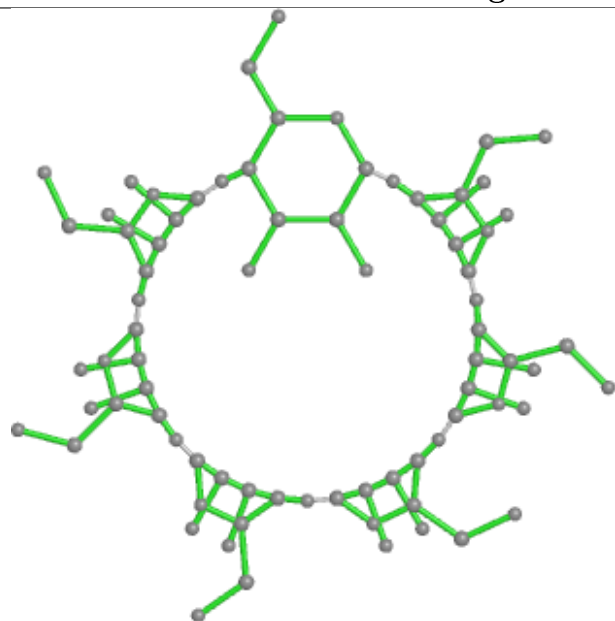
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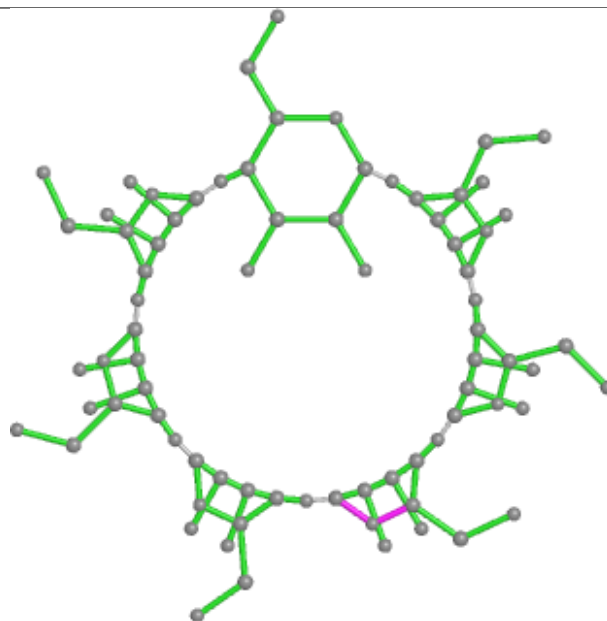
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	5	GLC	1	0
2	K	1	GLC	1	0
3	J	2	GLC	1	0
3	F	1	GLC	1	0
2	G	4	GLC	1	0
2	E	4	GLC	1	0
3	L	1	GLC	1	0
2	K	5	GLC	1	0
2	E	3	GLC	1	0

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

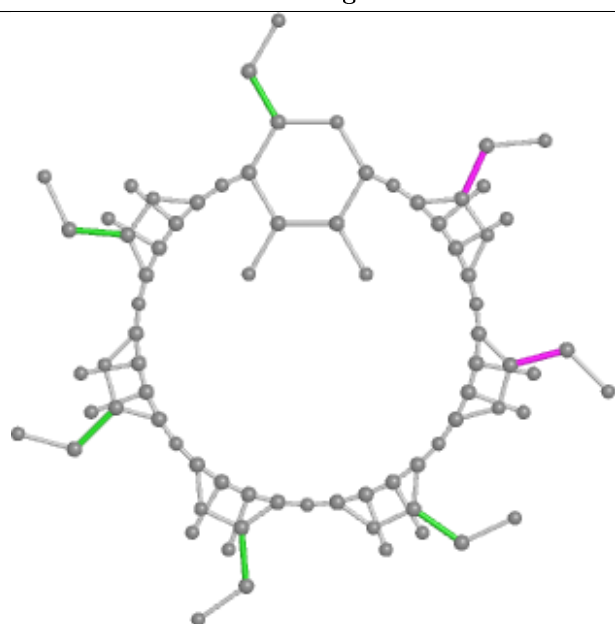
## Oligosaccharide Chain E



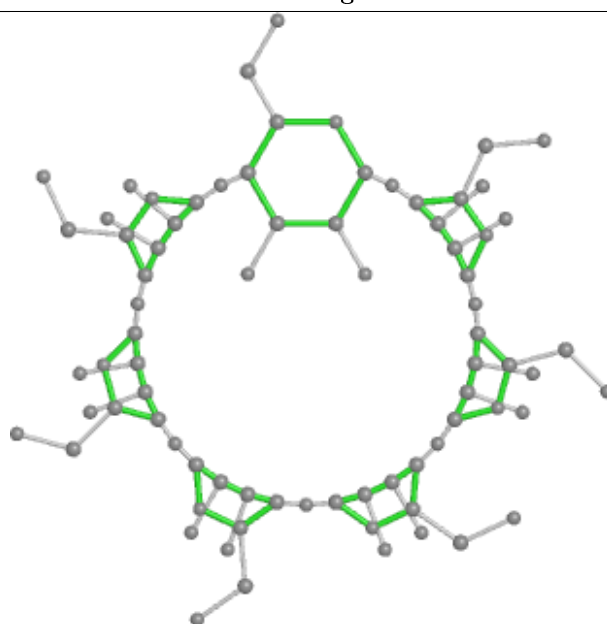
Bond lengths



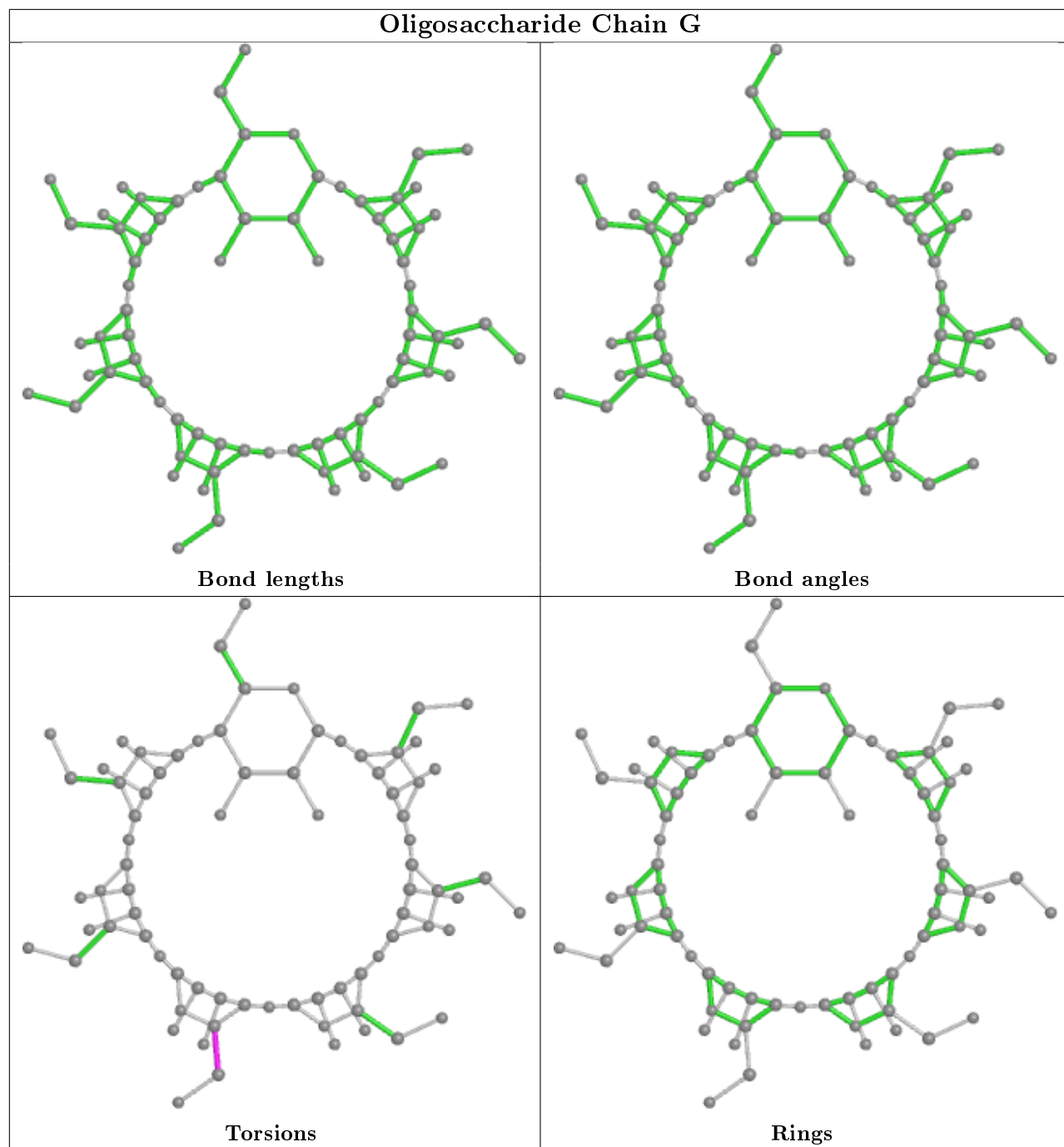
Bond angles

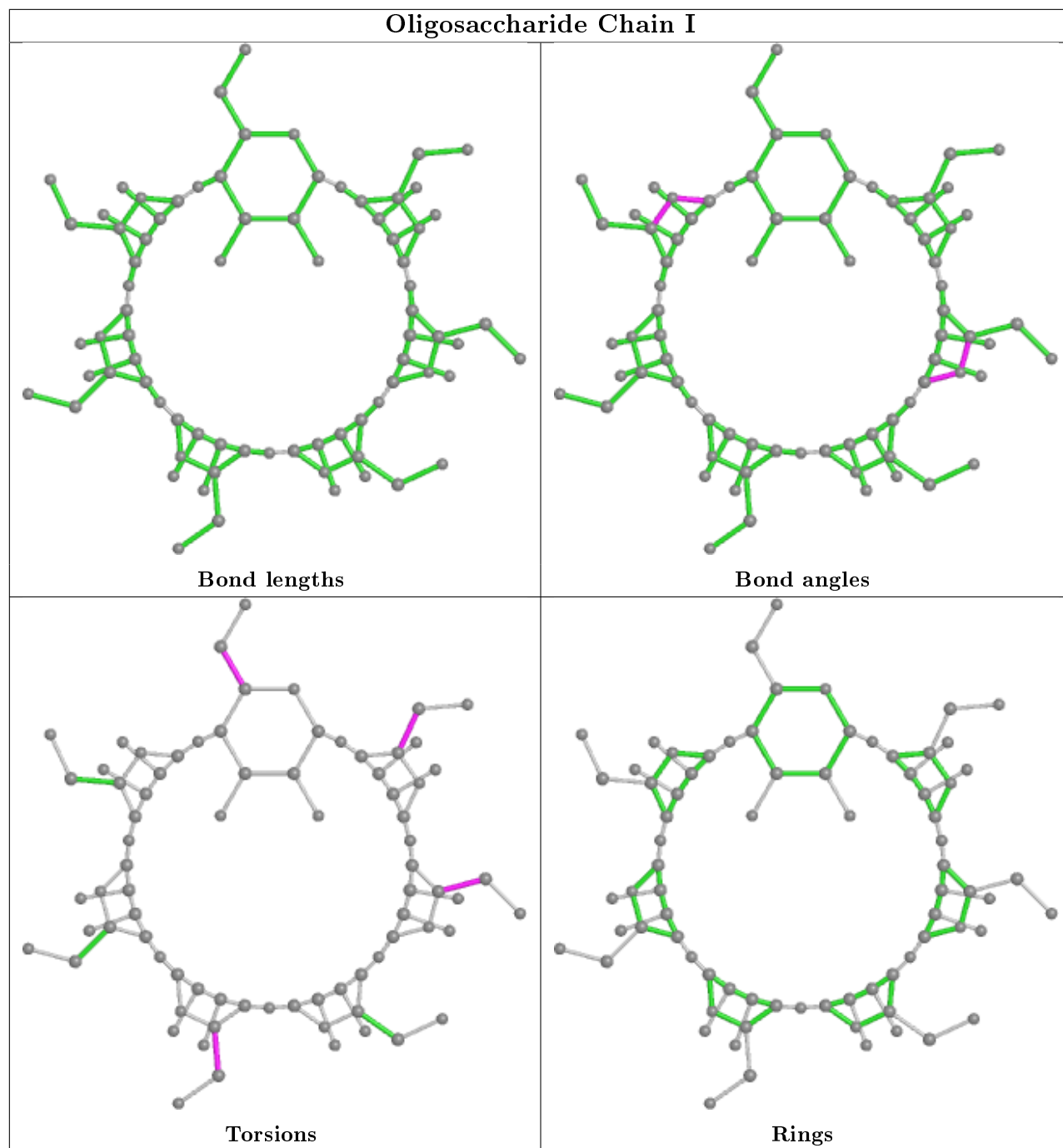


Torsions

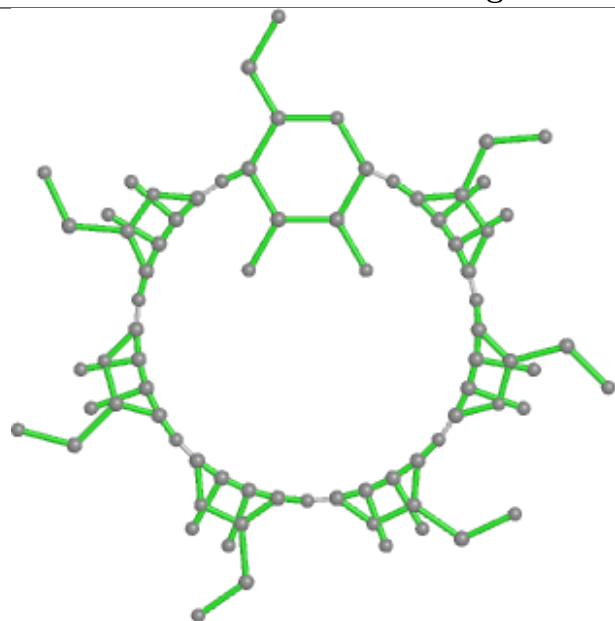


Rings

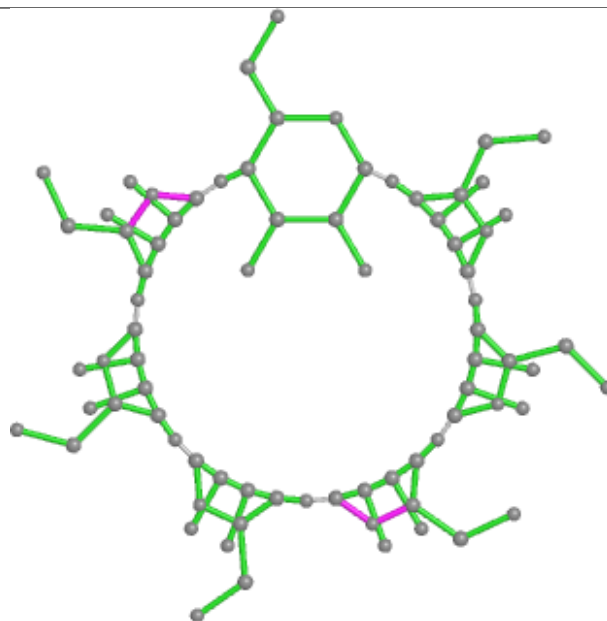




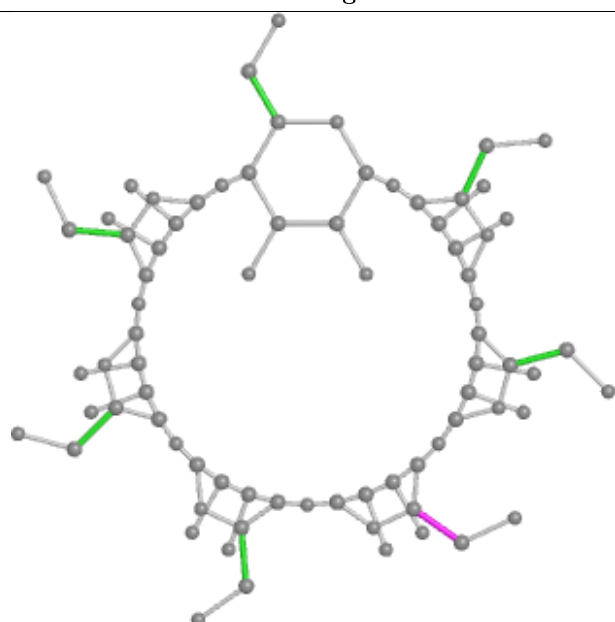
## Oligosaccharide Chain K



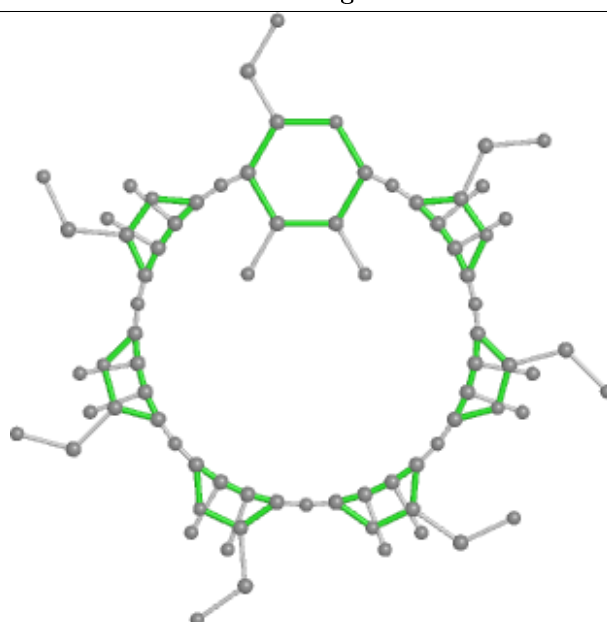
Bond lengths



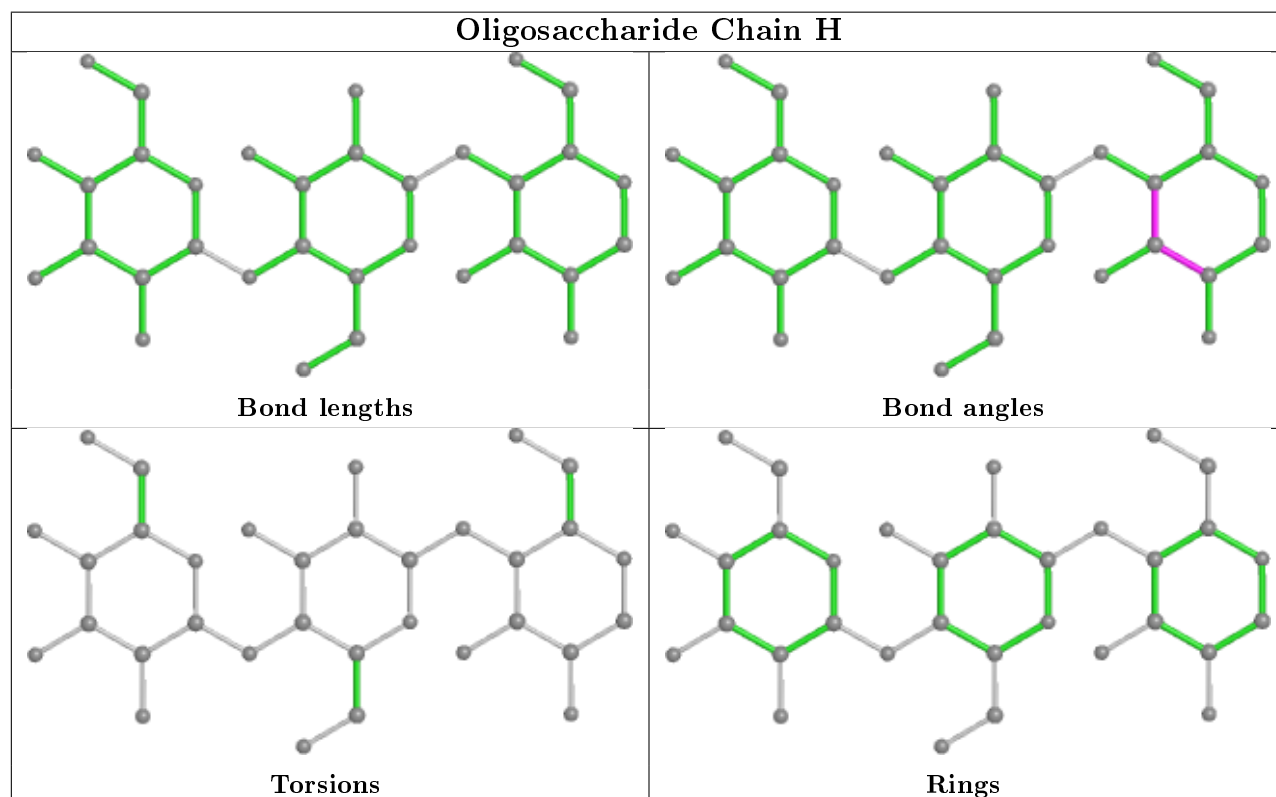
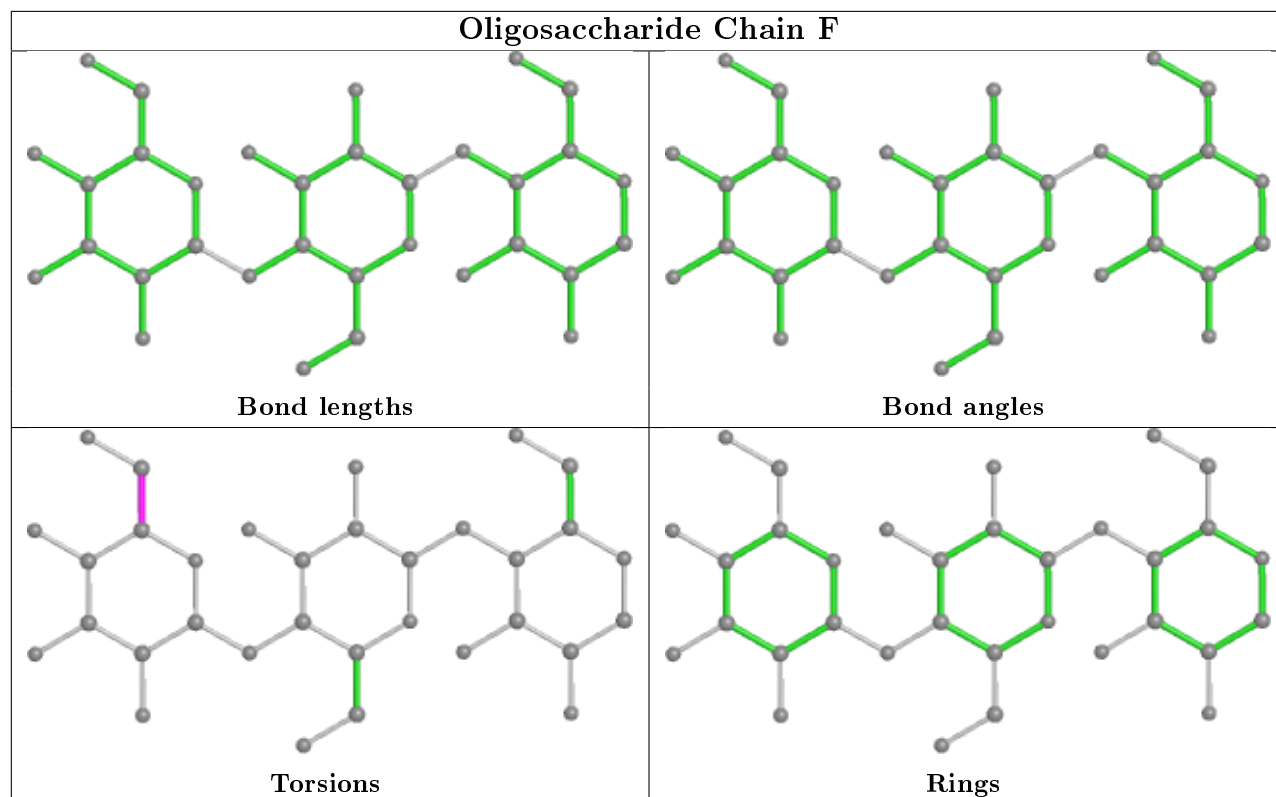
Bond angles

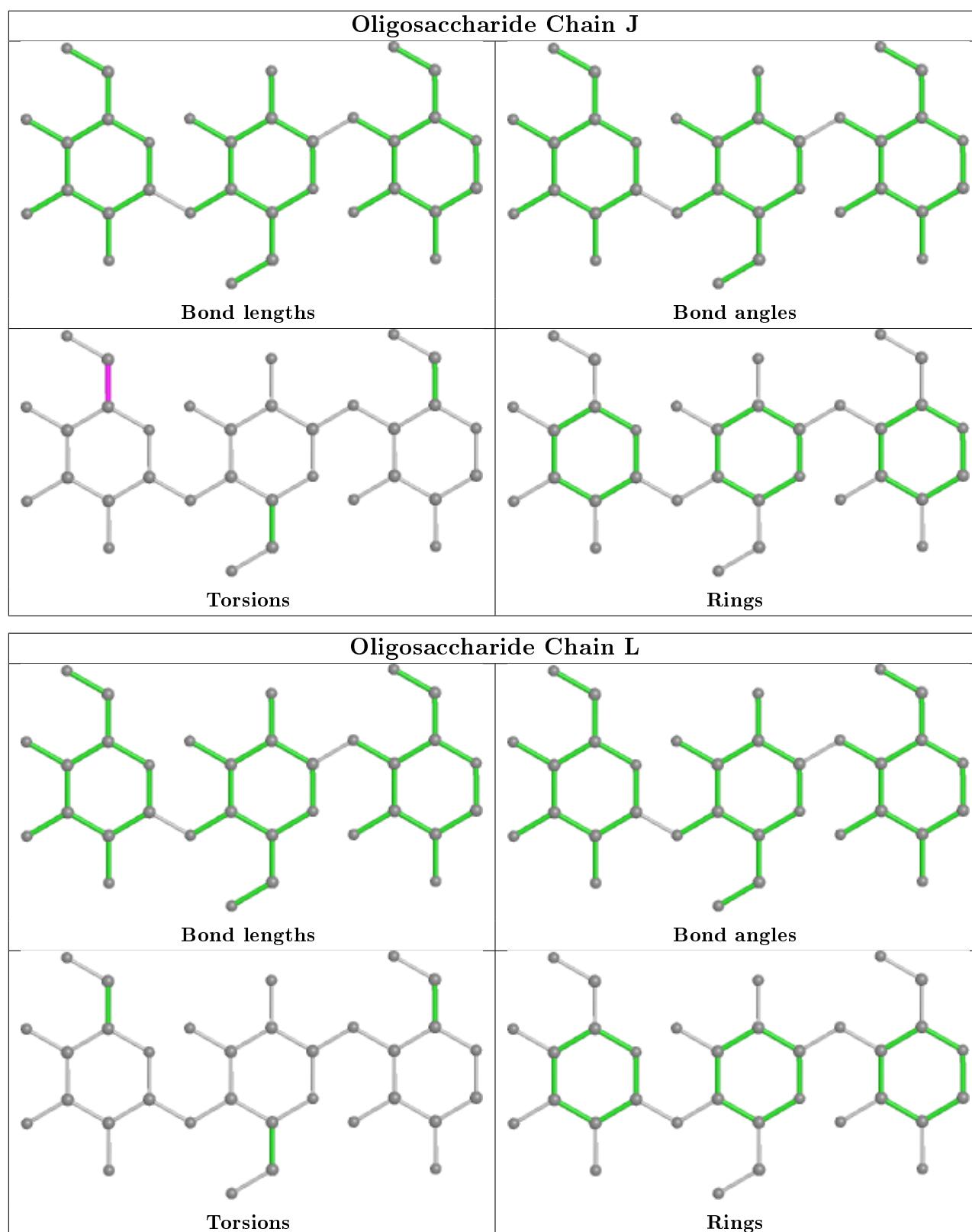


Torsions



Rings





## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
4	PO4	D	800	-	4,4,4	1.71	0	6,6,6	0.42	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	467/475 (98%)	-0.13	11 (2%) 59 66	16, 31, 46, 59	0
1	B	467/475 (98%)	-0.28	11 (2%) 59 66	12, 25, 44, 64	0
1	C	467/475 (98%)	-0.18	5 (1%) 80 85	15, 27, 52, 65	0
1	D	467/475 (98%)	-0.07	24 (5%) 28 35	12, 29, 63, 80	0
All	All	1868/1900 (98%)	-0.16	51 (2%) 54 62	12, 28, 52, 80	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	475	ALA	7.3
1	A	460	CYS	4.9
1	A	440	GLY	4.6
1	C	475	ALA	4.2
1	D	459	LEU	4.1
1	D	455	GLN	4.0
1	B	475	ALA	3.9
1	D	457	GLY	3.9
1	B	441	GLY	3.9
1	D	433	LEU	3.8
1	A	455	GLN	3.7
1	B	455	GLN	3.5
1	D	441	GLY	3.5
1	D	456	GLY	3.5
1	D	439	ARG	3.4
1	D	454	PRO	3.3
1	B	440	GLY	3.2
1	A	438	PRO	3.2
1	C	239	PHE	3.2
1	B	456	GLY	3.2
1	C	31	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	425	HIS	3.1
1	B	265	GLU	3.0
1	A	475	ALA	2.9
1	D	430	ASP	2.8
1	A	265	GLU	2.7
1	B	425	HIS	2.7
1	A	441	GLY	2.6
1	B	439	ARG	2.6
1	A	424	PRO	2.6
1	D	31	PRO	2.6
1	B	460	CYS	2.5
1	B	406	ASP	2.5
1	D	407	GLY	2.5
1	D	451	VAL	2.4
1	A	425	HIS	2.4
1	C	453	THR	2.4
1	D	424	PRO	2.3
1	D	431	PHE	2.3
1	D	458	ARG	2.2
1	D	460	CYS	2.2
1	A	31	PRO	2.2
1	C	440	GLY	2.2
1	D	434	HIS	2.2
1	D	428	ARG	2.1
1	D	406	ASP	2.1
1	D	265	GLU	2.1
1	D	284	GLN	2.1
1	A	2	ALA	2.1
1	B	457	GLY	2.0
1	D	285	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

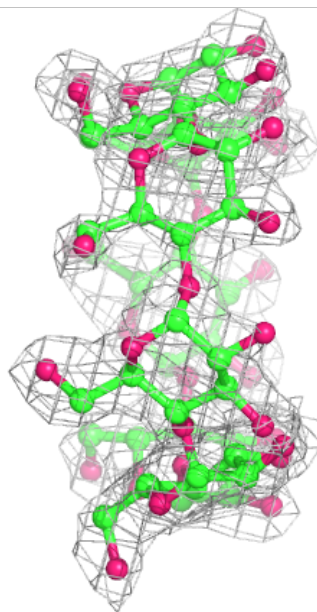
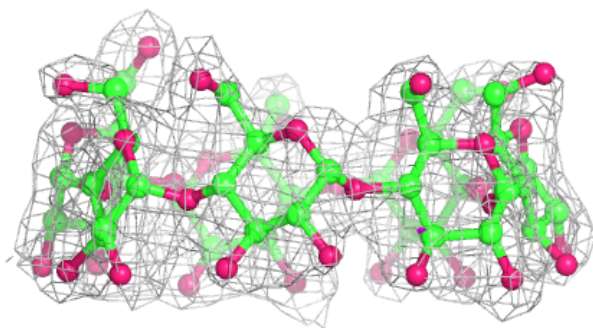
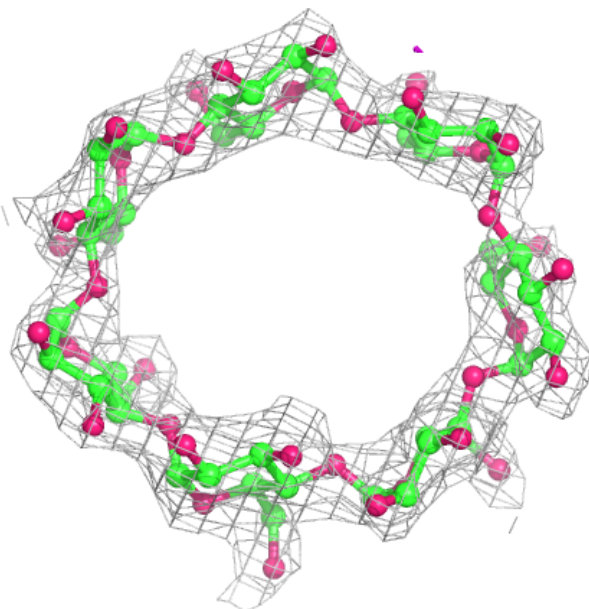
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	J	3	11/12	0.79	0.30	55,56,57,57	0
2	GLC	I	6	11/12	0.80	0.20	70,72,73,73	0
2	GLC	I	7	11/12	0.80	0.26	59,63,66,67	0
3	GLC	J	2	11/12	0.81	0.22	43,47,49,52	0
2	GLC	I	4	11/12	0.82	0.19	72,73,74,75	0
2	GLC	E	6	11/12	0.83	0.20	50,56,56,57	0
2	GLC	K	6	11/12	0.84	0.21	42,45,47,48	0
3	GLC	F	1	11/12	0.84	0.17	36,41,42,42	0
2	GLC	I	3	11/12	0.84	0.17	65,67,69,71	0
3	GLC	F	2	11/12	0.84	0.20	40,44,47,50	0
3	GLC	F	3	11/12	0.85	0.24	52,53,55,55	0
2	GLC	G	5	11/12	0.86	0.16	37,39,40,44	0
3	GLC	J	1	11/12	0.86	0.19	43,45,46,46	0
2	GLC	E	4	11/12	0.86	0.15	54,56,57,57	0
2	GLC	E	2	11/12	0.87	0.17	43,45,46,51	0
3	GLC	L	2	11/12	0.88	0.18	30,33,35,37	0
2	GLC	E	3	11/12	0.88	0.18	54,55,58,59	0
3	GLC	H	1	11/12	0.88	0.17	23,27,29,31	0
2	GLC	E	7	11/12	0.90	0.18	41,43,47,48	0
2	GLC	E	5	11/12	0.90	0.14	54,56,56,57	0
2	GLC	I	5	11/12	0.90	0.15	74,76,77,78	0
3	GLC	H	3	11/12	0.91	0.12	31,32,35,36	0
2	GLC	G	4	11/12	0.91	0.13	31,33,36,37	0
2	GLC	E	1	11/12	0.91	0.12	37,41,42,43	0
2	GLC	I	1	11/12	0.91	0.13	45,53,55,55	0
2	GLC	I	2	11/12	0.91	0.14	56,58,60,62	0
3	GLC	L	3	11/12	0.91	0.12	39,41,41,43	0
3	GLC	H	2	11/12	0.92	0.12	20,26,27,31	0
2	GLC	G	6	11/12	0.92	0.12	31,33,36,38	0
3	GLC	L	1	11/12	0.92	0.16	28,32,34,35	0
2	GLC	K	7	11/12	0.92	0.18	38,42,44,44	0
2	GLC	K	4	11/12	0.92	0.16	44,45,46,47	0
2	GLC	K	2	11/12	0.92	0.20	40,40,42,43	0
2	GLC	K	5	11/12	0.93	0.11	45,46,48,49	0
2	GLC	K	3	11/12	0.93	0.17	41,42,44,45	0
2	GLC	K	1	11/12	0.94	0.15	37,40,42,44	0
2	GLC	G	7	11/12	0.95	0.09	23,25,28,30	0
2	GLC	G	1	11/12	0.96	0.10	22,23,26,26	0
2	GLC	G	3	11/12	0.96	0.09	31,33,34,34	0
2	GLC	G	2	11/12	0.97	0.08	22,24,25,29	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.

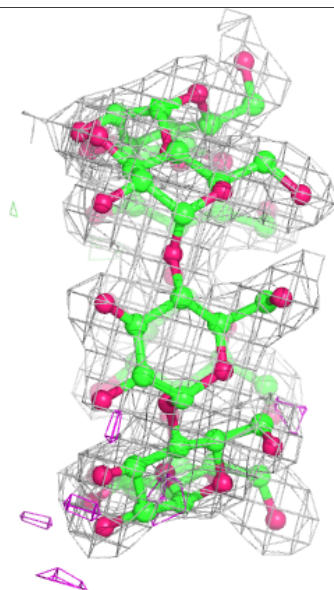
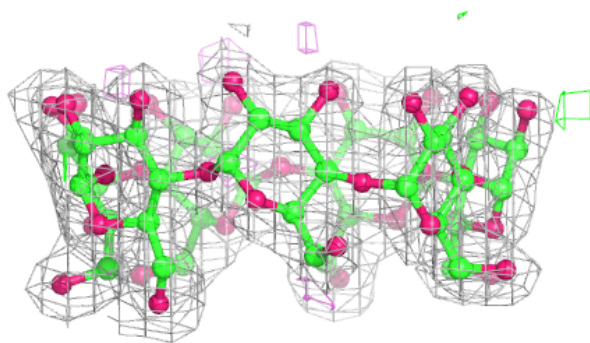
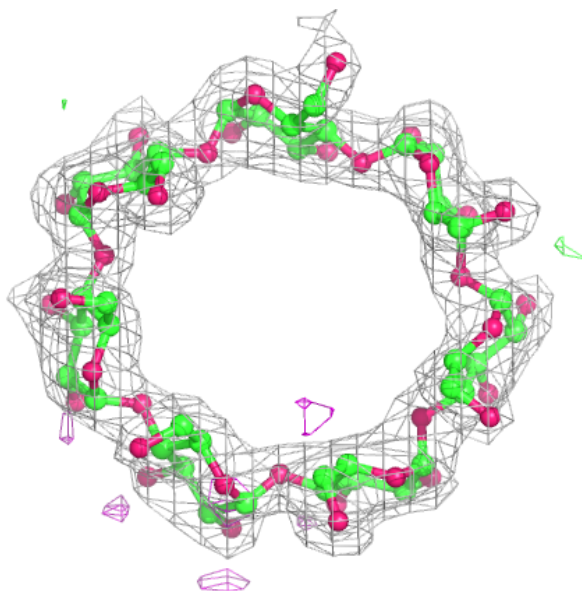
**Electron density around Chain E:**

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



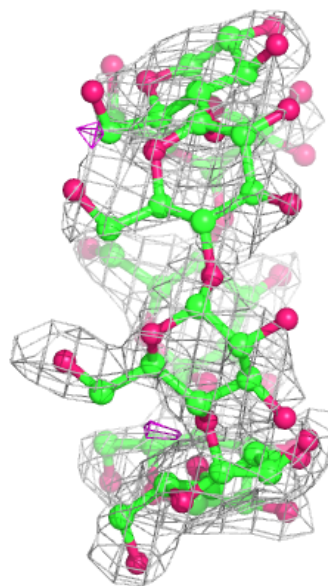
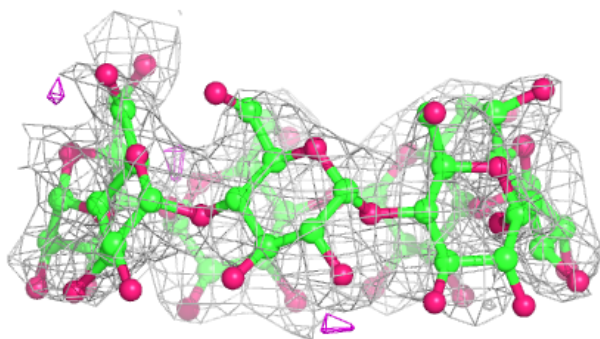
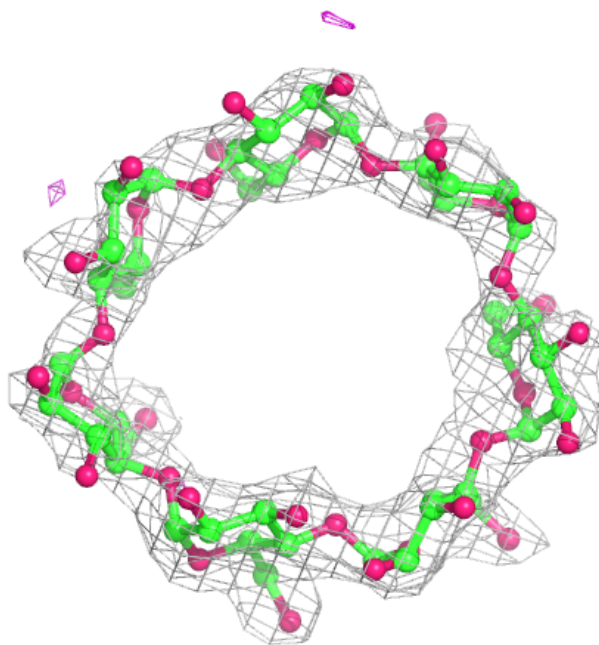
**Electron density around Chain G:**

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



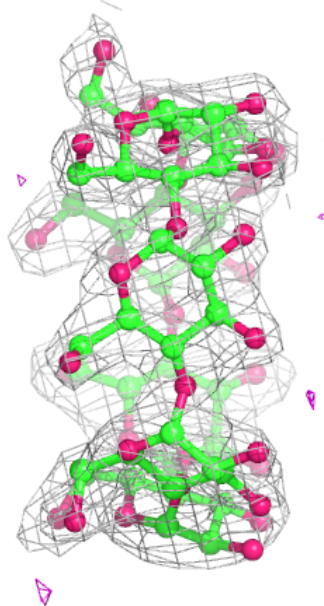
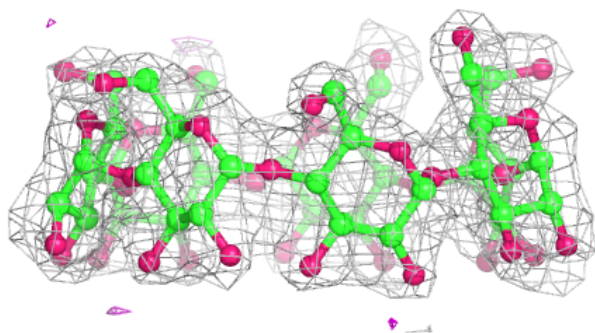
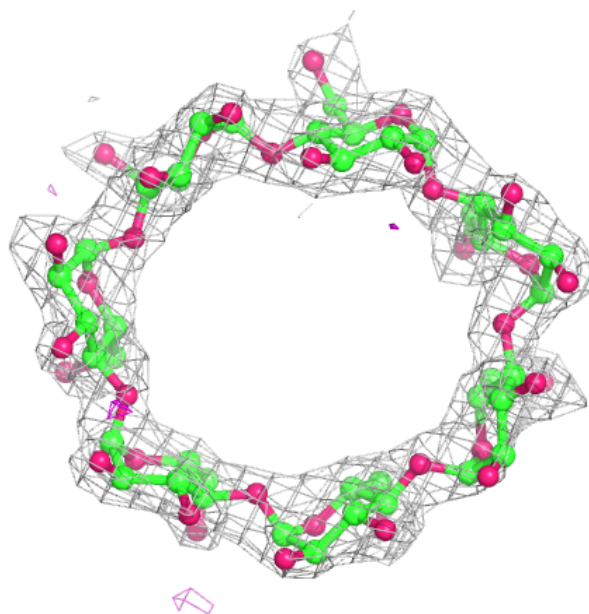
**Electron density around Chain I:**

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



**Electron density around Chain K:**

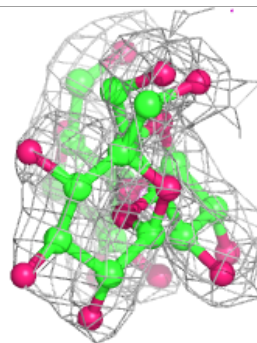
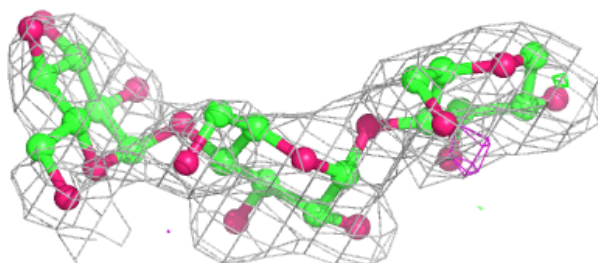
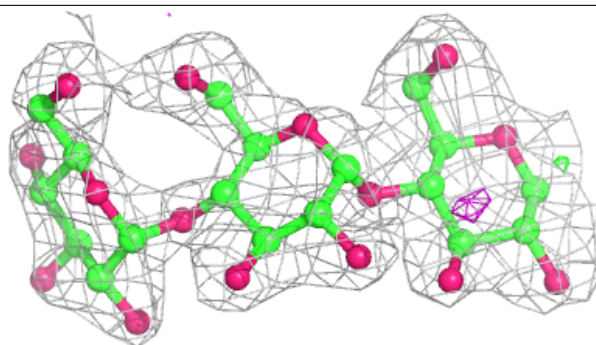
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



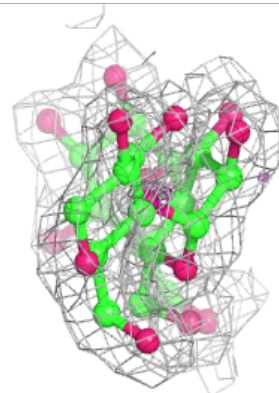
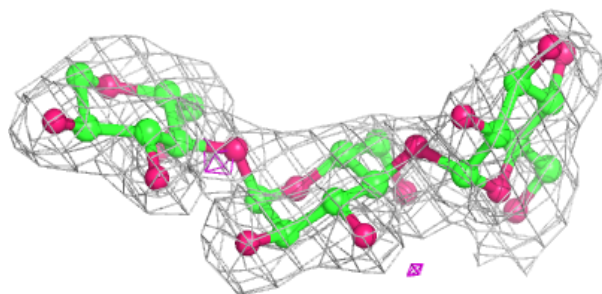
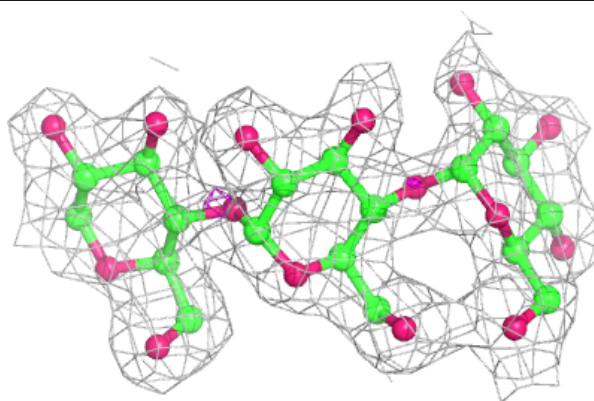


**Electron density around Chain F:**

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

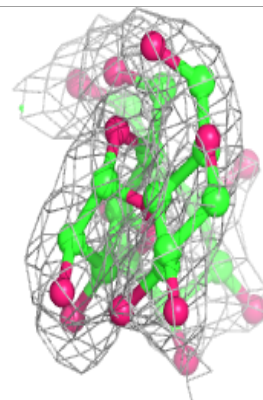
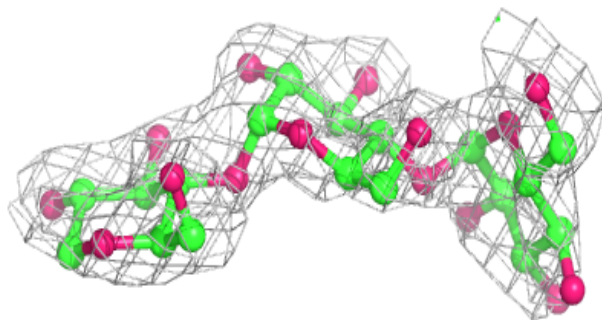
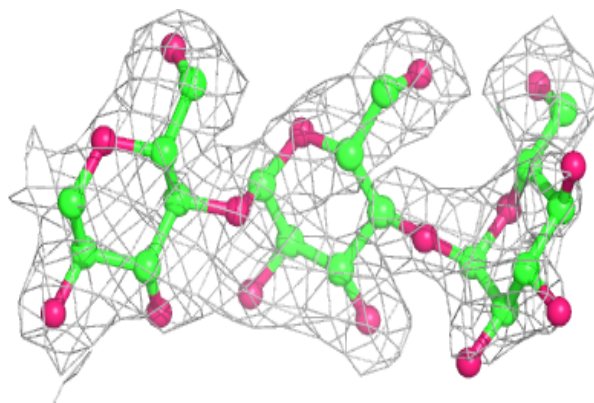
**Electron density around Chain H:**

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

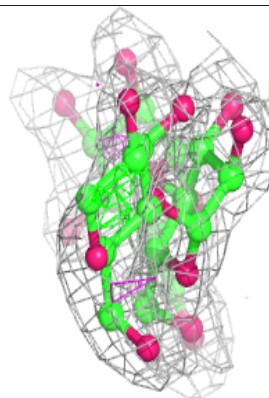
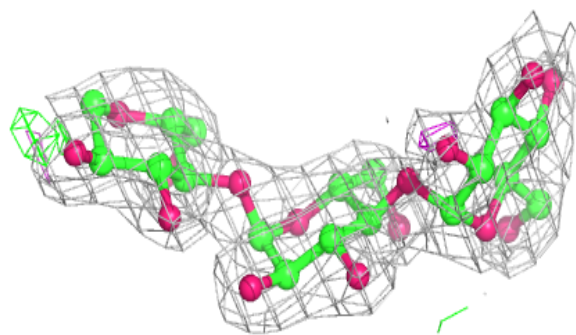
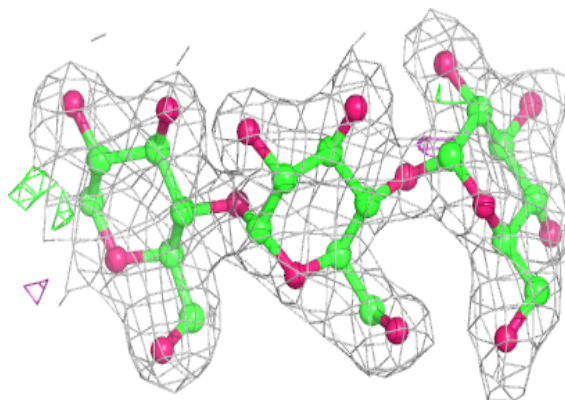


**Electron density around Chain J:**

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

**Electron density around Chain L:**

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



## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	PO4	D	800	5/5	0.96	0.12	55,55,56,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.