Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 05:35 PM EST

PDB ID	:	2YP1
Title	:	Crystallization of a 45 kDa peroxygenase- peroxidase from the mushroom Agrocybe aegerita and structure determination by SAD utilizing only the haem iron
Authors	:	Piontek, K.; Strittmatter, E.; Ullrich, R.; Plattner, D.A.; Hofrichter, M.
Deposited on	:	2012-10-29
Resolution	:	2.31 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:

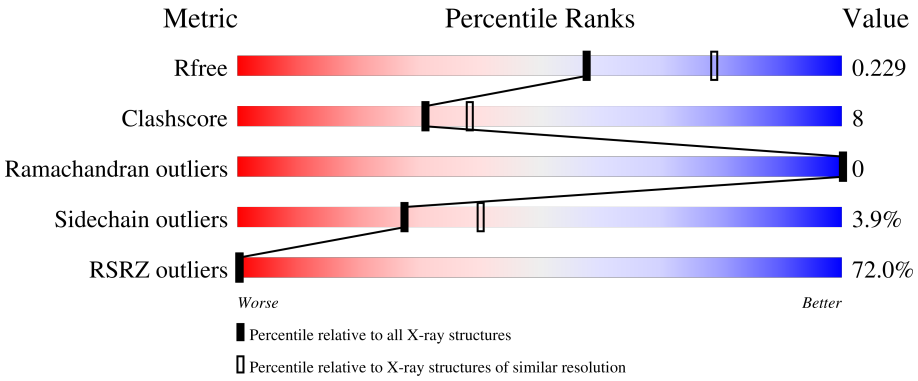
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	325	74% 84% 14% ••
1	B	325	57% 83% 15% •
1	C	325	65% 88% 11%
1	D	325	91% 78% 20% ••
2	E	6	33% 67%
3	F	5	20% 60% 20%

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Mol	Chain	Length	Quality of chain
3	J	5	40% 60%
4	G	2	100%
4	I	2	100%
4	K	2	100%
4	L	2	50% 50%
4	N	2	100%
4	P	2	100%
4	Q	2	50% 50%
4	R	2	100%
4	S	2	50% 50%
5	H	8	12% 75% 12%
5	M	8	12% 62% 25%
6	O	3	100%
6	T	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	A	1331	-	-	X	-
10	SO4	B	1331	-	-	X	-

2 Entry composition (i)

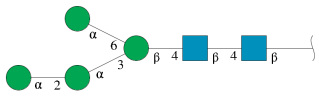
There are 12 unique types of molecules in this entry. The entry contains 12290 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AROMATIC PEROXYGENASE.

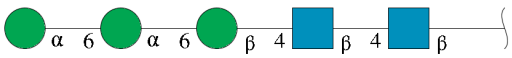
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2506	1589	434	475	8			
1	B	324	Total	C	N	O	S	0	4	0
			2537	1608	442	479	8			
1	C	325	Total	C	N	O	S	0	1	0
			2526	1599	440	479	8			
1	D	323	Total	C	N	O	S	0	1	0
			2507	1590	435	474	8			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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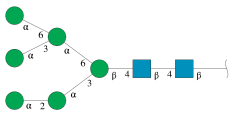
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	5	Total C N O 61 34 2 25	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C N O 28 16 2 10	0	0	0
4	I	2	Total C N O 28 16 2 10	0	0	0
4	K	2	Total C N O 28 16 2 10	0	0	0
4	L	2	Total C N O 28 16 2 10	0	0	0
4	N	2	Total C N O 28 16 2 10	0	0	0
4	P	2	Total C N O 28 16 2 10	0	0	0
4	Q	2	Total C N O 28 16 2 10	0	0	0
4	R	2	Total C N O 28 16 2 10	0	0	0
4	S	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	8	Total C N O 94 52 2 40	0	0	0

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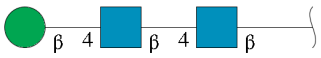
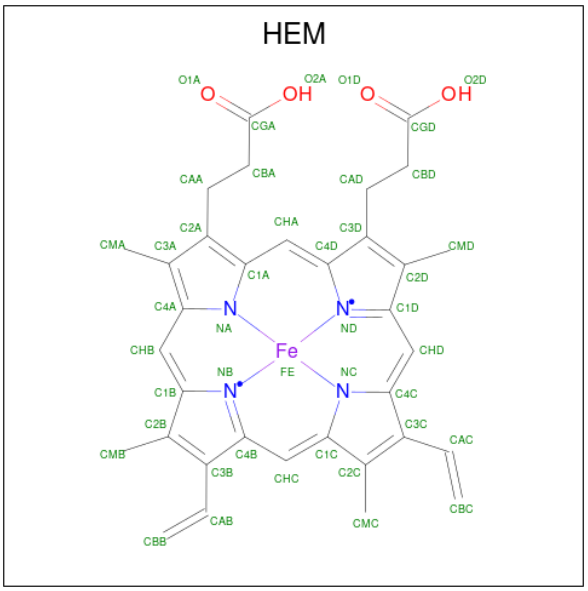
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	M	8	Total C N O 94 52 2 40	0	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	O	3	Total C N O 39 22 2 15	0	0	0
6	T	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C Fe N O 43 34 1 4 4	0	0
7	B	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0

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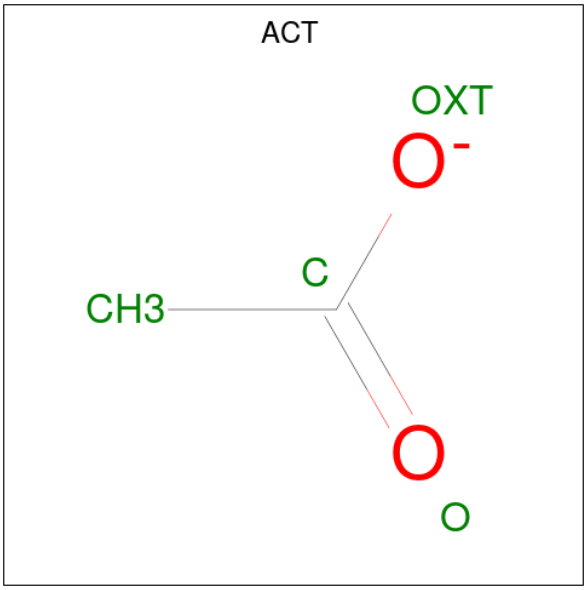
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		

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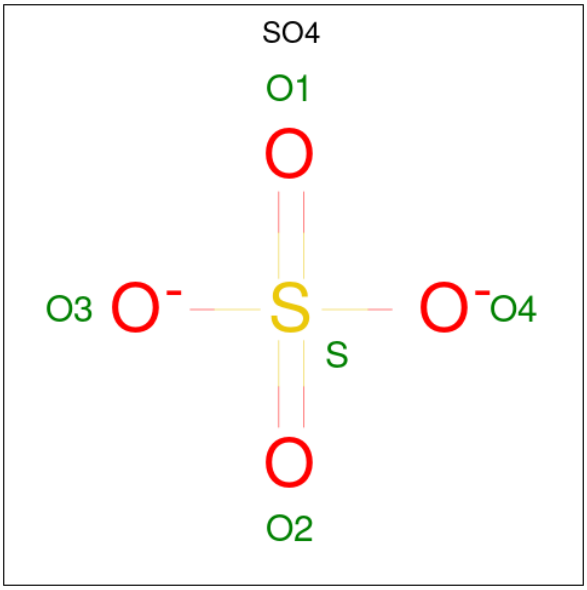
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 4 2 2	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	A	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0

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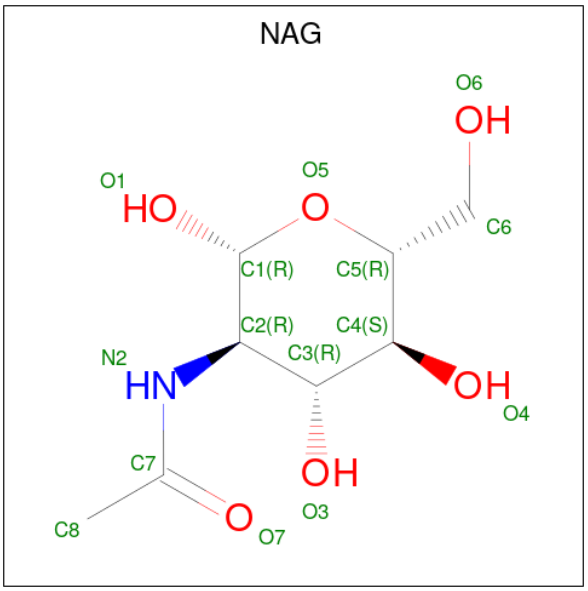
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	327	Total O 327 327	0	0
12	B	369	Total O 369 369	0	0

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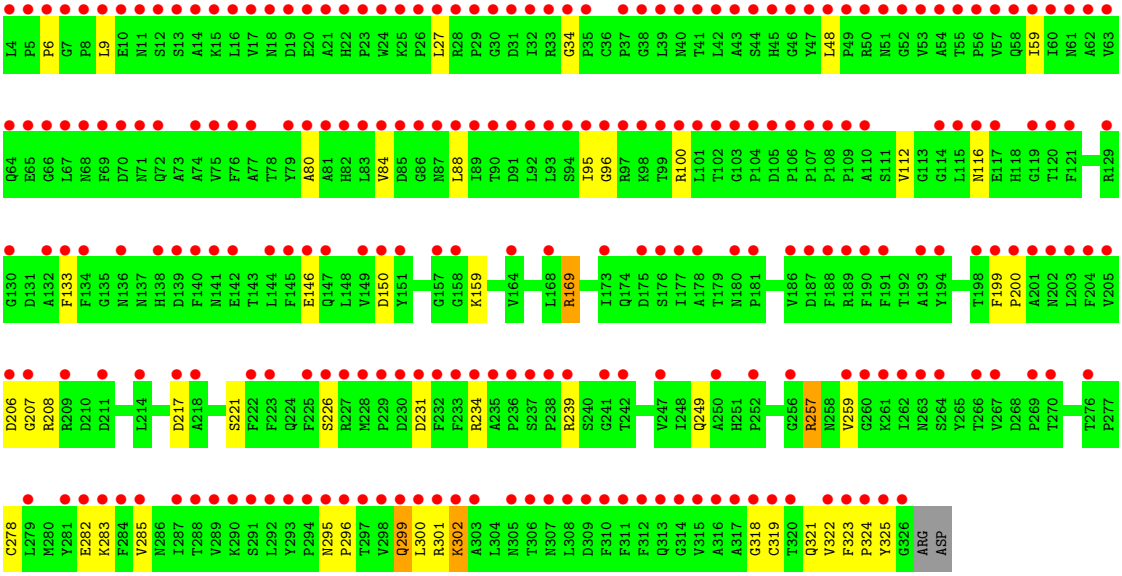
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	291	Total O 291 291	0	0
12	D	198	Total O 198 198	0	0

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. 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. 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.

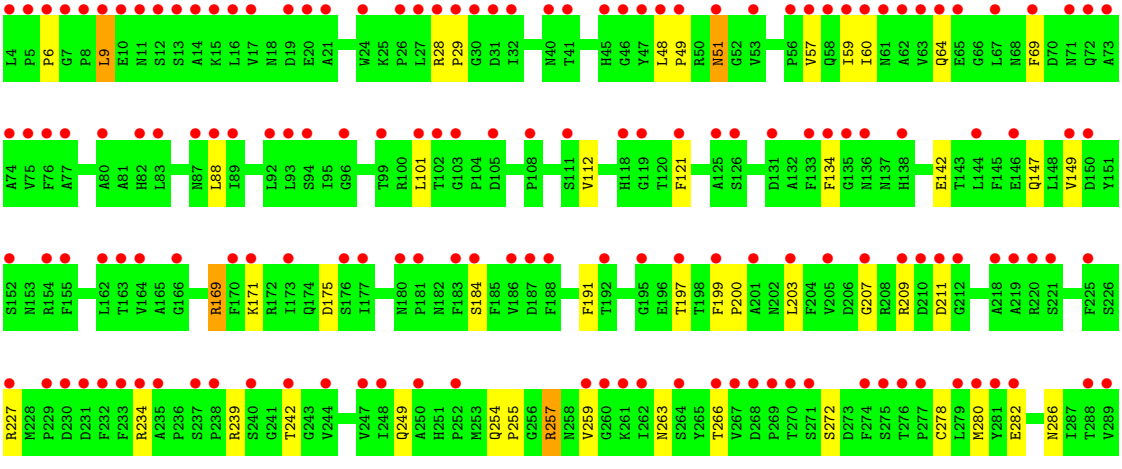
• Molecule 1: AROMATIC PEROXYGENASE

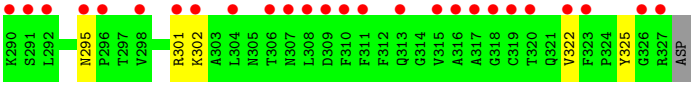
Chain A:



• Molecule 1: AROMATIC PEROXYGENASE

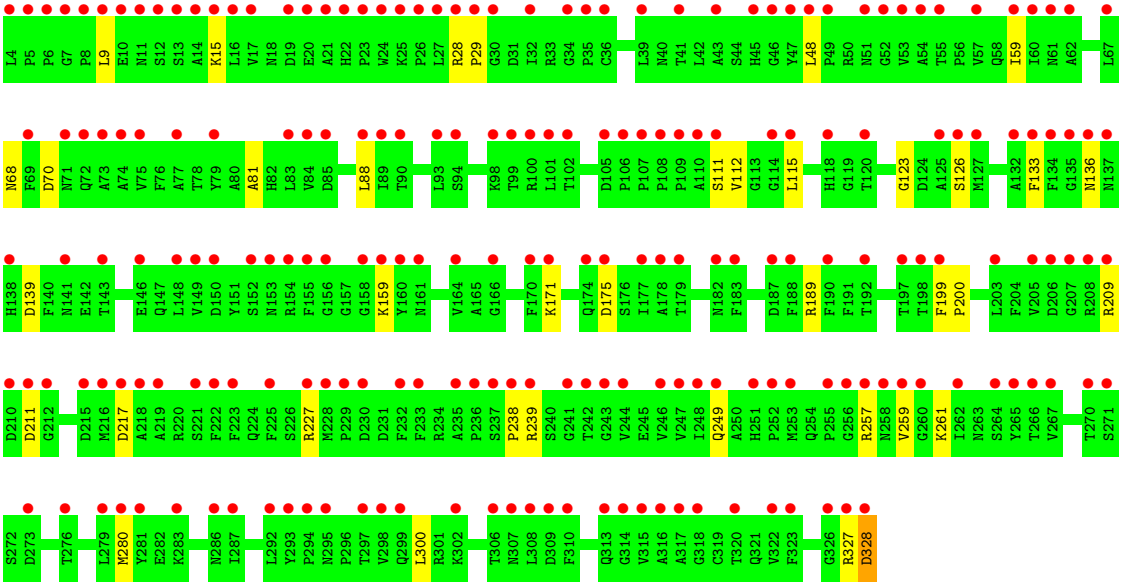
Chain B:





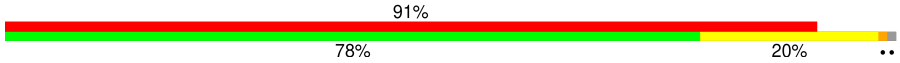
• Molecule 1: AROMATIC PEROXYGENASE

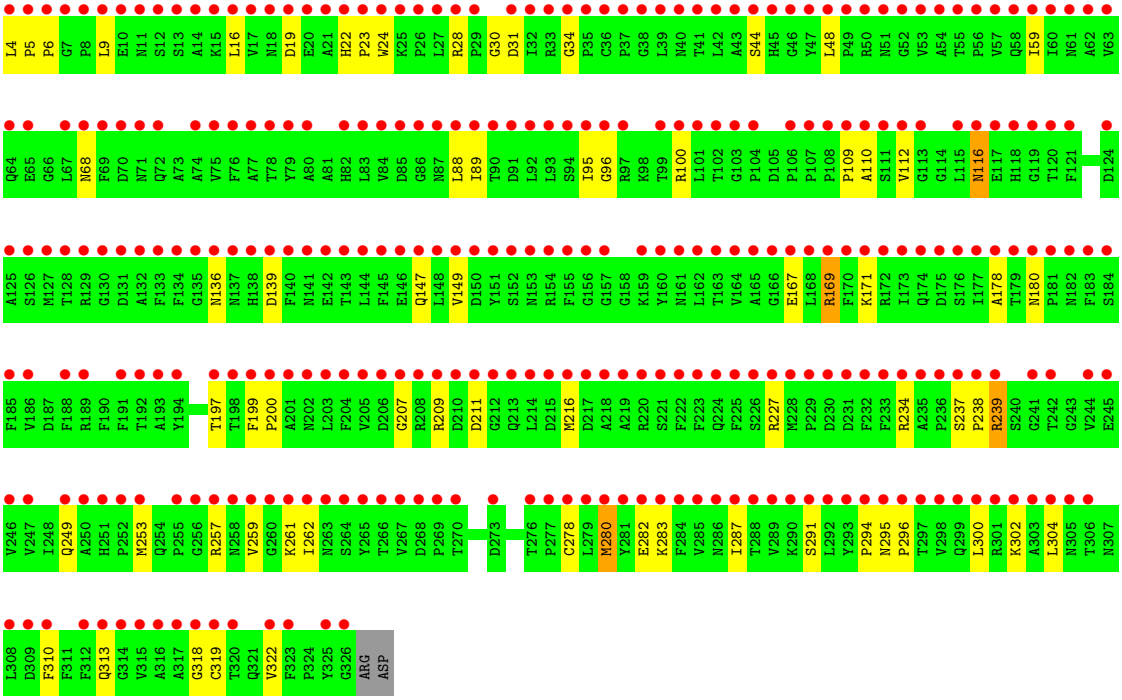
Chain C:



• Molecule 1: AROMATIC PEROXYGENASE

Chain D:



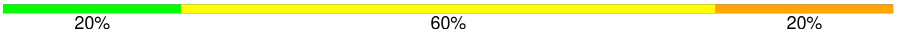


• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

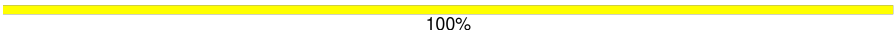
Chain K:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

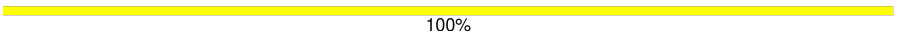
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

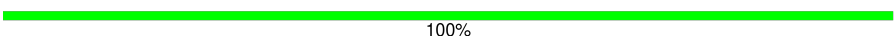


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

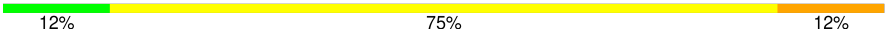


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

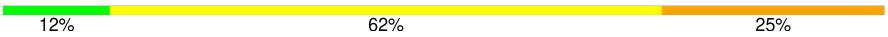
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



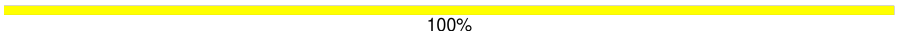
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



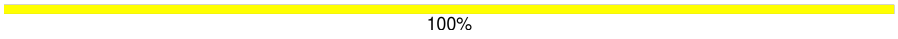
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.75Å 144.88Å 134.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.31 48.91 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-2.31) 99.7 (48.91-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.01 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.230 0.177 , 0.229	Depositor DCC
R_{free} test set	4843 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 68.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.62	EDS
Total number of atoms	12290	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACT, BMA, MG, MAN, SO4, NAG, HEM

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	0.48	0/2579	0.56	0/3512
1	B	0.52	0/2619	0.57	0/3564
1	C	0.52	0/2599	0.53	0/3538
1	D	0.44	0/2580	0.51	0/3513
All	All	0.49	0/10377	0.54	0/14127

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	30	GLY	Peptide

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	2506	0	2386	40	0
1	B	2537	0	2426	41	0
1	C	2526	0	2405	20	0
1	D	2507	0	2390	52	0
2	E	72	0	61	2	0
3	F	61	0	52	2	0
3	J	61	0	52	2	0
4	G	28	0	25	3	0
4	I	28	0	25	3	0
4	K	28	0	25	2	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
5	H	94	0	79	4	0
5	M	94	0	79	2	0
6	O	39	0	34	0	0
6	T	39	0	34	0	0
7	A	43	0	30	5	0
7	B	43	0	30	3	0
7	C	43	0	30	3	0
7	D	43	0	30	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	4	0	3	0	0
9	B	4	0	3	0	0
9	C	8	0	6	0	0
9	D	4	0	3	0	0
10	A	20	0	0	2	0
10	B	15	0	0	2	0
10	C	20	0	0	0	0
10	D	10	0	0	2	0
11	C	14	0	13	1	0
11	D	42	0	39	0	0
12	A	327	0	0	9	0
12	B	369	0	0	13	0
12	C	291	0	0	5	0
12	D	198	0	0	6	0
All	All	12290	0	10410	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (174) 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)
7:D:350:HEM:HMC2	7:D:350:HEM:HBC2	1.29	1.11
1:A:259:VAL:HG23	1:A:259:VAL:O	1.68	0.94
1:A:299:GLN:HG2	12:A:2271:HOH:O	1.73	0.88
1:A:299:GLN:NE2	12:A:2273:HOH:O	2.07	0.88
1:D:89:ILE:HD11	1:D:300:LEU:HD13	1.56	0.88
7:D:350:HEM:HBC2	7:D:350:HEM:CMC	2.02	0.85
1:D:100:ARG:N	10:D:1328:SO4:O1	2.13	0.81
1:D:259:VAL:O	1:D:259:VAL:CG1	2.29	0.81
1:B:278:CYS:HB2	10:B:1331:SO4:O2	1.81	0.80
5:H:6:MAN:C6	5:H:8:MAN:H3	2.11	0.80
1:D:296:PRO:HB2	1:D:300:LEU:HB3	1.65	0.79
5:H:6:MAN:H62	5:H:8:MAN:H3	1.66	0.76
7:A:350:HEM:HBC2	7:A:350:HEM:HHD	1.68	0.74
1:B:134:PHE:CD1	3:J:2:NAG:H62	2.21	0.74
1:B:282:GLU:HG3	1:B:322:VAL:HG11	1.69	0.74
1:D:282:GLU:HG2	1:D:322:VAL:HG11	1.71	0.71
1:B:302:LYS:HE3	12:B:2319:HOH:O	1.91	0.70
12:B:2351:HOH:O	4:K:2:NAG:O6	2.08	0.70
1:A:217[A]:ASP:OD2	12:A:2203:HOH:O	2.08	0.69
1:B:254:GLN:NE2	12:B:2267:HOH:O	2.25	0.69
5:M:6:MAN:H62	5:M:8:MAN:H3	1.74	0.69
1:B:259:VAL:HG12	1:B:259:VAL:O	1.90	0.69
1:A:133:PHE:CE1	4:G:1:NAG:H82	2.27	0.68
1:D:5:PRO:O	12:D:2003:HOH:O	2.11	0.68
1:D:31:ASP:N	12:D:2024:HOH:O	2.27	0.67
1:D:259:VAL:O	1:D:259:VAL:HG13	1.94	0.67
1:A:112:VAL:HG12	1:A:112:VAL:O	1.97	0.65
1:D:167:GLU:OE2	12:D:2103:HOH:O	2.14	0.64
1:A:48:LEU:HD21	1:A:59:ILE:HA	1.80	0.64
1:B:263:ASN:ND2	12:B:2277:HOH:O	2.16	0.63
1:D:147:GLN:OE1	1:D:171:LYS:HE3	1.98	0.63
1:D:88:LEU:HD23	1:D:304:LEU:HG	1.80	0.63
1:D:291:SER:HB2	12:D:2158:HOH:O	1.99	0.62
1:A:249:GLN:NE2	1:C:249:GLN:OE1	2.33	0.61
1:C:227:ARG:CD	12:C:2199:HOH:O	2.49	0.61
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.66	0.60
1:A:206:ASP:OD2	12:A:2183:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:GLY:HA2	1:D:116:ASN:ND2	2.17	0.59
1:C:259:VAL:HG12	1:C:259:VAL:O	2.02	0.58
1:B:249:GLN:OE1	12:B:2261:HOH:O	2.17	0.58
1:D:310:PHE:O	1:D:313[A]:GLN:HB2	2.03	0.58
1:B:278:CYS:HB2	10:B:1331:SO4:S	2.44	0.57
1:B:147:GLN:NE2	1:B:171:LYS:HE2	2.19	0.57
1:C:327:ARG:O	1:C:328:ASP:HB2	2.05	0.57
1:C:123:GLY:HA3	1:C:189:ARG:HD3	1.87	0.57
1:C:171:LYS:HE2	1:C:175:ASP:OD1	2.05	0.56
1:C:209:ARG:HD2	1:C:211:ASP:OD2	2.05	0.56
7:C:350:HEM:CMC	7:C:350:HEM:HBC2	2.36	0.56
1:A:208:ARG:NH2	1:A:231:ASP:O	2.39	0.56
1:B:184:SER:HA	1:B:257[A]:ARG:HB3	1.88	0.56
1:D:4:LEU:N	12:D:2002:HOH:O	2.38	0.56
1:A:259:VAL:O	1:A:259:VAL:CG2	2.42	0.55
7:A:350:HEM:HHD	7:A:350:HEM:CBC	2.37	0.55
1:D:5:PRO:HD3	1:D:310:PHE:CE1	2.41	0.55
1:D:209:ARG:HD2	1:D:211:ASP:OD2	2.07	0.54
5:M:6:MAN:H62	5:M:8:MAN:C3	2.36	0.54
1:B:254:GLN:HB3	1:B:255:PRO:HD2	1.89	0.54
4:I:1:NAG:C6	4:I:2:NAG:C1	2.83	0.54
1:C:48:LEU:HD21	1:C:59:ILE:HA	1.90	0.54
1:B:6:PRO:HD3	1:B:57:VAL:HG22	1.89	0.53
12:B:2100:HOH:O	1:D:313[B]:GLN:HG3	2.08	0.53
1:B:191:PHE:HB2	12:B:2090:HOH:O	2.07	0.53
1:D:180:ASN:C	1:D:180:ASN:OD1	2.45	0.53
1:A:296:PRO:HG2	1:A:301:ARG:HB2	1.89	0.53
1:D:16:LEU:HG	1:D:19:ASP:HB3	1.90	0.53
1:A:282:GLU:HG3	1:A:322:VAL:HG21	1.91	0.53
1:D:278:CYS:HB2	10:D:1329:SO4:O3	2.09	0.53
4:G:1:NAG:H61	4:G:2:NAG:C7	2.39	0.52
4:I:1:NAG:H62	4:I:2:NAG:C1	2.39	0.52
1:A:100:ARG:HD2	12:A:2099:HOH:O	2.10	0.52
1:B:207:GLY:HA3	1:B:234:ARG:O	2.10	0.52
1:A:207:GLY:HA3	1:A:234:ARG:O	2.10	0.51
7:D:350:HEM:HMC2	7:D:350:HEM:CBC	2.20	0.51
7:B:350:HEM:HHC	7:B:350:HEM:HBB2	1.91	0.51
1:D:68:ASN:O	1:D:238:PRO:HA	2.10	0.51
5:H:6:MAN:C6	5:H:8:MAN:C3	2.67	0.51
1:A:278:CYS:HB2	10:A:1331:SO4:O1	2.10	0.51
1:A:285:VAL:CG1	1:A:324:PRO:HD3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:350:HEM:HBC2	7:A:350:HEM:CHD	2.37	0.51
1:D:282:GLU:HG2	1:D:322:VAL:CG1	2.39	0.51
1:D:259:VAL:O	1:D:259:VAL:HG12	2.06	0.50
1:D:112:VAL:HG12	1:D:112:VAL:O	2.11	0.50
1:D:48:LEU:HD21	1:D:59:ILE:HA	1.94	0.50
1:A:283:LYS:NZ	12:A:2252:HOH:O	2.00	0.49
1:D:24:TRP:CG	1:D:227:ARG:HG3	2.47	0.49
1:B:9:LEU:HD13	1:B:64:GLN:HB3	1.94	0.49
1:B:48:LEU:HD21	1:B:59:ILE:HA	1.94	0.49
7:C:350:HEM:HBC2	7:C:350:HEM:HMC1	1.95	0.49
1:D:237:SER:O	1:D:239:ARG:NE	2.43	0.49
4:I:1:NAG:H62	4:I:2:NAG:O5	2.13	0.49
1:A:27:LEU:N	12:A:2028:HOH:O	2.30	0.49
1:B:48:LEU:O	1:B:49:PRO:C	2.51	0.49
1:B:112:VAL:O	1:B:112:VAL:HG12	2.11	0.48
1:C:126:SER:OG	7:C:350:HEM:O2A	2.31	0.48
1:C:227:ARG:HD2	12:C:2199:HOH:O	2.12	0.48
1:B:51:ASN:H	1:B:51:ASN:HD22	1.60	0.48
1:D:318:GLY:O	1:D:319:CYS:HB2	2.12	0.48
1:D:136:ASN:ND2	1:D:139:ASP:OD2	2.35	0.48
1:B:28:ARG:HB3	1:B:29:PRO:CD	2.44	0.47
1:D:22:HIS:N	1:D:23:PRO:CD	2.77	0.47
1:D:199:PHE:N	1:D:200:PRO:CD	2.77	0.47
1:D:28:ARG:O	12:D:2024:HOH:O	2.20	0.47
1:B:259:VAL:O	1:B:259:VAL:CG1	2.61	0.47
1:B:266:THR:HA	12:B:2278:HOH:O	2.14	0.47
1:D:207:GLY:HA3	1:D:234:ARG:O	2.14	0.47
1:B:60:ILE:O	1:B:64:GLN:HG3	2.15	0.47
1:C:28:ARG:HB3	1:C:29:PRO:HD2	1.96	0.47
1:A:301:ARG:NH2	1:A:325:TYR:O	2.43	0.47
1:B:249:GLN:NE2	1:D:249:GLN:OE1	2.44	0.47
2:E:3:BMA:C6	2:E:6:MAN:O2	2.62	0.47
1:A:133:PHE:CD1	4:G:1:NAG:H82	2.49	0.46
1:B:203:LEU:HD13	7:B:350:HEM:CBC	2.45	0.46
1:B:171:LYS:HE3	1:B:175:ASP:OD1	2.15	0.46
1:A:257:ARG:N	1:A:257:ARG:HD3	2.30	0.46
1:C:111:SER:HB2	12:C:2111:HOH:O	2.16	0.46
1:B:301:ARG:NH1	1:B:325:TYR:O	2.50	0.45
1:A:199:PHE:HB3	7:A:350:HEM:HBC2	1.99	0.45
1:B:191:PHE:HD1	12:B:2090:HOH:O	2.00	0.45
1:A:318:GLY:O	1:A:319:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:4:MAN:O5	3:J:5:MAN:H2	2.17	0.45
1:B:227:ARG:NH2	12:B:2241:HOH:O	2.17	0.45
1:A:80:ALA:O	1:A:84:VAL:HG22	2.17	0.44
1:A:257:ARG:N	1:A:257:ARG:CD	2.81	0.44
3:F:3:BMA:H61	3:F:4:MAN:C5	2.47	0.44
1:A:302:LYS:HA	1:A:302:LYS:HD2	1.48	0.44
1:C:189:ARG:HA	12:C:2128:HOH:O	2.17	0.44
1:B:203:LEU:HD13	7:B:350:HEM:HBC2	1.99	0.44
1:B:28:ARG:HE	1:B:28:ARG:HB2	1.57	0.43
1:D:253:MET:HA	1:D:253:MET:CE	2.48	0.43
1:D:280:MET:HE3	1:D:280:MET:C	2.39	0.43
1:C:81:ALA:HB1	1:C:115:LEU:HD21	2.00	0.43
1:D:149:VAL:HG22	1:D:216:MET:SD	2.58	0.43
5:H:6:MAN:H61	5:H:8:MAN:H2	1.37	0.43
1:A:146:GLU:HG2	1:B:149:VAL:HG11	2.00	0.43
1:C:136:ASN:ND2	1:C:139:ASP:OD2	2.45	0.43
1:A:34:GLY:HA3	1:A:95:ILE:O	2.19	0.43
1:C:68:ASN:O	1:C:238:PRO:HA	2.19	0.43
1:D:109:PRO:O	1:D:110:ALA:C	2.56	0.43
1:D:24:TRP:HA	1:D:44:SER:O	2.18	0.43
1:B:209:ARG:HD2	1:B:211:ASP:OD2	2.18	0.42
1:D:280:MET:HE3	1:D:280:MET:O	2.19	0.42
1:D:283:LYS:O	1:D:287:ILE:HB	2.19	0.42
1:A:217[A]:ASP:OD1	12:A:2201:HOH:O	2.21	0.42
1:D:5:PRO:HA	1:D:6:PRO:HD3	1.90	0.42
1:D:178:ALA:O	1:D:262:ILE:HB	2.19	0.42
1:D:280:MET:C	1:D:280:MET:CE	2.88	0.42
1:A:278:CYS:HB2	10:A:1331:SO4:S	2.59	0.42
1:A:150:ASP:OD1	1:B:142:GLU:OE2	2.37	0.42
1:A:323:PHE:HA	1:A:324:PRO:HD2	1.92	0.42
1:C:133:PHE:CE2	11:C:381:NAG:H82	2.55	0.42
1:C:199:PHE:N	1:C:200:PRO:CD	2.83	0.42
1:B:199:PHE:N	1:B:200:PRO:CD	2.82	0.42
2:E:1:NAG:H61	2:E:2:NAG:C1	2.49	0.42
1:B:302:LYS:CE	12:B:2319:HOH:O	2.58	0.41
1:A:169:ARG:HH11	1:A:169:ARG:HD3	1.75	0.41
1:A:96:GLY:HA2	1:A:116:ASN:ND2	2.35	0.41
1:D:24:TRP:CD1	1:D:227:ARG:HG3	2.55	0.41
1:D:34:GLY:HA3	1:D:95:ILE:O	2.20	0.41
1:D:169:ARG:HB2	1:D:197:THR:HG21	2.01	0.41
1:D:294:PRO:O	1:D:295:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ARG:HG2	1:D:211:ASP:OD2	2.21	0.41
1:A:199:PHE:HB3	7:A:350:HEM:CBC	2.50	0.41
1:A:321:GLN:HG2	1:A:323:PHE:CZ	2.56	0.41
1:B:242:THR:HG22	12:B:2259:HOH:O	2.21	0.41
1:D:89:ILE:CD1	1:D:300:LEU:HD13	2.40	0.41
1:D:278:CYS:SG	4:K:1:NAG:H83	2.61	0.41
1:B:169:ARG:HB2	1:B:197:THR:HG21	2.03	0.41
1:B:301:ARG:NH2	12:B:2316:HOH:O	2.53	0.41
1:A:6:PRO:HG3	12:A:2057:HOH:O	2.21	0.40
3:F:3:BMA:H61	3:F:4:MAN:H5	2.03	0.40
1:B:272:SER:OG	1:B:280:MET:HB2	2.21	0.40
1:A:199:PHE:N	1:A:200:PRO:CD	2.84	0.40
1:C:15:LYS:HE3	12:C:2019:HOH:O	2.20	0.40
1:C:112:VAL:HG12	1:C:112:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/325 (99%)	301 (94%)	21 (6%)	0	100	100
1	B	326/325 (100%)	307 (94%)	19 (6%)	0	100	100
1	C	324/325 (100%)	304 (94%)	20 (6%)	0	100	100
1	D	322/325 (99%)	298 (92%)	24 (8%)	0	100	100
All	All	1294/1300 (100%)	1210 (94%)	84 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	270/271 (100%)	258 (96%)	12 (4%)	24	34
1	B	274/271 (101%)	262 (96%)	12 (4%)	24	34
1	C	272/271 (100%)	261 (96%)	11 (4%)	27	39
1	D	270/271 (100%)	262 (97%)	8 (3%)	36	51
All	All	1086/1084 (100%)	1043 (96%)	43 (4%)	27	39

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	88	LEU
1	A	159	LYS
1	A	169	ARG
1	A	221	SER
1	A	226	SER
1	A	239	ARG
1	A	257	ARG
1	A	295	ASN
1	A	299	GLN
1	A	300	LEU
1	A	302	LYS
1	B	9	LEU
1	B	51	ASN
1	B	69	PHE
1	B	88	LEU
1	B	101	LEU
1	B	121	PHE
1	B	169	ARG
1	B	239	ARG
1	B	257[A]	ARG
1	B	257[B]	ARG
1	B	286	ASN
1	B	295	ASN

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Mol	Chain	Res	Type
1	C	9	LEU
1	C	70	ASP
1	C	88	LEU
1	C	159	LYS
1	C	217	ASP
1	C	239	ARG
1	C	257	ARG
1	C	261	LYS
1	C	280	MET
1	C	300	LEU
1	C	328	ASP
1	D	9	LEU
1	D	116	ASN
1	D	169	ARG
1	D	239	ARG
1	D	257	ARG
1	D	261	LYS
1	D	280	MET
1	D	302	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	116	ASN
1	A	138	HIS
1	A	249	GLN
1	A	299	GLN
1	B	51	ASN
1	B	147	GLN
1	C	61	ASN
1	C	249	GLN
1	D	116	ASN
1	D	263	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

56 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	NAG	E	1	1,2	14,14,15	0.44	0	17,19,21	1.39	3 (17%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	1.12	1 (5%)
2	BMA	E	3	2	11,11,12	0.55	0	15,15,17	0.94	1 (6%)
2	MAN	E	4	2	11,11,12	0.52	0	15,15,17	0.94	0
2	MAN	E	5	2	11,11,12	0.58	0	15,15,17	0.73	0
2	MAN	E	6	2	11,11,12	0.54	0	15,15,17	1.14	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.69	0	17,19,21	1.26	2 (11%)
3	NAG	F	2	3	14,14,15	0.79	0	17,19,21	1.31	4 (23%)
3	BMA	F	3	3	11,11,12	0.56	0	15,15,17	1.00	0
3	MAN	F	4	3	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
3	MAN	F	5	3	11,11,12	0.54	0	15,15,17	0.87	0
4	NAG	G	1	1,4	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
4	NAG	G	2	4	14,14,15	0.53	0	17,19,21	1.55	4 (23%)
5	NAG	H	1	1,5	14,14,15	0.65	0	17,19,21	1.64	2 (11%)
5	NAG	H	2	5	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
5	BMA	H	3	5	11,11,12	0.68	0	15,15,17	1.14	1 (6%)
5	MAN	H	4	5	11,11,12	0.58	0	15,15,17	1.08	1 (6%)
5	MAN	H	5	5	11,11,12	0.42	0	15,15,17	1.07	1 (6%)
5	MAN	H	6	5	11,11,12	0.57	0	15,15,17	0.83	0
5	MAN	H	7	5	11,11,12	0.53	0	15,15,17	0.87	0
5	MAN	H	8	5	11,11,12	0.57	0	15,15,17	1.12	1 (6%)
4	NAG	I	1	1,4	14,14,15	0.49	0	17,19,21	1.94	3 (17%)
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	J	1	1,3	14,14,15	0.60	0	17,19,21	1.18	2 (11%)
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	2.01	5 (29%)
3	BMA	J	3	3	11,11,12	0.56	0	15,15,17	1.22	2 (13%)
3	MAN	J	4	3	11,11,12	0.59	0	15,15,17	1.14	2 (13%)
3	MAN	J	5	3	11,11,12	0.61	0	15,15,17	1.68	3 (20%)
4	NAG	K	1	1,4	14,14,15	0.55	0	17,19,21	1.80	4 (23%)
4	NAG	K	2	4	14,14,15	0.59	0	17,19,21	1.56	2 (11%)
4	NAG	L	1	1,4	14,14,15	0.77	0	17,19,21	1.28	1 (5%)
4	NAG	L	2	4	14,14,15	0.55	0	17,19,21	0.87	0
5	NAG	M	1	1,5	14,14,15	0.65	0	17,19,21	1.80	4 (23%)
5	NAG	M	2	5	14,14,15	0.74	0	17,19,21	1.17	2 (11%)
5	BMA	M	3	5	11,11,12	0.78	0	15,15,17	1.22	1 (6%)
5	MAN	M	4	5	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
5	MAN	M	5	5	11,11,12	0.43	0	15,15,17	1.44	1 (6%)
5	MAN	M	6	5	11,11,12	0.52	0	15,15,17	1.96	4 (26%)
5	MAN	M	7	5	11,11,12	0.48	0	15,15,17	0.81	0
5	MAN	M	8	5	11,11,12	0.73	0	15,15,17	1.41	2 (13%)
4	NAG	N	1	1,4	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
4	NAG	N	2	4	14,14,15	0.51	0	17,19,21	0.76	1 (5%)
6	NAG	O	1	1,6	14,14,15	0.59	0	17,19,21	0.85	1 (5%)
6	NAG	O	2	6	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
6	BMA	O	3	6	11,11,12	0.51	0	15,15,17	1.80	3 (20%)
4	NAG	P	1	1,4	14,14,15	0.71	0	17,19,21	1.78	6 (35%)
4	NAG	P	2	4	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
4	NAG	Q	1	1,4	14,14,15	0.56	0	17,19,21	1.59	3 (17%)
4	NAG	Q	2	4	14,14,15	0.49	0	17,19,21	0.77	0
4	NAG	R	1	1,4	14,14,15	0.59	0	17,19,21	0.74	0
4	NAG	R	2	4	14,14,15	0.57	0	17,19,21	0.70	0
4	NAG	S	1	1,4	14,14,15	0.66	0	17,19,21	1.24	3 (17%)
4	NAG	S	2	4	14,14,15	0.49	0	17,19,21	0.57	0
6	NAG	T	1	1,6	14,14,15	0.64	0	17,19,21	1.49	3 (17%)
6	NAG	T	2	6	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
6	BMA	T	3	6	11,11,12	0.51	0	15,15,17	1.27	2 (13%)

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	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	1/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
5	MAN	H	7	5	-	1/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	2/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1
5	MAN	M	5	5	-	2/2/19/22	0/1/1/1
5	MAN	M	6	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	2	NAG	C2-N2-C7	-5.23	115.89	122.90
4	I	1	NAG	C1-O5-C5	5.23	119.19	112.19
5	M	1	NAG	C1-O5-C5	4.94	118.81	112.19
4	K	2	NAG	O5-C1-C2	-4.69	104.04	111.29
3	J	5	MAN	C3-C4-C5	4.60	118.57	110.23
4	Q	1	NAG	C1-O5-C5	4.57	118.31	112.19
5	H	1	NAG	C1-O5-C5	4.49	118.20	112.19
6	O	3	BMA	C1-O5-C5	4.48	118.19	112.19
5	M	5	MAN	C1-O5-C5	4.23	117.85	112.19
5	M	6	MAN	C3-C4-C5	4.17	117.79	110.23
5	M	6	MAN	C1-O5-C5	4.11	117.69	112.19
4	K	1	NAG	C2-N2-C7	-3.79	117.82	122.90
6	O	3	BMA	C1-C2-C3	3.66	114.97	109.64
4	P	1	NAG	O5-C1-C2	-3.61	105.71	111.29
5	H	1	NAG	C2-N2-C7	-3.60	118.07	122.90
5	M	6	MAN	C6-C5-C4	-3.52	104.38	113.02
5	M	8	MAN	C1-C2-C3	3.51	114.75	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	3	BMA	C1-O5-C5	3.49	116.87	112.19
3	J	2	NAG	C4-C3-C2	-3.44	105.97	111.02
6	T	1	NAG	O5-C1-C2	-3.34	106.13	111.29
5	H	2	NAG	C1-O5-C5	-3.34	107.72	112.19
4	I	1	NAG	C4-C3-C2	-3.25	106.25	111.02
5	H	8	MAN	C1-C2-C3	-3.25	104.91	109.64
6	T	2	NAG	O5-C1-C2	-3.12	106.46	111.29
3	J	5	MAN	C1-O5-C5	3.11	116.36	112.19
4	G	2	NAG	C1-C2-N2	3.07	115.27	110.43
3	J	1	NAG	C2-N2-C7	-3.04	118.83	122.90
4	K	2	NAG	C1-O5-C5	-3.01	108.15	112.19
4	L	1	NAG	C2-N2-C7	-2.98	118.90	122.90
4	K	1	NAG	C1-O5-C5	2.95	116.14	112.19
4	P	2	NAG	C2-N2-C7	-2.94	118.97	122.90
4	G	2	NAG	O5-C1-C2	-2.89	106.82	111.29
4	K	1	NAG	C1-C2-N2	2.86	114.94	110.43
5	M	8	MAN	O2-C2-C3	-2.79	104.36	110.15
2	E	1	NAG	O5-C1-C2	-2.77	107.00	111.29
3	J	2	NAG	C1-C2-N2	2.76	114.79	110.43
5	H	5	MAN	C1-O5-C5	2.76	115.89	112.19
4	Q	1	NAG	C3-C4-C5	-2.75	105.25	110.23
5	M	1	NAG	C6-C5-C4	-2.74	106.28	113.02
3	F	2	NAG	C2-N2-C7	-2.73	119.24	122.90
4	P	1	NAG	C1-C2-N2	2.71	114.71	110.43
5	M	4	MAN	C2-C3-C4	-2.71	106.09	110.86
6	T	1	NAG	O5-C5-C4	2.68	117.35	110.83
4	P	1	NAG	C2-N2-C7	-2.65	119.36	122.90
3	J	2	NAG	C1-O5-C5	2.64	115.72	112.19
4	P	1	NAG	O4-C4-C3	-2.63	104.18	110.38
3	J	3	BMA	C1-O5-C5	2.62	115.70	112.19
4	G	1	NAG	C3-C4-C5	-2.62	105.49	110.23
2	E	6	MAN	C2-C3-C4	-2.59	106.31	110.86
3	J	1	NAG	O5-C1-C2	-2.58	107.31	111.29
4	S	1	NAG	O5-C1-C2	-2.56	107.33	111.29
3	J	5	MAN	O5-C5-C4	2.56	117.05	110.83
3	J	2	NAG	O5-C1-C2	-2.55	107.34	111.29
2	E	3	BMA	C1-O5-C5	2.54	115.59	112.19
3	F	4	MAN	C1-C2-C3	2.49	113.27	109.64
3	J	4	MAN	C1-C2-C3	2.49	113.26	109.64
5	M	2	NAG	C3-C4-C5	-2.48	105.74	110.23
2	E	2	NAG	O5-C1-C2	-2.45	107.51	111.29
4	G	2	NAG	C3-C4-C5	2.44	114.65	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	3	BMA	C1-C2-C3	2.43	113.19	109.64
4	Q	1	NAG	C2-N2-C7	-2.40	119.68	122.90
2	E	1	NAG	C2-N2-C7	-2.39	119.70	122.90
4	K	1	NAG	O5-C1-C2	-2.37	107.62	111.29
4	I	1	NAG	O5-C5-C4	2.37	116.59	110.83
3	F	2	NAG	O5-C1-C2	-2.35	107.65	111.29
3	F	1	NAG	O5-C5-C4	2.35	116.53	110.83
6	T	3	BMA	C1-O5-C5	2.29	115.26	112.19
6	T	1	NAG	C1-C2-N2	2.29	114.04	110.43
5	M	2	NAG	C1-O5-C5	-2.27	109.14	112.19
5	H	3	BMA	C1-C2-C3	2.27	112.95	109.64
4	N	2	NAG	O5-C1-C2	-2.27	107.79	111.29
6	O	2	NAG	O5-C5-C6	2.26	112.06	107.66
4	G	2	NAG	C4-C3-C2	2.24	114.30	111.02
4	S	1	NAG	C1-O5-C5	2.23	115.17	112.19
4	I	2	NAG	C1-O5-C5	2.18	115.11	112.19
4	P	1	NAG	C4-C3-C2	2.18	114.21	111.02
2	E	1	NAG	O7-C7-C8	-2.18	118.18	122.05
5	M	1	NAG	C3-C4-C5	2.16	114.16	110.23
4	P	1	NAG	O4-C4-C5	-2.15	104.03	109.32
5	H	4	MAN	C2-C3-C4	-2.12	107.13	110.86
4	S	1	NAG	C3-C4-C5	2.11	114.06	110.23
4	N	1	NAG	O5-C5-C6	2.11	111.77	107.66
5	M	6	MAN	O3-C3-C4	-2.08	105.47	110.38
6	T	3	BMA	O5-C5-C6	2.08	111.71	107.66
3	F	2	NAG	C1-C2-N2	2.08	113.70	110.43
5	M	1	NAG	O7-C7-C8	-2.07	118.36	122.05
3	F	2	NAG	C4-C3-C2	2.06	114.04	111.02
3	J	4	MAN	C2-C3-C4	2.06	114.48	110.86
6	O	3	BMA	C2-C3-C4	-2.03	107.28	110.86
6	O	1	NAG	O5-C1-C2	-2.02	108.17	111.29
3	F	1	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C3-C2-N2-C7
3	F	4	MAN	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	O	2	NAG	O5-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	J	5	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
3	J	5	MAN	C4-C5-C6-O6
6	T	3	BMA	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
5	M	6	MAN	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
5	M	6	MAN	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	M	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	5	MAN	C4-C5-C6-O6
6	T	3	BMA	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
5	M	5	MAN	C4-C5-C6-O6
5	M	8	MAN	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
5	H	7	MAN	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
5	M	5	MAN	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6	MAN	C1-C2-C3-C4-C5-O5

19 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
2	E	2	NAG	1	0
3	J	4	MAN	1	0
2	E	1	NAG	1	0
3	J	2	NAG	1	0
5	M	8	MAN	2	0
2	E	3	BMA	1	0
2	E	6	MAN	1	0
3	F	3	BMA	2	0
4	G	2	NAG	1	0
5	H	6	MAN	4	0
4	K	2	NAG	1	0
4	I	1	NAG	3	0

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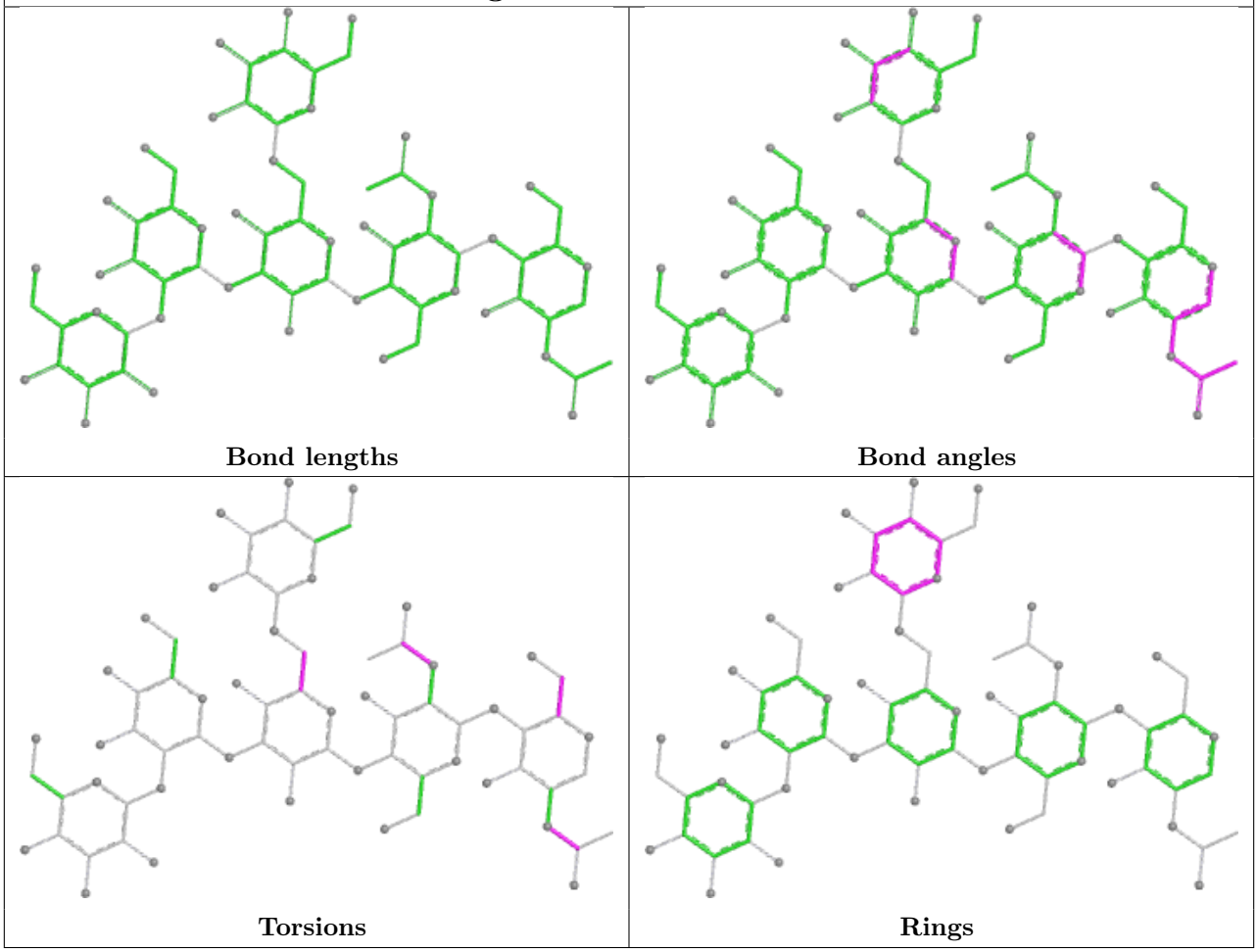
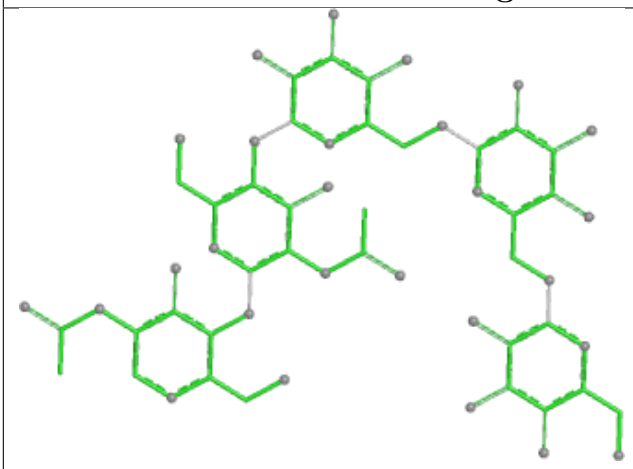
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	5	MAN	1	0
4	G	1	NAG	3	0
3	F	4	MAN	2	0
4	I	2	NAG	3	0
5	M	6	MAN	2	0
5	H	8	MAN	4	0

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

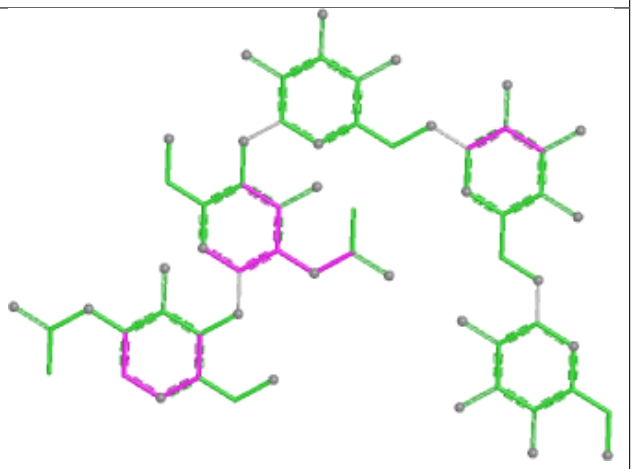
Oligosaccharide Chain E



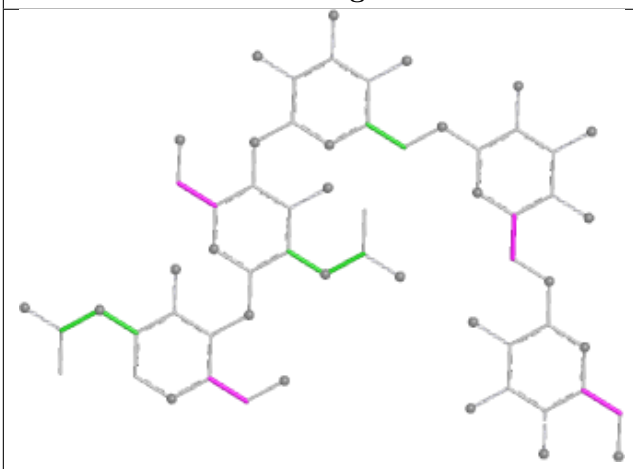
Oligosaccharide Chain F



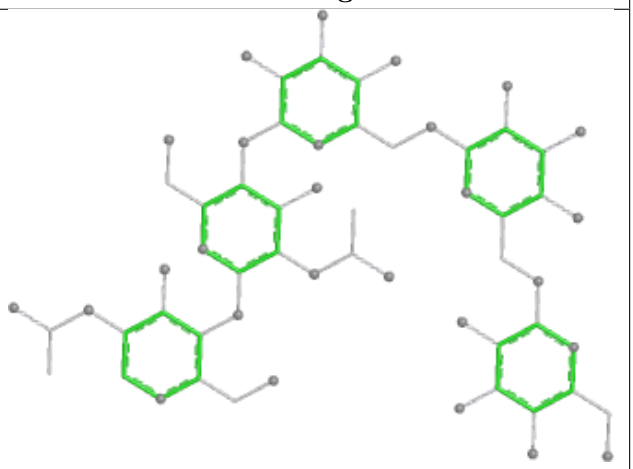
Bond lengths



Bond angles

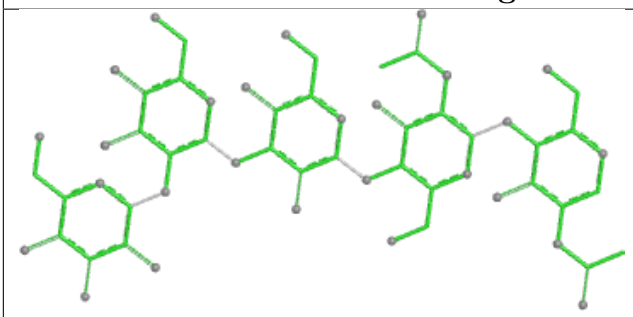


Torsions

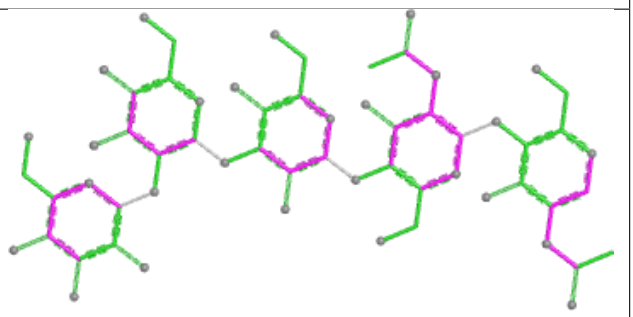


Rings

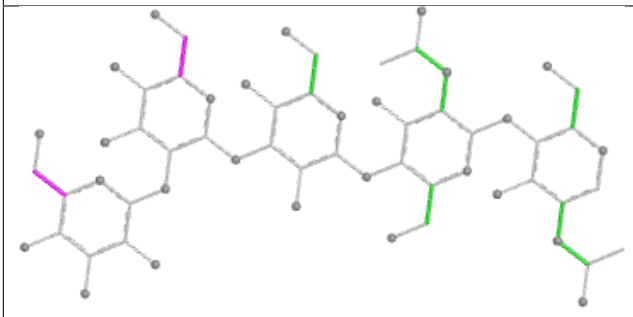
Oligosaccharide Chain J



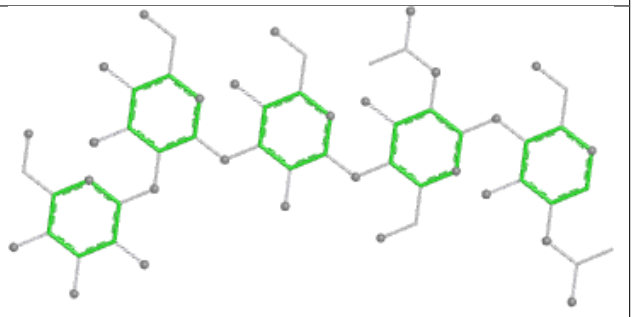
Bond lengths



Bond angles

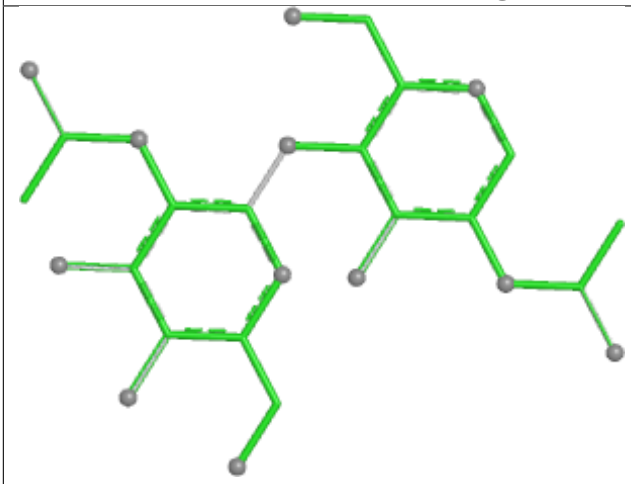


Torsions

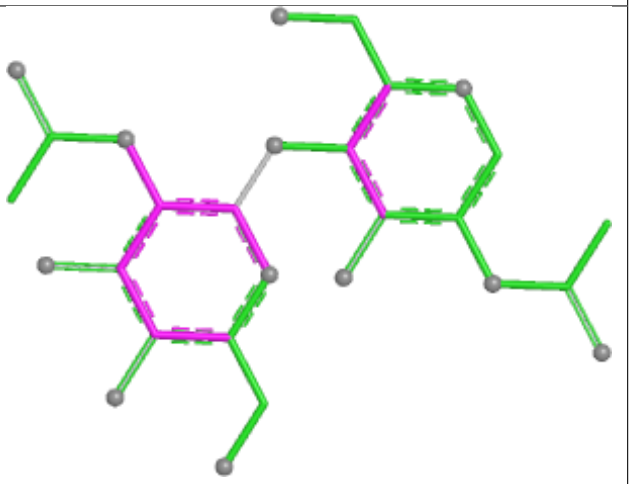


Rings

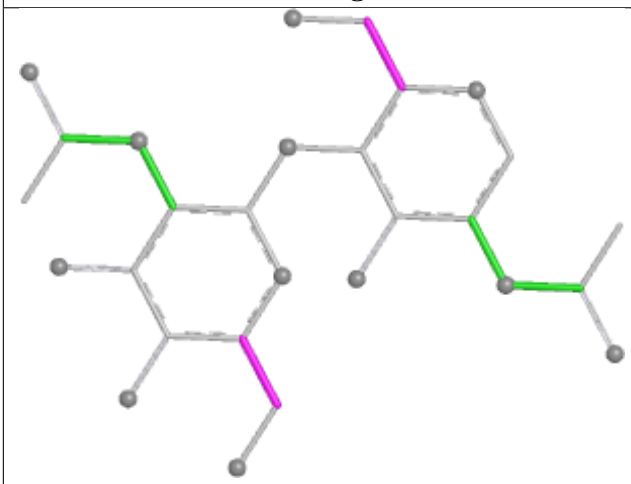
Oligosaccharide Chain G



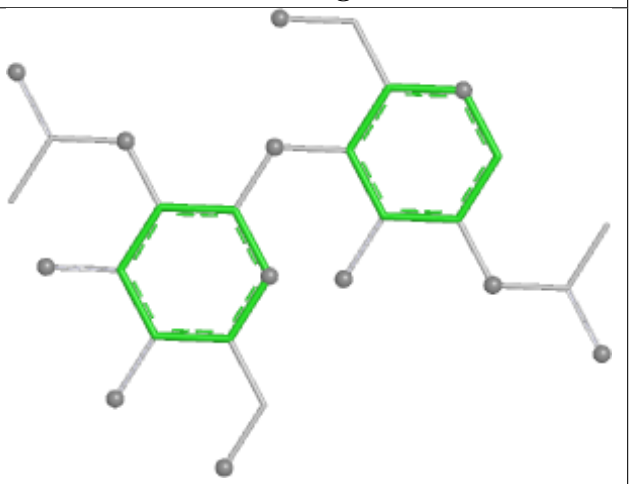
Bond lengths



Bond angles

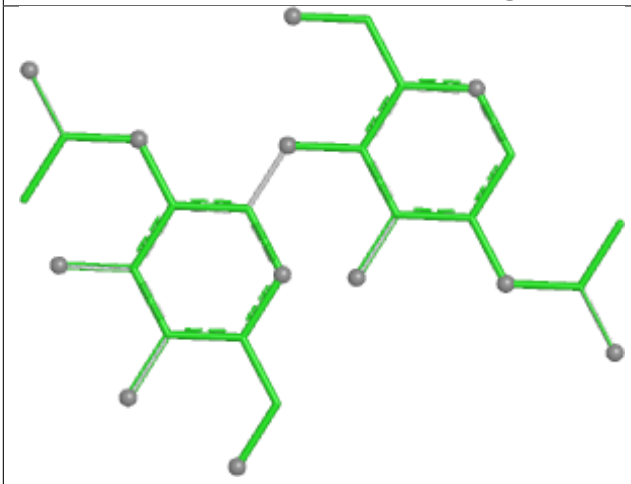


Torsions

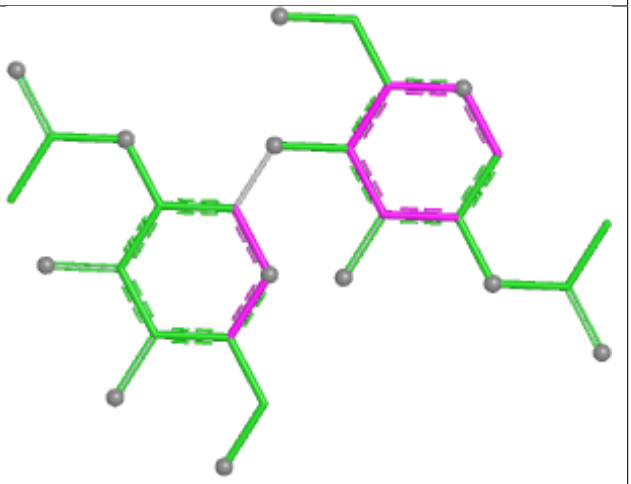


Rings

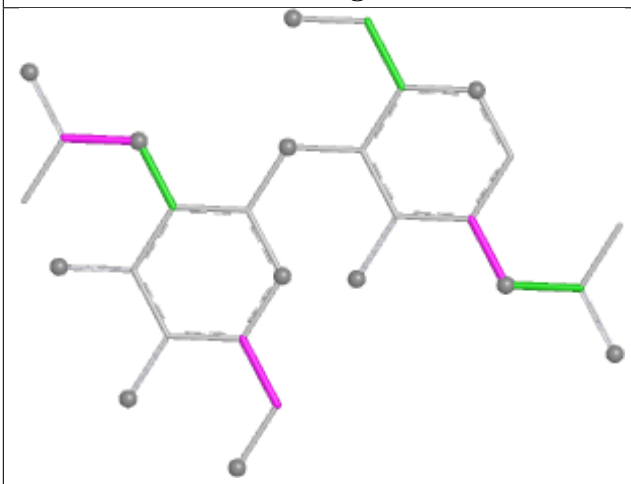
Oligosaccharide Chain I



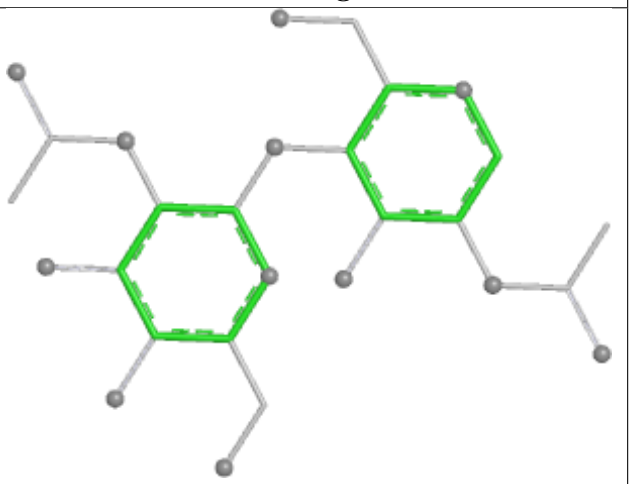
Bond lengths



Bond angles

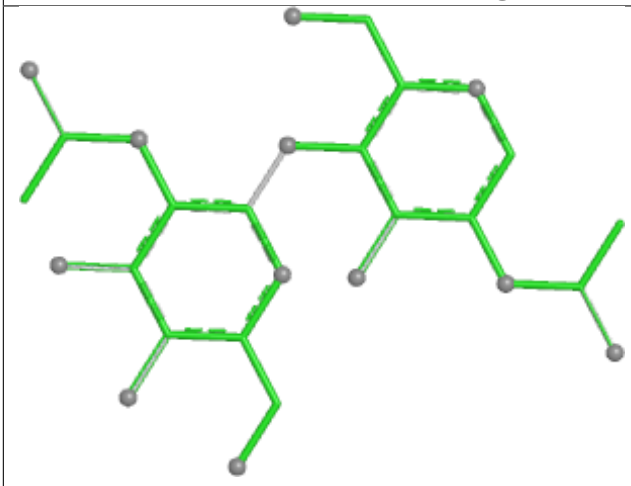


Torsions

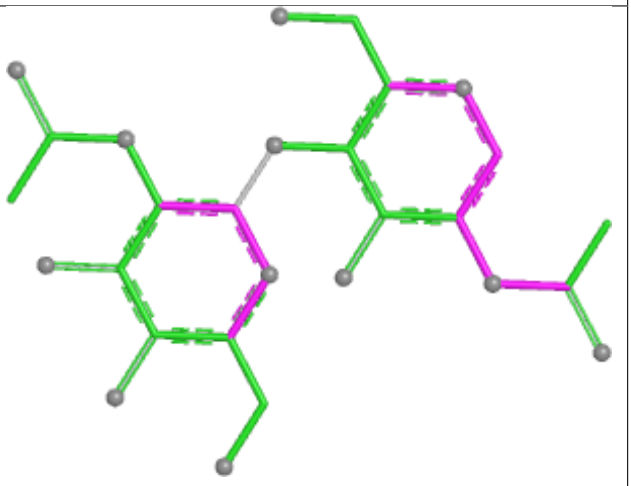


Rings

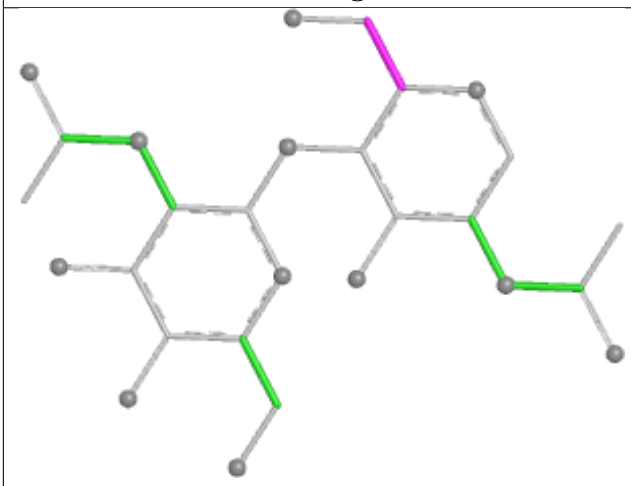
Oligosaccharide Chain K



Bond lengths



Bond angles



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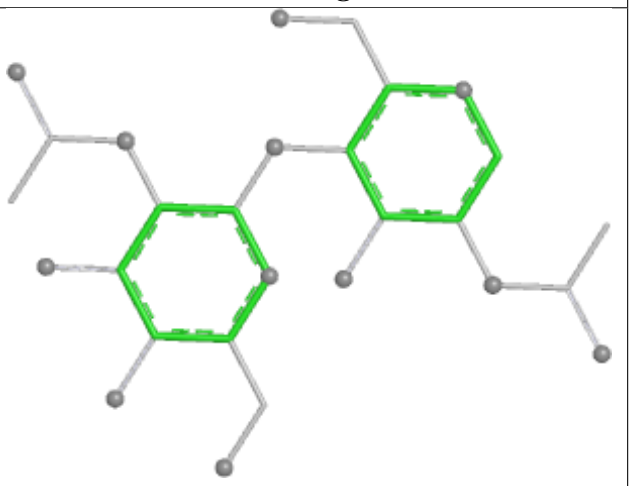
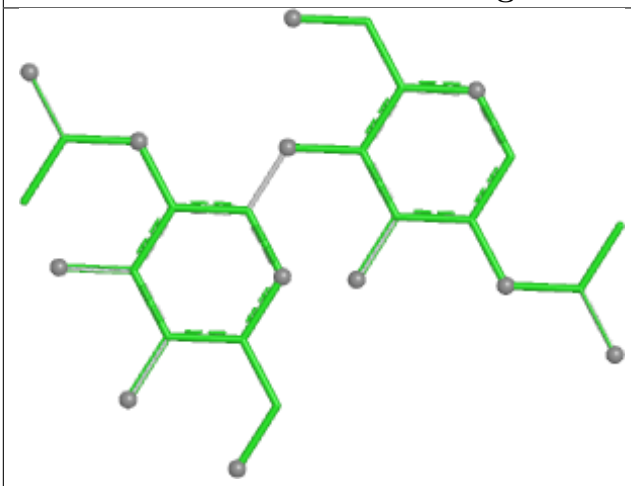
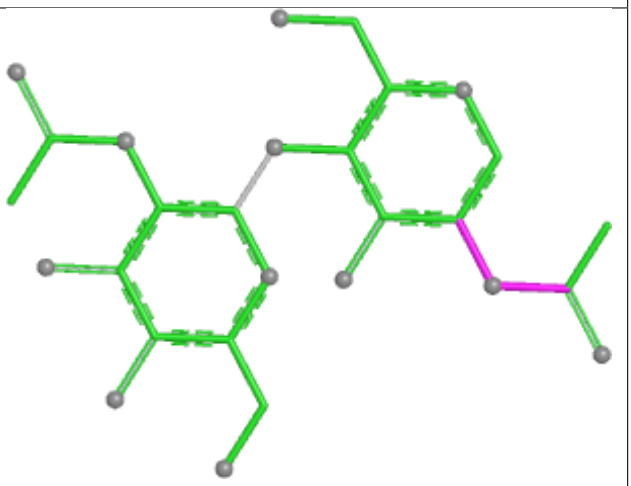


Rings

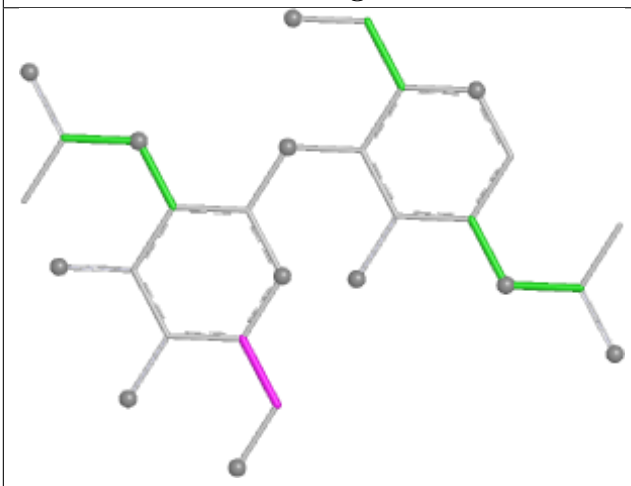
Oligosaccharide Chain L



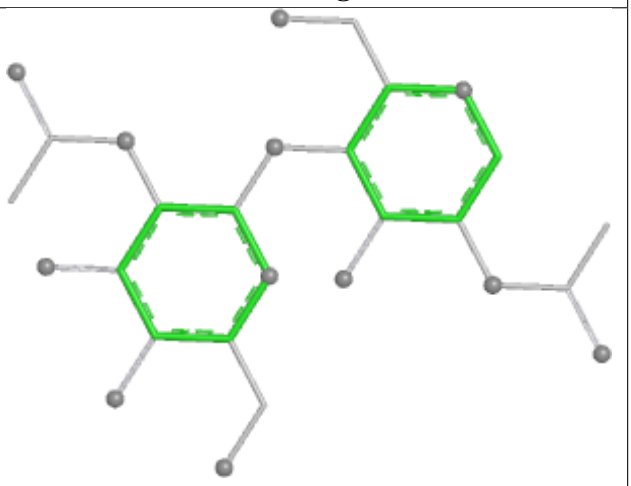
Bond lengths



Bond angles

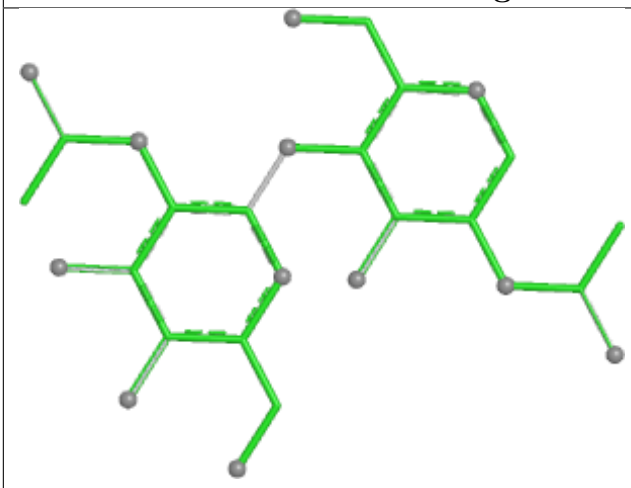


Torsions

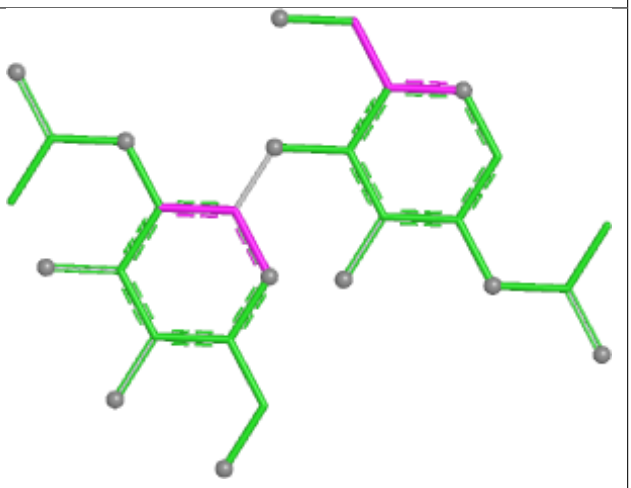


Rings

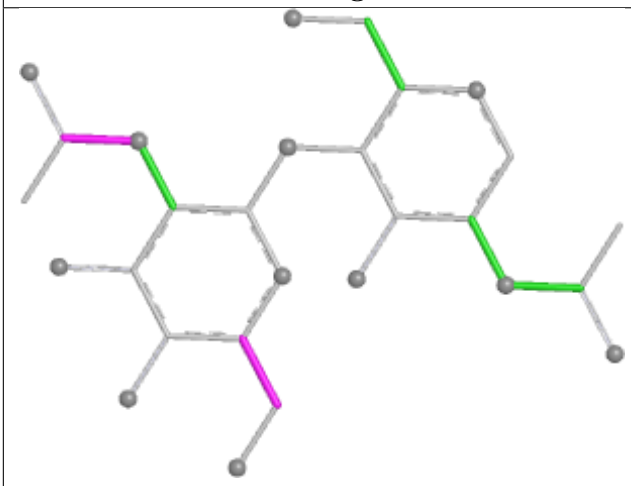
Oligosaccharide Chain N



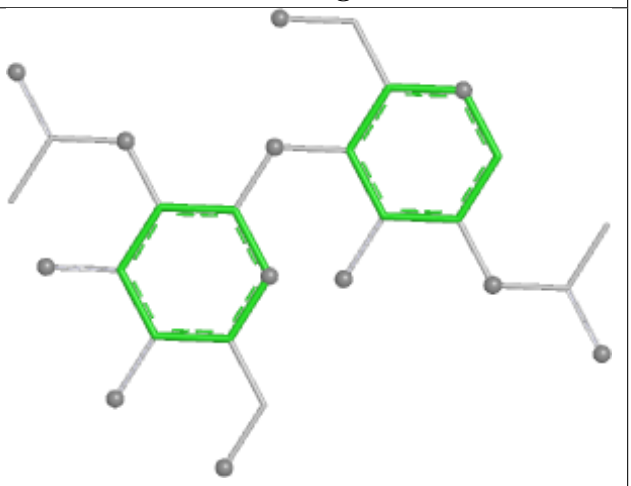
Bond lengths



Bond angles

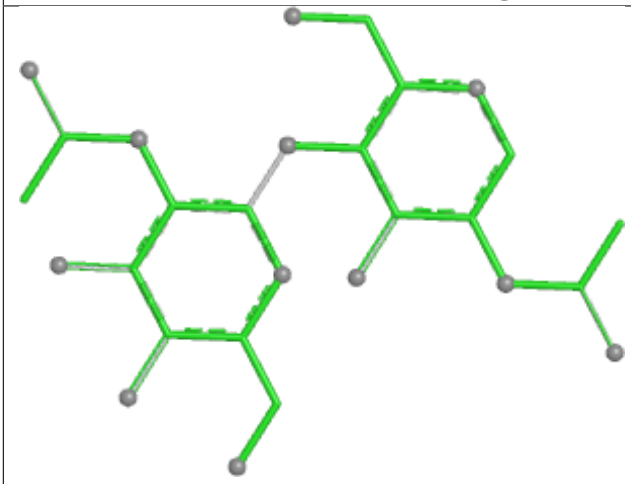


Torsions

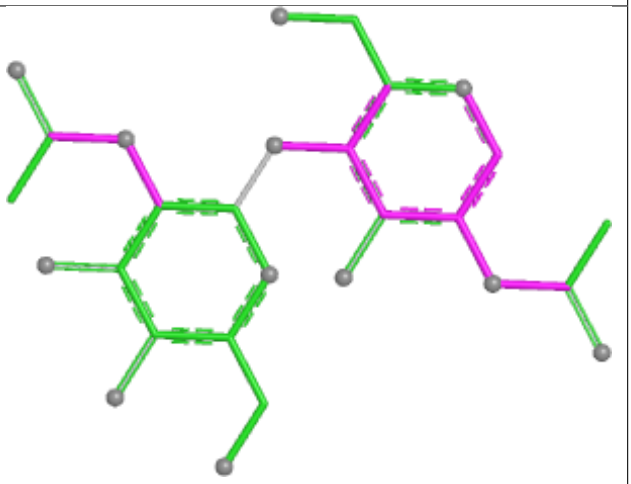


Rings

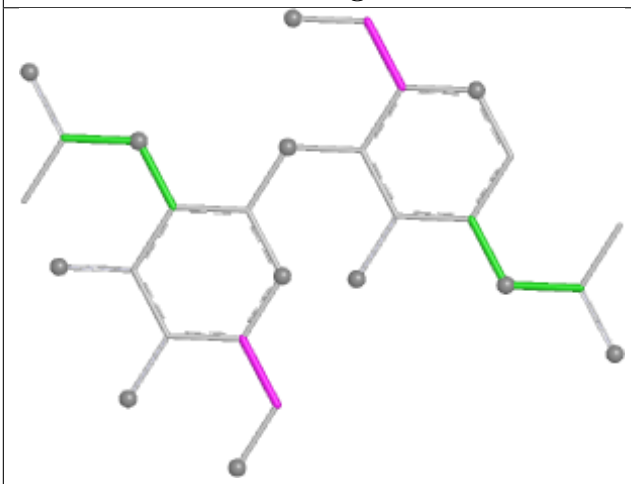
Oligosaccharide Chain P



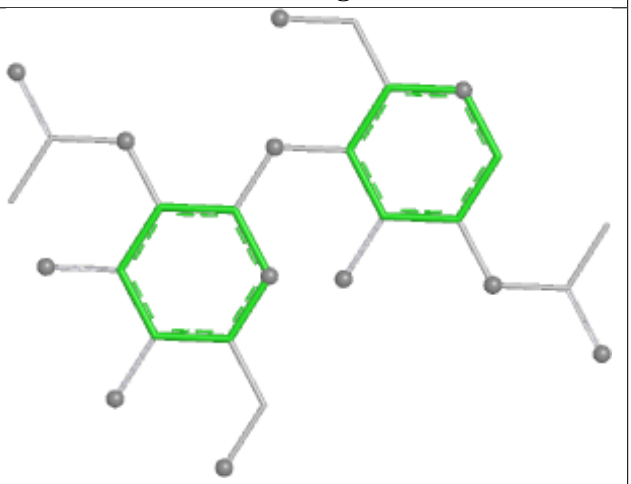
Bond lengths



Bond angles

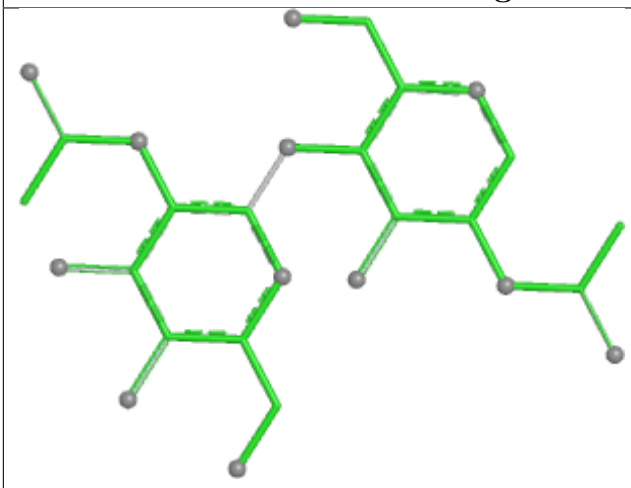


Torsions

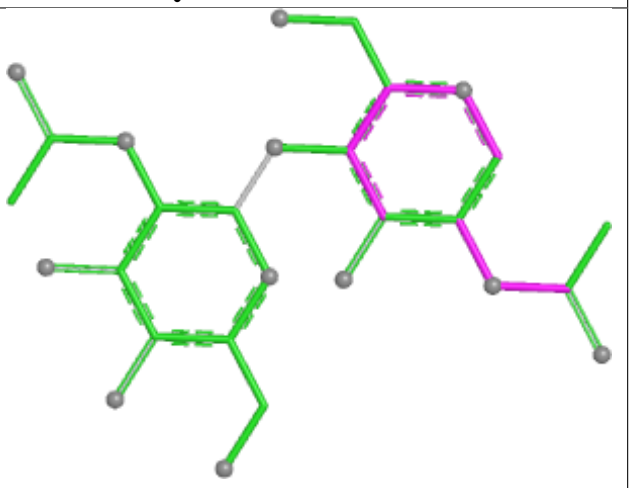


Rings

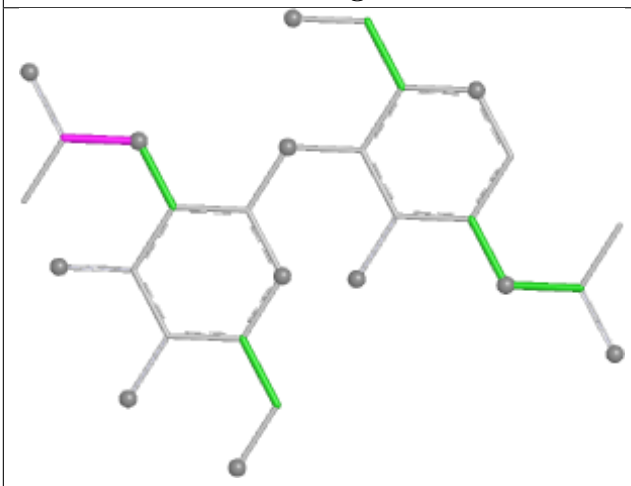
Oligosaccharide Chain Q



Bond lengths



Bond angles



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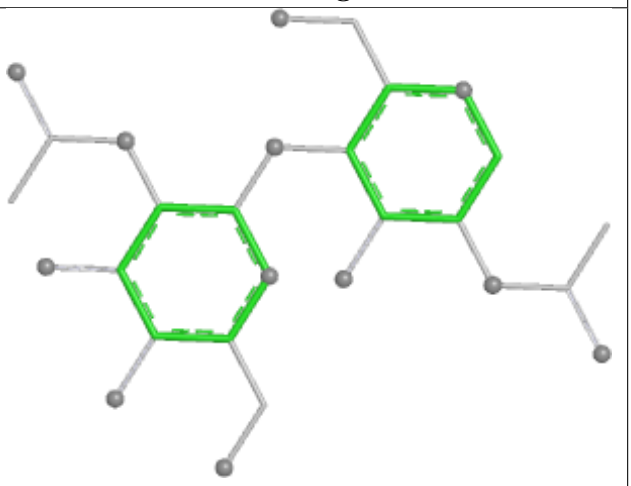
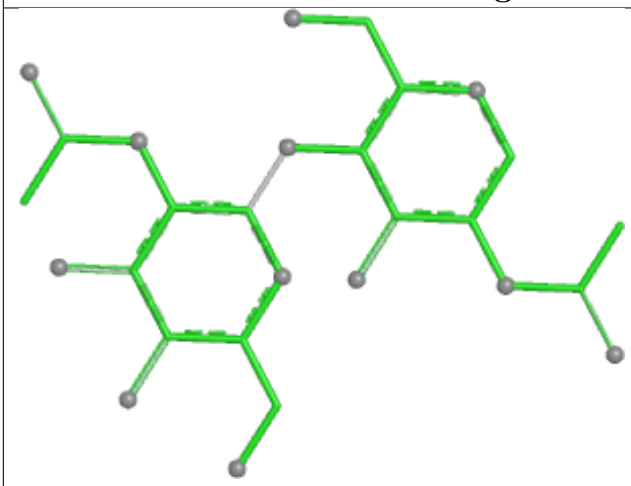
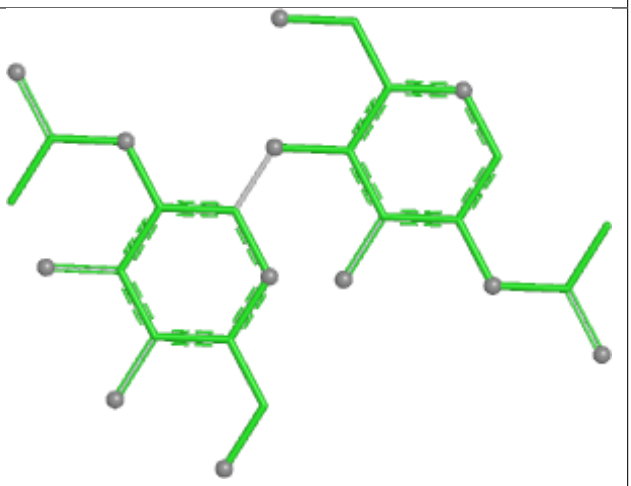


Rings

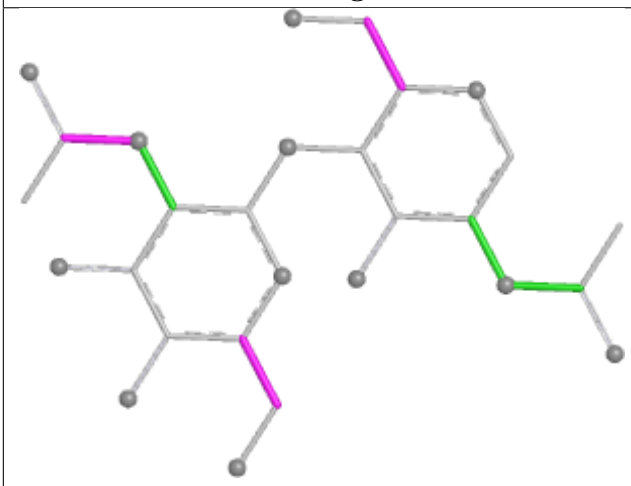
Oligosaccharide Chain R



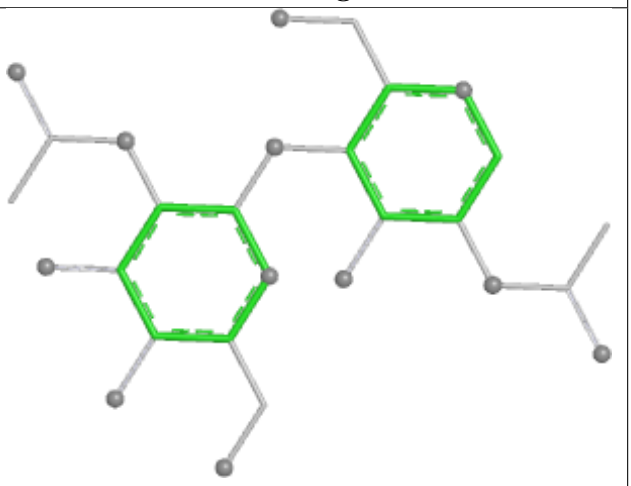
Bond lengths



Bond angles

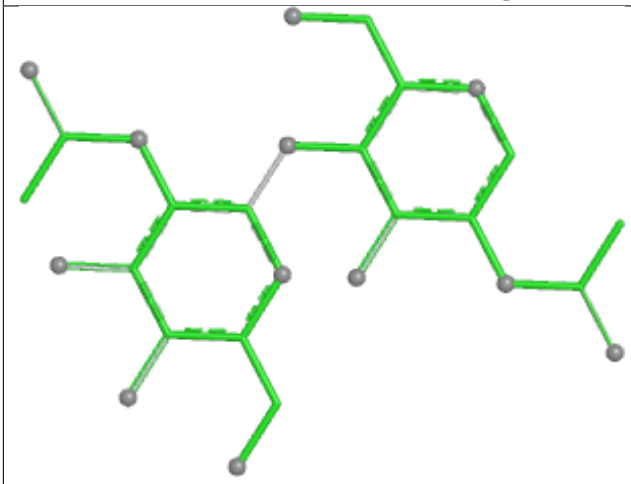


Torsions

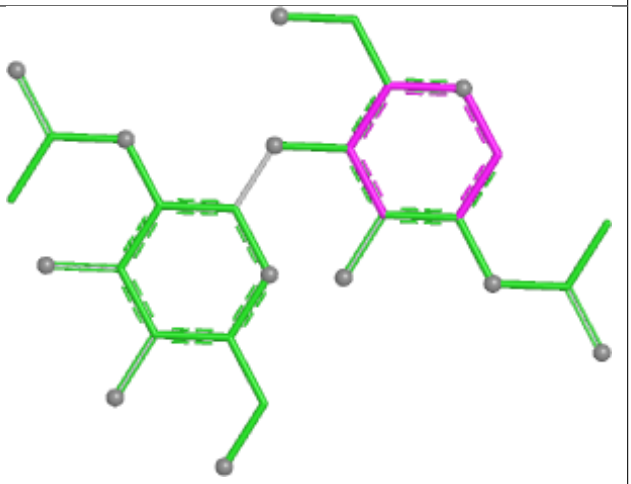


Rings

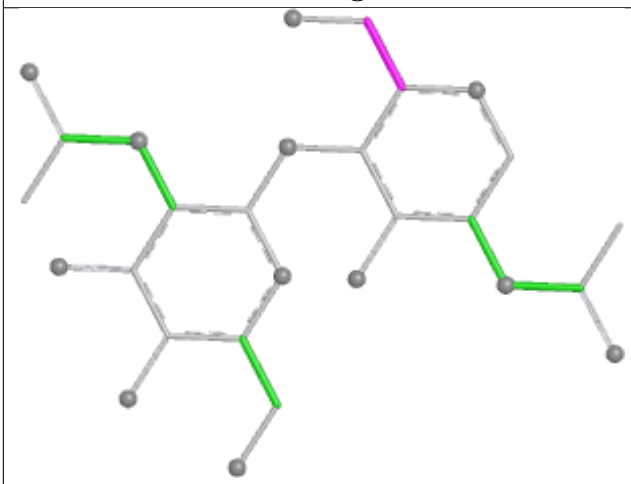
Oligosaccharide Chain S



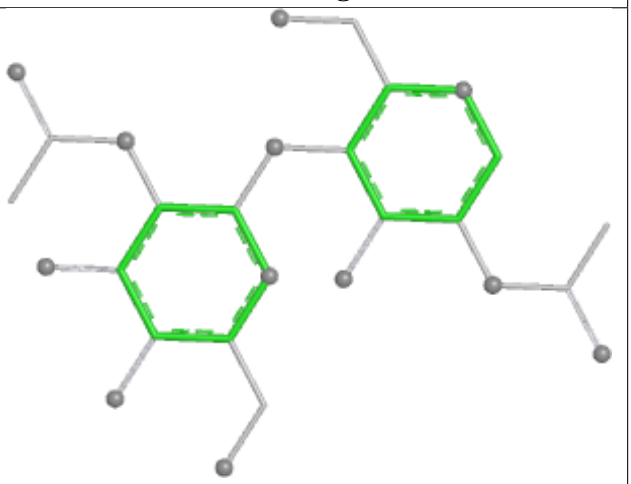
Bond lengths



Bond angles

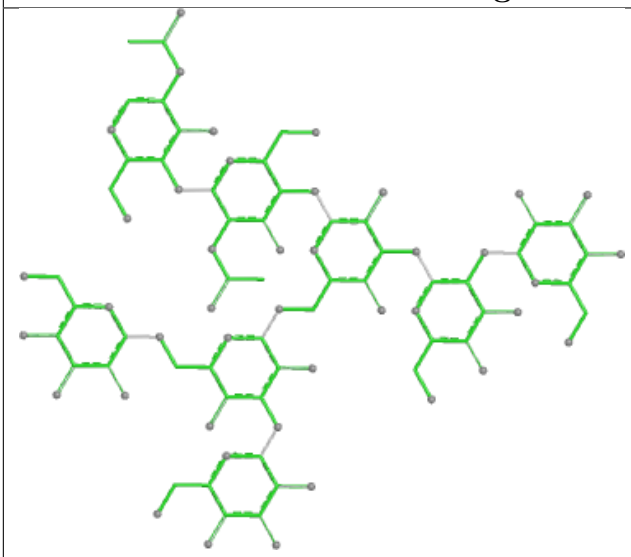


Torsions

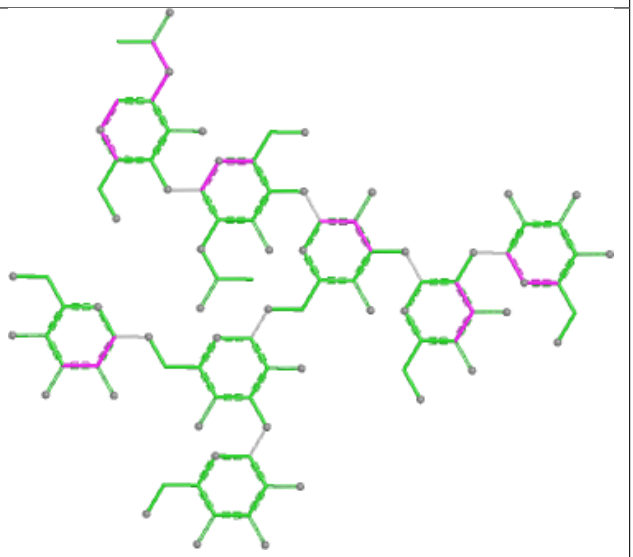


Rings

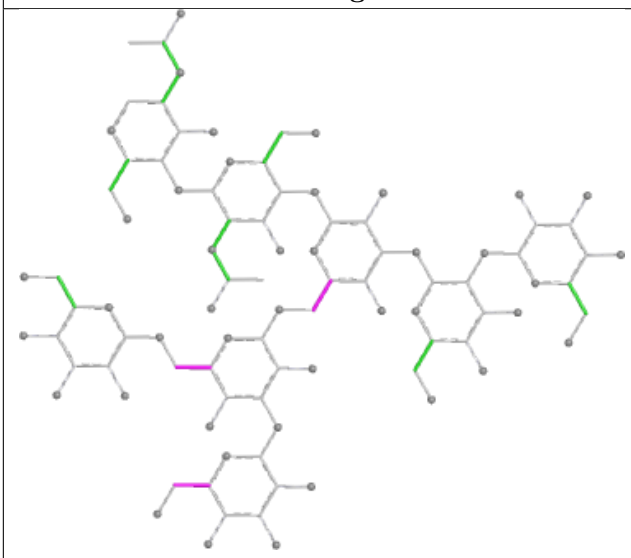
Oligosaccharide Chain H



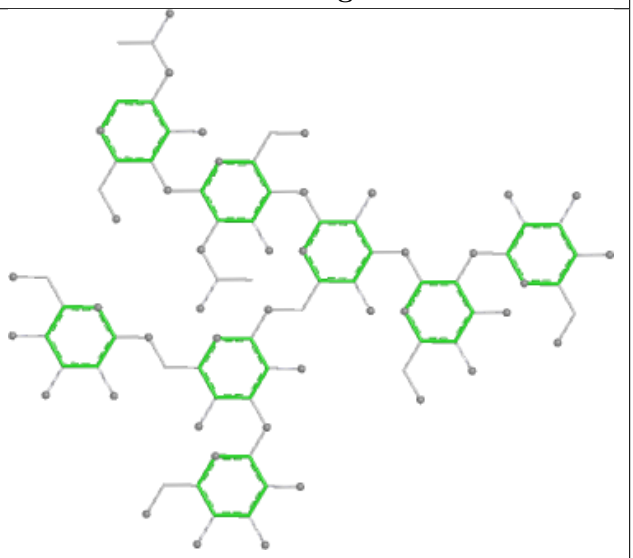
Bond lengths



Bond angles

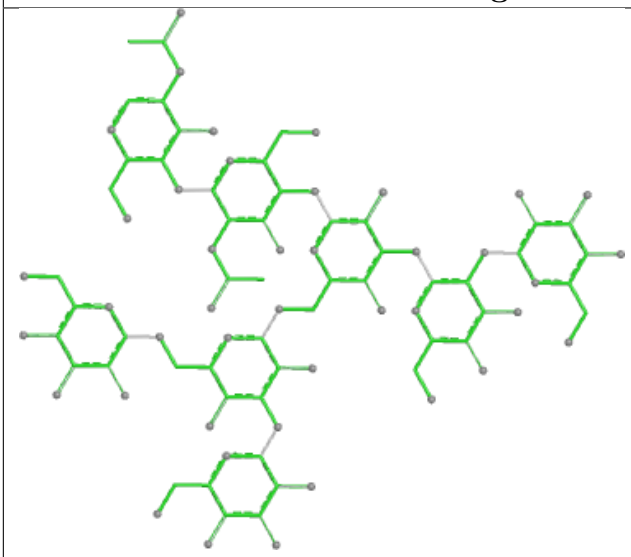


Torsions

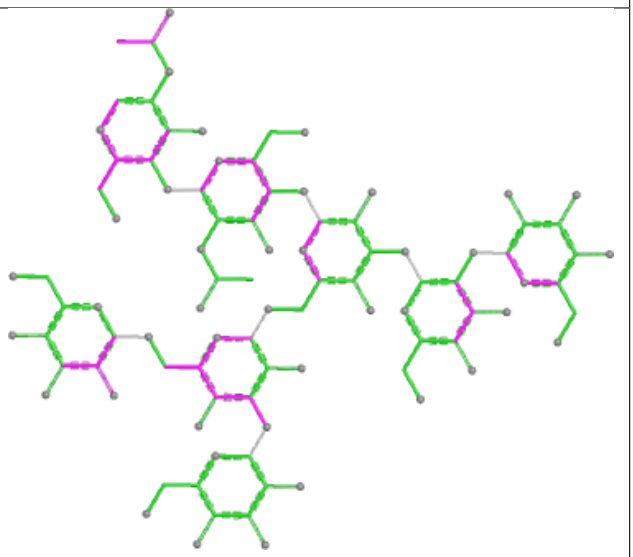


Rings

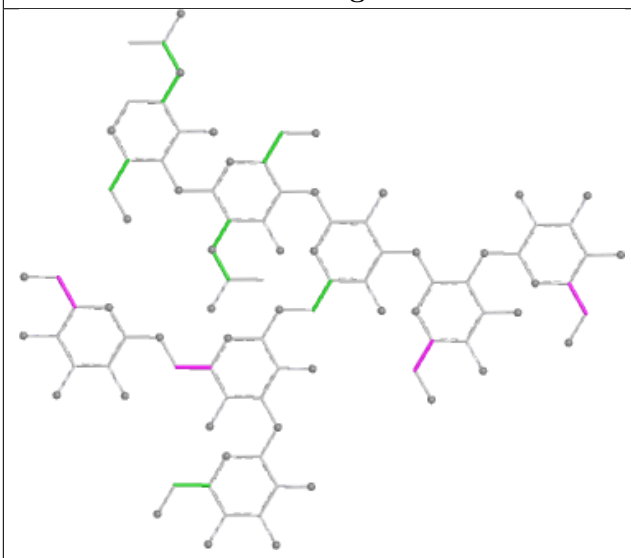
Oligosaccharide Chain M



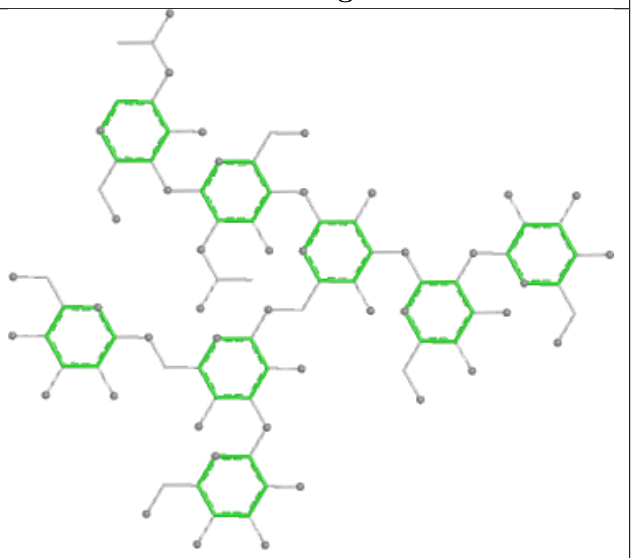
Bond lengths



Bond angles

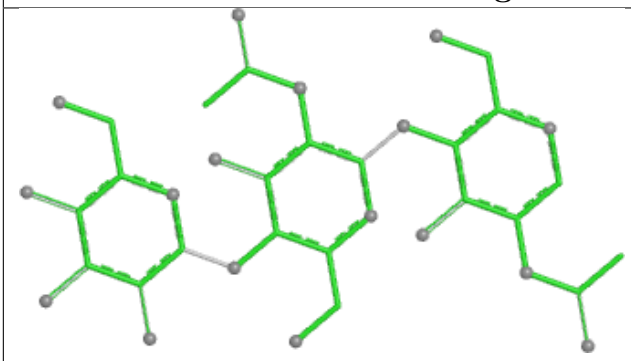


Torsions

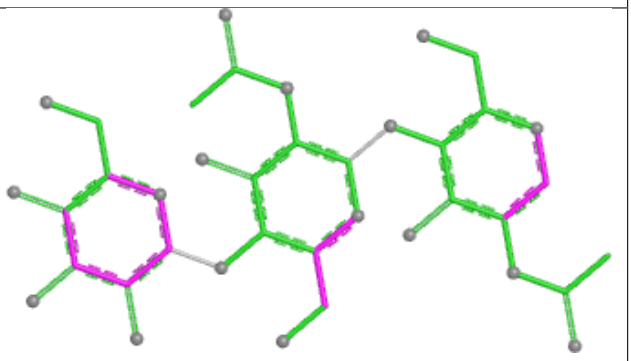


Rings

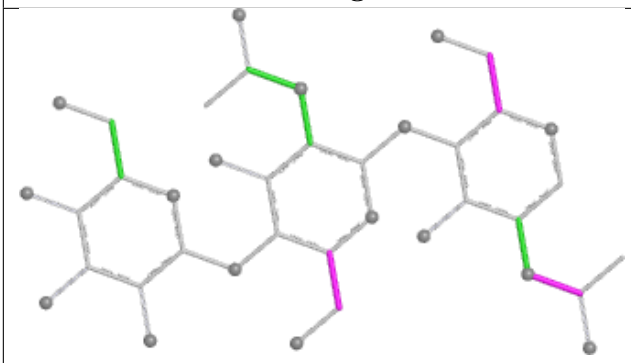
Oligosaccharide Chain O



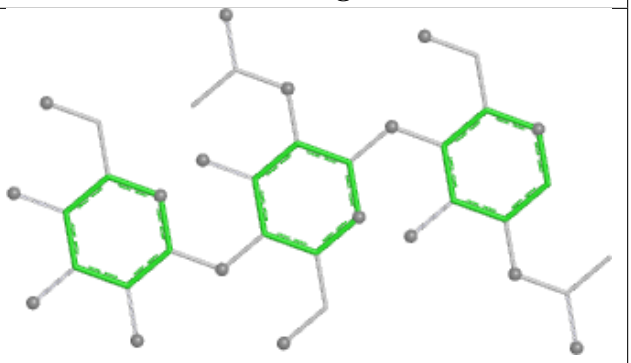
Bond lengths



Bond angles

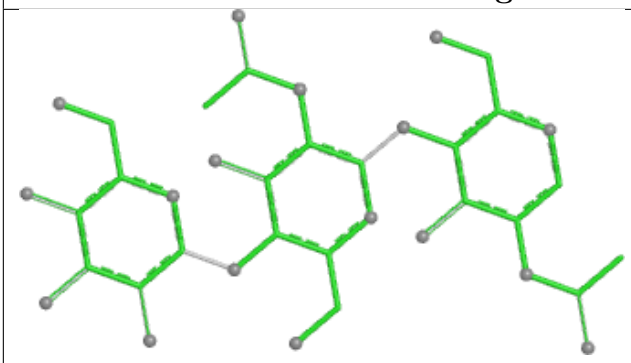


Torsions

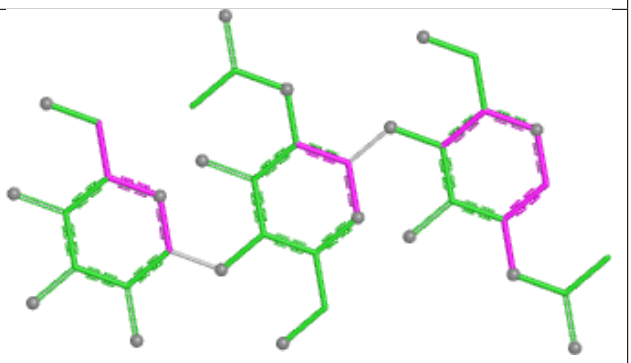


Rings

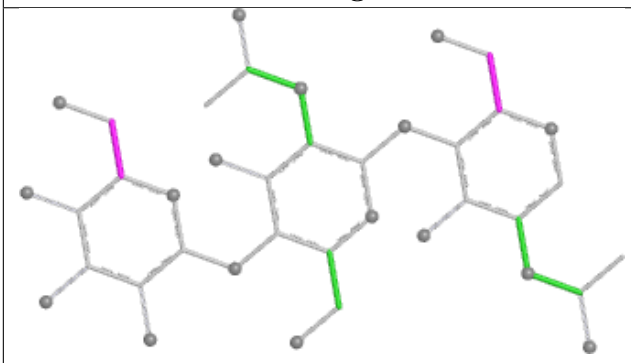
Oligosaccharide Chain T



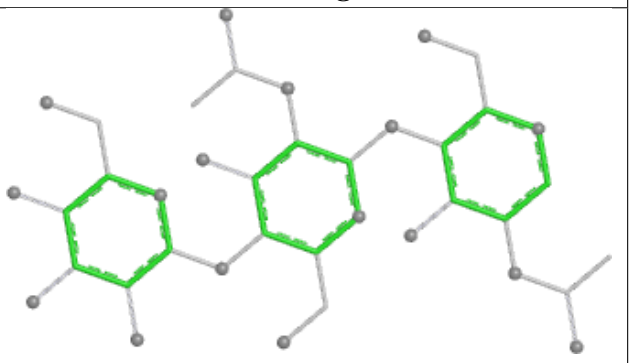
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 for Mogul analysis.

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	$\#\|Z\| > 2$
10	SO4	A	1330	-	4,4,4	0.27	0	6,6,6	0.18	0
10	SO4	A	1329	-	4,4,4	0.24	0	6,6,6	0.27	0
7	HEM	A	350	1,8	42,50,50	2.01	9 (21%)	46,82,82	1.46	5 (10%)
9	ACT	C	1334	-	3,3,3	0.76	0	3,3,3	1.35	0
7	HEM	D	350	1,8	42,50,50	1.83	5 (11%)	46,82,82	1.69	10 (21%)
10	SO4	C	1330	-	4,4,4	0.22	0	6,6,6	0.21	0
10	SO4	C	1332	-	4,4,4	0.29	0	6,6,6	0.21	0
10	SO4	B	1329	-	4,4,4	0.27	0	6,6,6	0.32	0
9	ACT	C	1329	-	3,3,3	0.71	0	3,3,3	1.48	0
11	NAG	D	391	1	14,14,15	0.54	0	17,19,21	1.45	4 (23%)
11	NAG	D	381	1	14,14,15	0.65	0	17,19,21	0.70	0
10	SO4	C	1333	-	4,4,4	0.21	0	6,6,6	0.07	0
11	NAG	D	411	1	14,14,15	0.55	0	17,19,21	0.83	0
10	SO4	A	1331	-	4,4,4	0.28	0	6,6,6	0.17	0
10	SO4	C	1331	-	4,4,4	0.24	0	6,6,6	0.13	0
10	SO4	A	1328	-	4,4,4	0.31	0	6,6,6	0.19	0
10	SO4	B	1331	-	4,4,4	0.27	0	6,6,6	0.19	0
11	NAG	C	381	1	14,14,15	0.63	0	17,19,21	1.37	2 (11%)
7	HEM	B	350	1,9,8	42,50,50	1.96	5 (11%)	46,82,82	1.51	8 (17%)
9	ACT	D	1327	-	3,3,3	0.71	0	3,3,3	1.39	0
10	SO4	D	1328	-	4,4,4	0.20	0	6,6,6	0.28	0
10	SO4	B	1330	-	4,4,4	0.23	0	6,6,6	0.17	0
9	ACT	A	1327	-	3,3,3	0.72	0	3,3,3	1.26	0
9	ACT	B	1328	7	3,3,3	0.80	0	3,3,3	1.25	0
10	SO4	D	1329	-	4,4,4	0.27	0	6,6,6	0.18	0
7	HEM	C	350	1,8	42,50,50	1.87	8 (19%)	46,82,82	1.55	8 (17%)

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
11	NAG	D	411	1	-	0/6/23/26	0/1/1/1
7	HEM	A	350	1,8	-	4/12/54/54	-
11	NAG	D	391	1	-	2/6/23/26	0/1/1/1
11	NAG	D	381	1	-	0/6/23/26	0/1/1/1
11	NAG	C	381	1	-	2/6/23/26	0/1/1/1
7	HEM	B	350	1,9,8	-	3/12/54/54	-
7	HEM	C	350	1,8	-	4/12/54/54	-
7	HEM	D	350	1,8	-	3/12/54/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	350	HEM	C3D-C2D	7.43	1.52	1.36
7	A	350	HEM	C3D-C2D	7.41	1.52	1.36
7	D	350	HEM	C3D-C2D	7.29	1.52	1.36
7	B	350	HEM	C3D-C2D	6.88	1.51	1.36
7	A	350	HEM	C3C-C2C	-5.49	1.32	1.40
7	B	350	HEM	C3C-C2C	-5.46	1.33	1.40
7	D	350	HEM	C3C-C2C	-4.56	1.34	1.40
7	C	350	HEM	C3C-C2C	-3.92	1.35	1.40
7	B	350	HEM	C3C-CAC	3.33	1.55	1.47
7	A	350	HEM	C3C-CAC	3.24	1.54	1.47
7	D	350	HEM	C3C-CAC	2.99	1.54	1.47
7	C	350	HEM	C3C-CAC	2.90	1.54	1.47
7	C	350	HEM	CAB-C3B	2.83	1.54	1.47
7	B	350	HEM	CAB-C3B	2.74	1.54	1.47
7	A	350	HEM	CMB-C2B	2.72	1.56	1.50
7	A	350	HEM	CAB-C3B	2.68	1.54	1.47
7	C	350	HEM	FE-ND	2.64	2.12	1.98
7	D	350	HEM	CAB-C3B	2.61	1.54	1.47
7	C	350	HEM	CMB-C2B	2.57	1.56	1.50
7	A	350	HEM	C3C-C4C	2.44	1.44	1.41
7	A	350	HEM	CMC-C2C	2.43	1.57	1.51
7	A	350	HEM	CMA-C3A	2.32	1.56	1.51
7	B	350	HEM	CMB-C2B	2.23	1.55	1.50
7	A	350	HEM	FE-ND	2.18	2.10	1.98
7	C	350	HEM	CMD-C2D	2.04	1.55	1.50
7	C	350	HEM	C3C-C4C	2.01	1.44	1.41
7	D	350	HEM	CMA-C3A	2.01	1.55	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	350	HEM	C4D-ND-C1D	4.56	110.60	105.21
7	D	350	HEM	C4D-ND-C1D	4.52	110.56	105.21
7	D	350	HEM	C4C-CHD-C1D	4.46	128.44	122.56
7	B	350	HEM	C4D-ND-C1D	4.40	110.42	105.21
7	C	350	HEM	C4D-ND-C1D	3.95	109.88	105.21
11	C	381	NAG	C4-C3-C2	3.67	116.39	111.02
7	B	350	HEM	C3B-C4B-NB	-3.32	107.08	109.47
7	C	350	HEM	C2C-C3C-C4C	3.22	109.15	106.90
11	D	391	NAG	C1-O5-C5	3.17	116.44	112.19
7	A	350	HEM	C2C-C3C-C4C	3.17	109.11	106.90
7	C	350	HEM	C4A-C3A-C2A	3.13	109.17	107.00
7	D	350	HEM	C2C-C3C-C4C	3.12	109.08	106.90
7	C	350	HEM	C4C-CHD-C1D	3.07	126.61	122.56
7	B	350	HEM	C1B-NB-C4B	2.85	108.58	105.21
7	D	350	HEM	CAD-CBD-CGD	-2.84	106.12	113.67
7	C	350	HEM	CMD-C2D-C1D	2.83	129.46	125.03
7	A	350	HEM	CAD-C3D-C4D	2.79	129.56	124.70
11	D	391	NAG	C1-C2-N2	2.78	114.81	110.43
7	B	350	HEM	C4C-CHD-C1D	2.71	126.14	122.56
11	D	391	NAG	C4-C3-C2	-2.69	107.08	111.02
7	A	350	HEM	CMD-C2D-C1D	2.66	129.19	125.03
7	D	350	HEM	CHD-C1D-ND	2.56	127.19	124.44
7	D	350	HEM	C3B-C2B-C1B	2.55	108.33	106.41
7	B	350	HEM	C2B-C1B-NB	-2.49	106.98	109.84
7	D	350	HEM	CHB-C1B-NB	2.44	127.40	124.37
7	A	350	HEM	C4C-CHD-C1D	2.42	125.75	122.56
7	B	350	HEM	C2C-C3C-C4C	2.32	108.52	106.90
7	B	350	HEM	C3B-C2B-C1B	2.29	108.13	106.41
11	C	381	NAG	C3-C4-C5	2.23	114.27	110.23
7	D	350	HEM	CMA-C3A-C4A	-2.22	125.21	128.46
7	D	350	HEM	CAD-C3D-C4D	2.21	128.54	124.70
7	B	350	HEM	C4B-CHC-C1C	2.16	125.41	122.56
7	C	350	HEM	CBD-CAD-C3D	-2.15	106.59	112.53
7	D	350	HEM	C3B-C4B-NB	-2.11	107.96	109.47
7	C	350	HEM	CMA-C3A-C4A	-2.10	125.39	128.46
7	C	350	HEM	C1D-C2D-C3D	-2.09	104.79	106.98
11	D	391	NAG	C3-C4-C5	-2.07	106.47	110.23

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	C	381	NAG	O5-C5-C6-O6
7	A	350	HEM	C2A-CAA-CBA-CGA
7	D	350	HEM	C2A-CAA-CBA-CGA
11	D	391	NAG	O5-C5-C6-O6
11	D	391	NAG	C4-C5-C6-O6
7	B	350	HEM	C2A-CAA-CBA-CGA
7	C	350	HEM	C2A-CAA-CBA-CGA
7	A	350	HEM	CAA-CBA-CGA-O2A
7	C	350	HEM	CAA-CBA-CGA-O1A
7	B	350	HEM	CAA-CBA-CGA-O1A
7	A	350	HEM	C2B-C3B-CAB-CBB
7	D	350	HEM	CAA-CBA-CGA-O1A
7	C	350	HEM	C4B-C3B-CAB-CBB
7	A	350	HEM	CAA-CBA-CGA-O1A
7	B	350	HEM	CAA-CBA-CGA-O2A
7	C	350	HEM	CAA-CBA-CGA-O2A
7	D	350	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

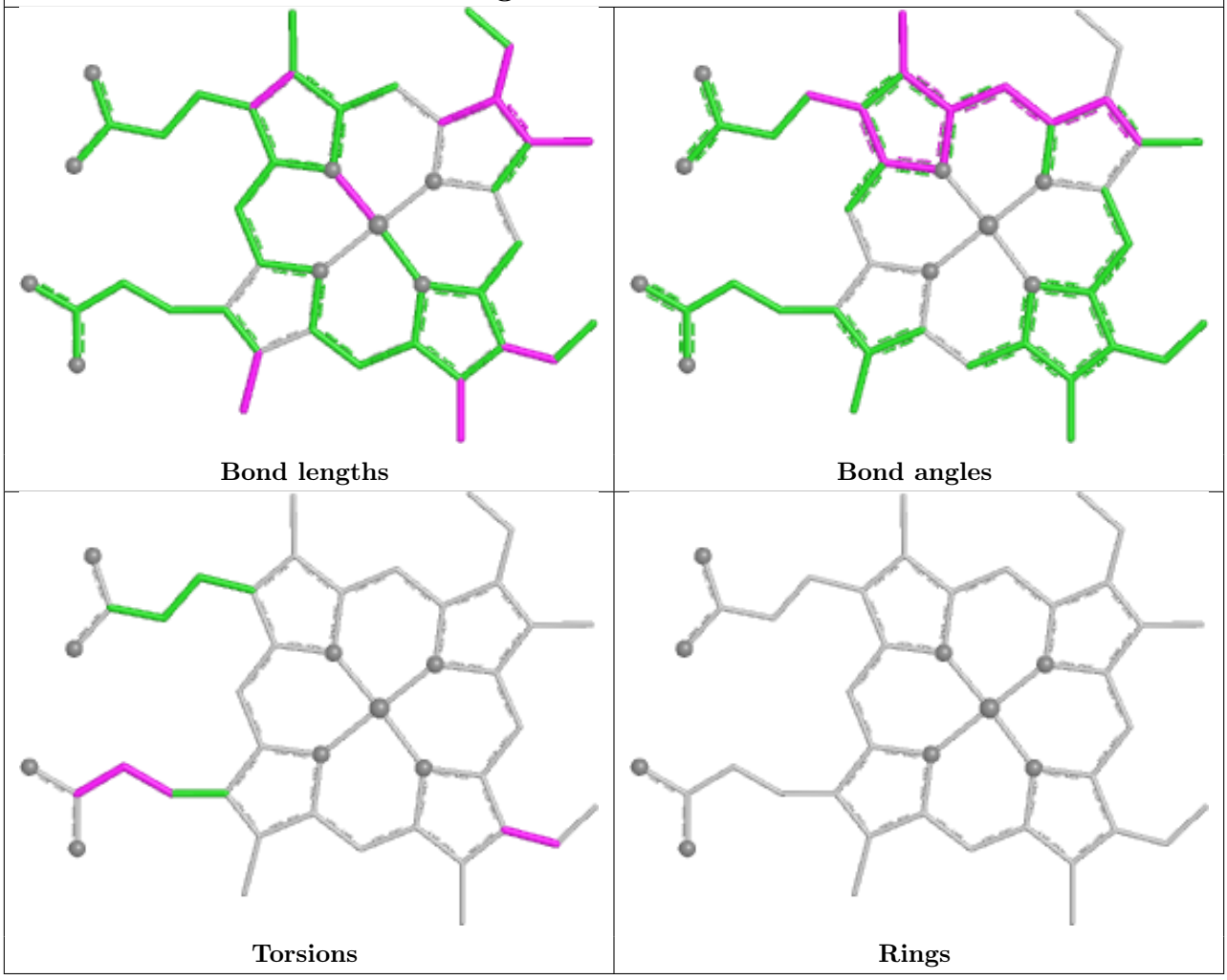
9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	350	HEM	5	0
7	D	350	HEM	3	0
10	A	1331	SO4	2	0
10	B	1331	SO4	2	0
11	C	381	NAG	1	0
7	B	350	HEM	3	0
10	D	1328	SO4	1	0
10	D	1329	SO4	1	0
7	C	350	HEM	3	0

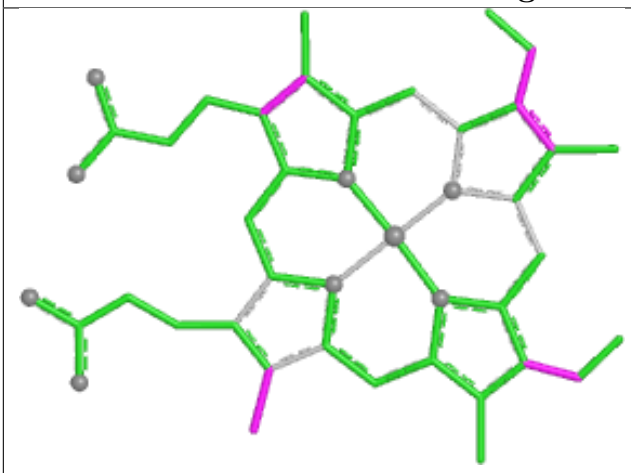
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

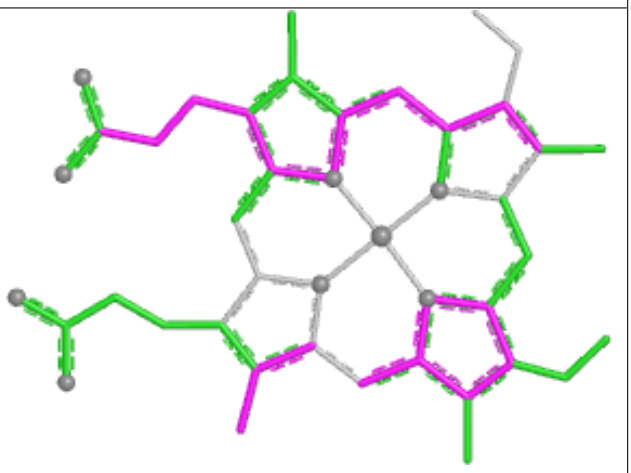
Ligand HEM A 350



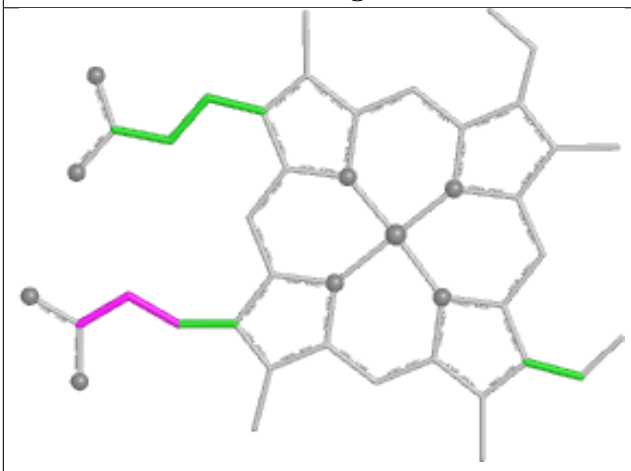
Ligand HEM D 350



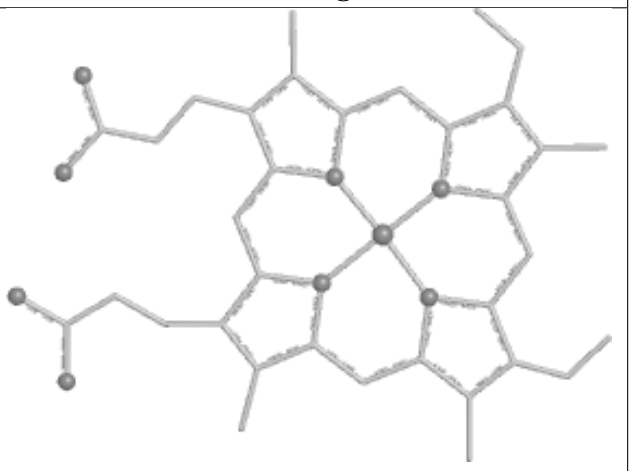
Bond lengths



Bond angles

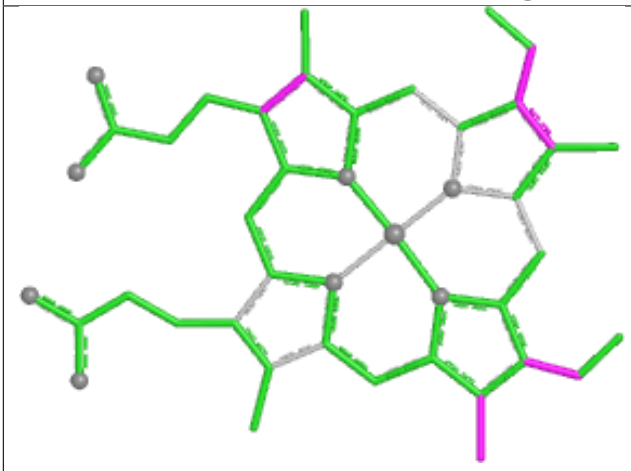


Torsions

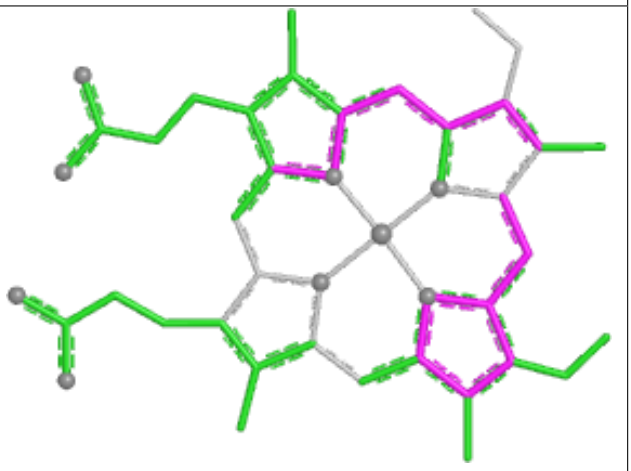


Rings

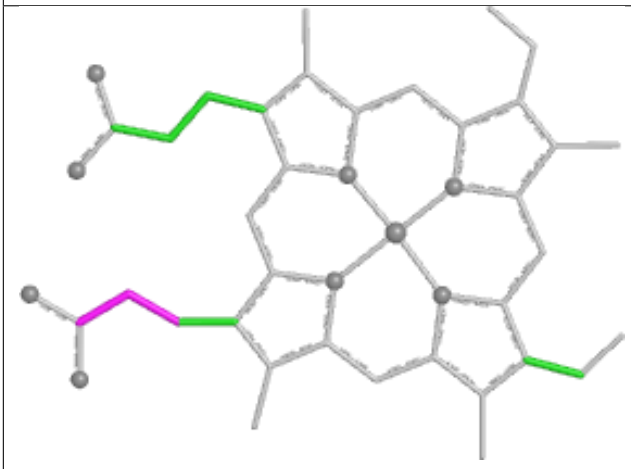
Ligand HEM B 350



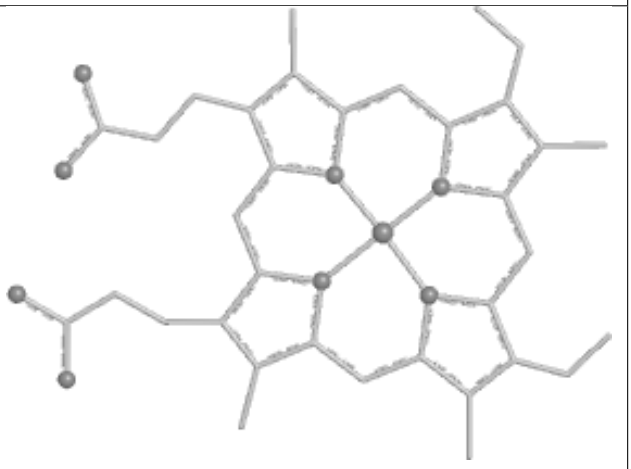
Bond lengths



Bond angles

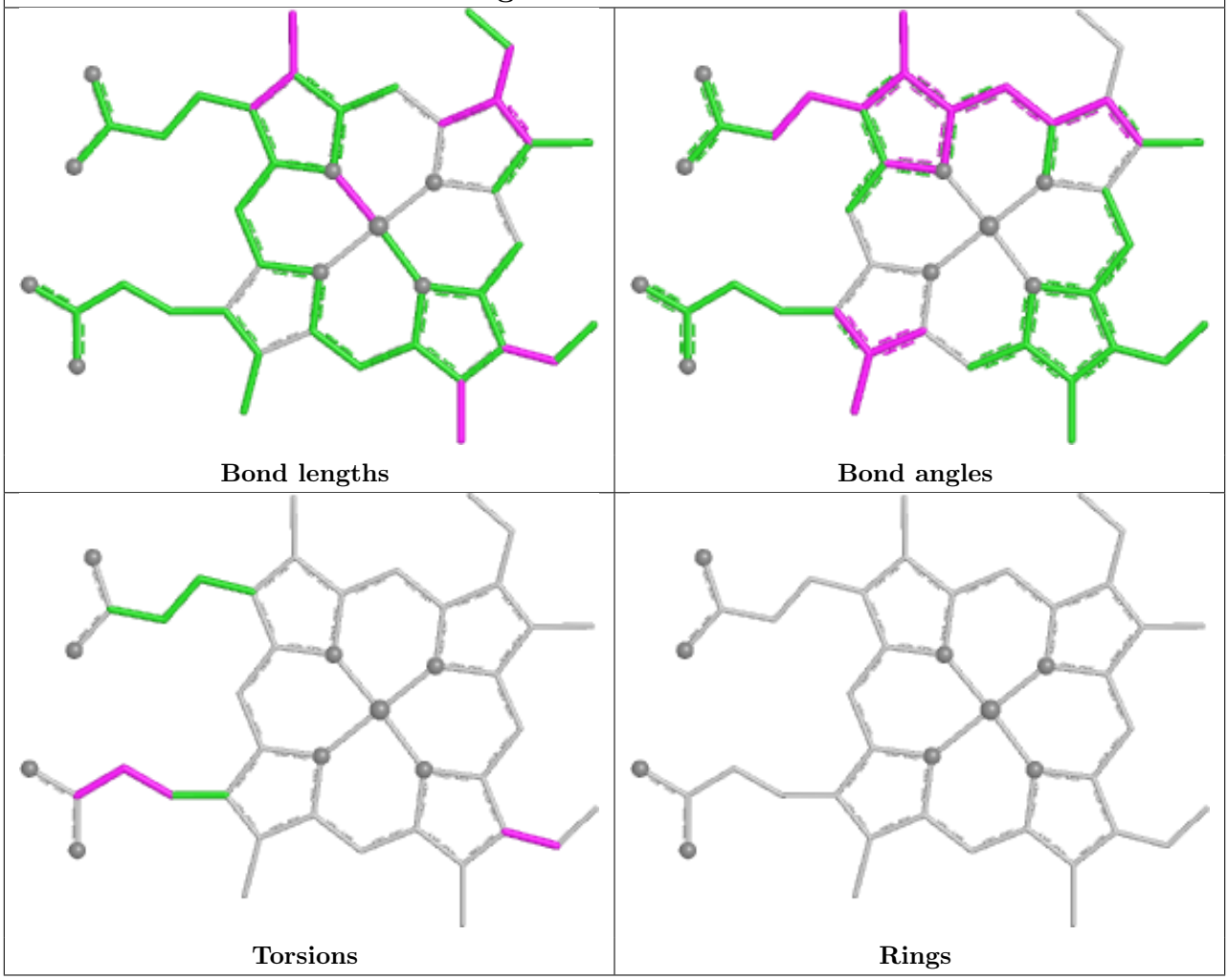


Torsions



Rings

Ligand HEM C 350



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Warning: The R factor obtained from EDS is 0.3888, which does not match the depositor's R factor of 0.1774. Please interpret the results in this section carefully.

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^{th} 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	323/325 (99%)	3.18	241 (74%)	0	0	12, 26, 42, 56	1 (0%)
1	B	324/325 (99%)	2.38	185 (57%)	0	0	10, 21, 34, 53	4 (1%)
1	C	325/325 (100%)	2.56	210 (64%)	0	0	14, 24, 37, 68	1 (0%)
1	D	323/325 (99%)	3.68	297 (91%)	0	0	15, 32, 47, 59	1 (0%)
All	All	1295/1300 (99%)	2.95	933 (72%)	0	0	10, 26, 43, 68	7 (0%)

All (933) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	THR	11.2
1	A	30	GLY	10.8
1	D	326	GLY	10.5
1	D	260	GLY	8.8
1	A	13	SER	8.4
1	A	31	ASP	8.4
1	D	4	LEU	8.3
1	A	28	ARG	8.1
1	A	90	THR	8.0
1	A	310	PHE	8.0
1	D	19	ASP	7.8
1	C	14	ALA	7.8
1	B	21	ALA	7.5
1	A	54	ALA	7.4
1	A	4	LEU	7.4
1	D	24	TRP	7.4
1	D	179	THR	7.3
1	B	264	SER	7.3
1	D	133	PHE	7.3

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Mol	Chain	Res	Type	RSRZ
1	D	132	ALA	7.3
1	A	303	ALA	7.2
1	D	90	THR	7.2
1	C	4	LEU	7.2
1	C	259	VAL	7.1
1	A	99	THR	7.1
1	B	197	THR	7.1
1	A	299	GLN	7.1
1	D	135	GLY	7.1
1	A	228	MET	7.0
1	C	30	GLY	7.0
1	C	5	PRO	7.0
1	B	15	LYS	6.9
1	D	101	LEU	6.9
1	D	212	GLY	6.8
1	D	184	SER	6.8
1	D	303	ALA	6.7
1	A	10	GLU	6.7
1	D	186	VAL	6.7
1	D	6	PRO	6.7
1	A	9	LEU	6.7
1	D	300	LEU	6.7
1	A	89	ILE	6.7
1	D	21	ALA	6.5
1	A	226	SER	6.5
1	D	259	VAL	6.5
1	D	302	LYS	6.5
1	A	63	VAL	6.5
1	A	52	GLY	6.4
1	D	42	LEU	6.4
1	D	134	PHE	6.3
1	A	29	PRO	6.2
1	B	9	LEU	6.1
1	D	109	PRO	6.1
1	A	266	THR	6.1
1	A	326	GLY	6.1
1	D	20	GLU	6.1
1	B	29	PRO	6.0
1	C	205	VAL	5.9
1	B	327	ARG	5.9
1	D	265	TYR	5.9
1	C	71	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	22	HIS	5.9
1	D	107	PRO	5.9
1	D	25	LYS	5.9
1	B	4	LEU	5.8
1	A	64	GLN	5.8
1	A	51	ASN	5.8
1	A	19	ASP	5.7
1	A	32	ILE	5.7
1	D	246	VAL	5.7
1	B	181	PRO	5.7
1	B	309	ASP	5.6
1	C	328	ASP	5.6
1	D	70	ASP	5.6
1	A	296	PRO	5.6
1	A	101	LEU	5.6
1	D	180	ASN	5.5
1	A	43	ALA	5.5
1	D	269	PRO	5.5
1	D	215	ASP	5.4
1	A	92	LEU	5.4
1	A	300	LEU	5.4
1	A	14	ALA	5.4
1	B	119	GLY	5.4
1	B	65	GLU	5.4
1	D	106	PRO	5.4
1	A	233	PHE	5.4
1	D	216	MET	5.4
1	A	5	PRO	5.3
1	C	106	PRO	5.3
1	A	59	ILE	5.3
1	D	140	PHE	5.3
1	C	327	ARG	5.3
1	D	298	VAL	5.3
1	A	66	GLY	5.3
1	A	322	VAL	5.3
1	D	225	PHE	5.3
1	D	12	SER	5.2
1	B	72	GLN	5.2
1	A	295	ASN	5.2
1	C	135	GLY	5.2
1	D	261	LYS	5.2
1	D	116	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	44	SER	5.2
1	D	301	ARG	5.2
1	A	103	GLY	5.2
1	A	6	PRO	5.1
1	D	130	GLY	5.1
1	D	95	ILE	5.1
1	A	200	PRO	5.1
1	C	236	PRO	5.1
1	D	229	PRO	5.1
1	A	88	LEU	5.1
1	D	10	GLU	5.1
1	D	120	THR	5.1
1	A	23	PRO	5.1
1	D	178	ALA	5.1
1	D	207	GLY	5.1
1	D	296	PRO	5.1
1	D	39	LEU	5.0
1	D	67	LEU	5.0
1	D	32	ILE	5.0
1	D	8	PRO	5.0
1	D	262	ILE	5.0
1	D	323	PHE	5.0
1	C	317	ALA	5.0
1	D	53	VAL	5.0
1	B	101	LEU	5.0
1	A	20	GLU	4.9
1	D	313[A]	GLN	4.9
1	D	100	ARG	4.9
1	B	276	THR	4.9
1	A	44	SER	4.9
1	D	57	VAL	4.9
1	A	16	LEU	4.9
1	D	65	GLU	4.8
1	A	21	ALA	4.8
1	D	148	LEU	4.8
1	B	10	GLU	4.8
1	D	113	GLY	4.8
1	D	222	PHE	4.8
1	C	299	GLN	4.8
1	D	292	LEU	4.8
1	D	112	VAL	4.7
1	B	11	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	82	HIS	4.7
1	B	46	GLY	4.7
1	A	302	LYS	4.7
1	B	27	LEU	4.7
1	C	298	VAL	4.7
1	D	9	LEU	4.7
1	D	235	ALA	4.7
1	D	27	LEU	4.7
1	C	9	LEU	4.6
1	A	116	ASN	4.6
1	B	295	ASN	4.6
1	D	224	GLN	4.6
1	D	299	GLN	4.6
1	D	200	PRO	4.6
1	D	92	LEU	4.6
1	A	309	ASP	4.6
1	B	317	ALA	4.6
1	A	53	VAL	4.6
1	B	8	PRO	4.6
1	C	190	PHE	4.6
1	A	230	ASP	4.6
1	D	111	SER	4.6
1	D	264	SER	4.6
1	B	7	GLY	4.6
1	A	292	LEU	4.6
1	D	286	ASN	4.6
1	D	233	PHE	4.5
1	D	295	ASN	4.5
1	D	149	VAL	4.5
1	A	47	TYR	4.5
1	A	294	PRO	4.5
1	A	86	GLY	4.5
1	D	41	THR	4.5
1	D	139	ASP	4.5
1	D	18	ASN	4.5
1	D	54	ALA	4.5
1	A	15	LYS	4.5
1	B	269	PRO	4.5
1	D	177	ILE	4.5
1	A	100	ARG	4.5
1	D	28	ARG	4.5
1	D	209	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	155	PHE	4.5
1	B	14	ALA	4.4
1	B	304	LEU	4.4
1	C	39	LEU	4.4
1	B	203	LEU	4.4
1	D	136	ASN	4.4
1	C	16	LEU	4.4
1	A	91	ASP	4.3
1	C	105	ASP	4.3
1	C	138	HIS	4.3
1	C	11	ASN	4.3
1	A	237	SER	4.3
1	C	207	GLY	4.3
1	D	102	THR	4.3
1	C	225	PHE	4.3
1	D	249	GLN	4.3
1	D	168	LEU	4.3
1	D	110	ALA	4.3
1	A	46	GLY	4.3
1	D	164	VAL	4.3
1	B	308	LEU	4.3
1	A	70	ASP	4.3
1	B	268	ASP	4.3
1	A	24	TRP	4.3
1	D	183	PHE	4.3
1	C	15	LYS	4.3
1	D	287	ILE	4.3
1	B	150[A]	ASP	4.2
1	C	152	SER	4.2
1	D	5	PRO	4.2
1	A	235	ALA	4.2
1	B	207	GLY	4.2
1	D	52	GLY	4.2
1	D	97	ARG	4.2
1	A	57	VAL	4.2
1	A	285	VAL	4.2
1	C	149	VAL	4.2
1	D	11	ASN	4.2
1	A	104	PRO	4.2
1	C	7	GLY	4.2
1	A	17	VAL	4.2
1	D	217	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	20	GLU	4.2
1	A	205	VAL	4.2
1	B	12	SER	4.2
1	D	226	SER	4.2
1	D	310	PHE	4.1
1	D	159	LYS	4.1
1	D	306	THR	4.1
1	C	8	PRO	4.1
1	A	7	GLY	4.1
1	A	323	PHE	4.1
1	B	201	ALA	4.1
1	B	233	PHE	4.1
1	D	47	TYR	4.1
1	C	10	GLU	4.1
1	C	212	GLY	4.1
1	D	7	GLY	4.1
1	D	218	ALA	4.1
1	A	311	PHE	4.1
1	A	289	VAL	4.1
1	A	206	ASP	4.1
1	D	45	HIS	4.1
1	D	309	ASP	4.1
1	C	306	THR	4.1
1	B	326	GLY	4.0
1	C	155	PHE	4.0
1	D	284	PHE	4.0
1	D	214	LEU	4.0
1	D	282	GLU	4.0
1	B	19	ASP	4.0
1	B	210	ASP	4.0
1	C	238	PRO	4.0
1	B	176	SER	4.0
1	C	13	SER	4.0
1	D	237	SER	4.0
1	C	28	ARG	4.0
1	D	88	LEU	4.0
1	A	315	VAL	4.0
1	A	307	ASN	4.0
1	D	26	PRO	4.0
1	D	87	ASN	4.0
1	D	91	ASP	4.0
1	D	305	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	4.0
1	A	225	PHE	4.0
1	B	311	PHE	4.0
1	A	217[A]	ASP	4.0
1	B	5	PRO	4.0
1	B	51	ASN	4.0
1	C	294	PRO	4.0
1	C	241	GLY	4.0
1	C	249	GLN	4.0
1	D	250	ALA	4.0
1	D	36	CYS	4.0
1	D	23	PRO	3.9
1	D	127	MET	3.9
1	D	86	GLY	3.9
1	D	157	GLY	3.9
1	C	313	GLN	3.9
1	D	13	SER	3.9
1	C	134	PHE	3.9
1	A	256	GLY	3.9
1	C	237	SER	3.9
1	D	138	HIS	3.9
1	D	142	GLU	3.9
1	D	232	PHE	3.9
1	D	37	PRO	3.9
1	A	306	THR	3.9
1	C	320	THR	3.9
1	C	264	SER	3.9
1	A	132	ALA	3.9
1	C	110	ALA	3.9
1	C	326	GLY	3.9
1	D	325	TYR	3.9
1	A	74	ALA	3.9
1	C	125	ALA	3.9
1	B	232	PHE	3.8
1	A	207	GLY	3.8
1	D	156	GLY	3.8
1	A	41	THR	3.8
1	D	78	THR	3.8
1	A	209	ARG	3.8
1	C	27	LEU	3.8
1	C	203	LEU	3.8
1	D	227	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	199	PHE	3.8
1	C	217	ASP	3.8
1	D	221	SER	3.8
1	B	316	ALA	3.8
1	D	144	LEU	3.8
1	B	310	PHE	3.8
1	D	231	ASP	3.8
1	A	34	GLY	3.8
1	C	235	ALA	3.8
1	D	80	ALA	3.8
1	D	93	LEU	3.8
1	D	223	PHE	3.8
1	C	221	SER	3.7
1	A	325	TYR	3.7
1	D	79	TYR	3.7
1	A	193	ALA	3.7
1	A	115	LEU	3.7
1	B	88	LEU	3.7
1	D	16	LEU	3.7
1	A	290	LYS	3.7
1	C	230	ASP	3.7
1	D	241	GLY	3.7
1	B	235	ALA	3.7
1	B	16	LEU	3.7
1	C	23	PRO	3.7
1	D	49	PRO	3.7
1	B	89	ILE	3.7
1	C	210	ASP	3.7
1	B	63	VAL	3.7
1	C	242	THR	3.7
1	D	151	TYR	3.7
1	D	108	PRO	3.7
1	D	137	ASN	3.7
1	A	105	ASP	3.7
1	C	260	GLY	3.7
1	A	320	THR	3.7
1	B	289	VAL	3.7
1	B	275	SER	3.7
1	D	290	LYS	3.7
1	D	146	GLU	3.7
1	A	270	THR	3.6
1	C	94	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	61	ASN	3.6
1	D	220	ARG	3.6
1	D	257	ARG	3.6
1	D	34	GLY	3.6
1	D	131	ASP	3.6
1	A	75	VAL	3.6
1	A	259	VAL	3.6
1	C	57	VAL	3.6
1	A	8	PRO	3.6
1	A	110	ALA	3.6
1	D	308	LEU	3.6
1	D	50	ARG	3.6
1	D	234	ARG	3.6
1	D	278	CYS	3.6
1	A	318	GLY	3.6
1	D	31	ASP	3.6
1	D	230	ASP	3.6
1	D	208	ARG	3.6
1	D	74	ALA	3.6
1	A	287	ILE	3.6
1	D	99	THR	3.6
1	B	298	VAL	3.6
1	D	22	HIS	3.6
1	C	178	ALA	3.6
1	C	85	ASP	3.5
1	A	164	VAL	3.5
1	A	291	SER	3.5
1	A	42	LEU	3.5
1	C	98	LYS	3.5
1	B	313	GLN	3.5
1	C	243	GLY	3.5
1	D	38	GLY	3.5
1	B	102	THR	3.5
1	A	106	PRO	3.5
1	A	18	ASN	3.5
1	C	262	ILE	3.5
1	A	288	THR	3.5
1	B	322	VAL	3.5
1	D	267	VAL	3.5
1	A	181	PRO	3.5
1	A	93	LEU	3.5
1	C	297	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	261	LYS	3.5
1	D	152	SER	3.4
1	A	27	LEU	3.4
1	D	43	ALA	3.4
1	D	154	ARG	3.4
1	C	170	PHE	3.4
1	C	233	PHE	3.4
1	C	17	VAL	3.4
1	C	29	PRO	3.4
1	B	48	LEU	3.4
1	C	218	ALA	3.4
1	B	105	ASP	3.4
1	B	320	THR	3.4
1	D	204	PHE	3.4
1	B	154	ARG	3.4
1	B	318	GLY	3.4
1	D	256	GLY	3.4
1	C	248	ILE	3.4
1	A	121	PHE	3.4
1	B	133	PHE	3.4
1	B	47	TYR	3.4
1	C	72	GLN	3.4
1	B	126	SER	3.4
1	A	141	ASN	3.4
1	C	61	ASN	3.4
1	A	81	ALA	3.4
1	D	201	ALA	3.4
1	B	270	THR	3.3
1	D	94	SER	3.3
1	D	304	LEU	3.3
1	B	20[A]	GLU	3.3
1	D	182	ASN	3.3
1	C	228	MET	3.3
1	A	313	GLN	3.3
1	D	294	PRO	3.3
1	D	172	ARG	3.3
1	A	65	GLU	3.3
1	C	307	ASN	3.3
1	D	228	MET	3.3
1	A	316	ALA	3.3
1	B	77	ALA	3.3
1	A	58	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	107	PRO	3.3
1	C	232	PHE	3.3
1	B	13	SER	3.3
1	B	281	TYR	3.3
1	B	96	GLY	3.3
1	D	51	ASN	3.3
1	A	227	ARG	3.3
1	C	26	PRO	3.3
1	A	142	GLU	3.3
1	A	12	SER	3.3
1	D	291	SER	3.3
1	A	175	ASP	3.2
1	C	107	PRO	3.2
1	C	108	PRO	3.2
1	C	310	PHE	3.2
1	D	69	PHE	3.2
1	D	121	PHE	3.2
1	A	67	LEU	3.2
1	A	279	LEU	3.2
1	C	101	LEU	3.2
1	B	125	ALA	3.2
1	A	301	ARG	3.2
1	A	45	HIS	3.2
1	C	253	MET	3.2
1	A	39	LEU	3.2
1	C	24	TRP	3.2
1	A	136	ASN	3.2
1	A	117	GLU	3.2
1	A	324	PRO	3.2
1	D	163	THR	3.2
1	D	188	PHE	3.2
1	A	314	GLY	3.2
1	B	267	VAL	3.2
1	C	315	VAL	3.2
1	D	96	GLY	3.2
1	A	85	ASP	3.2
1	D	77	ALA	3.2
1	D	150	ASP	3.2
1	D	192	THR	3.2
1	C	246	VAL	3.1
1	D	71	ASN	3.1
1	D	263	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	160	TYR	3.1
1	B	6	PRO	3.1
1	C	6	PRO	3.1
1	C	55	THR	3.1
1	C	89	ILE	3.1
1	A	140	PHE	3.1
1	A	222	PHE	3.1
1	C	83	LEU	3.1
1	C	88	LEU	3.1
1	D	64	GLN	3.1
1	D	145	PHE	3.1
1	A	202	ASN	3.1
1	B	244	VAL	3.1
1	A	218	ALA	3.1
1	A	108	PRO	3.1
1	D	55	THR	3.1
1	C	32	ILE	3.1
1	C	154	ARG	3.1
1	A	283	LYS	3.1
1	D	174	GLN	3.1
1	D	279	LEU	3.1
1	A	190	PHE	3.1
1	D	185	PHE	3.1
1	C	137	ASN	3.1
1	D	14	ALA	3.1
1	A	319	CYS	3.1
1	D	266	THR	3.1
1	A	232	PHE	3.1
1	C	133	PHE	3.1
1	C	258	ASN	3.1
1	D	40	ASN	3.1
1	D	165	ALA	3.1
1	D	270	THR	3.1
1	C	114	GLY	3.0
1	A	71	ASN	3.0
1	A	263	ASN	3.0
1	B	271	SER	3.0
1	C	12	SER	3.0
1	C	126	SER	3.0
1	C	183	PHE	3.0
1	D	17	VAL	3.0
1	C	74	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	193	ALA	3.0
1	A	269	PRO	3.0
1	B	67	LEU	3.0
1	B	237	SER	3.0
1	B	282	GLU	3.0
1	A	133	PHE	3.0
1	C	219	ALA	3.0
1	A	49	PRO	3.0
1	A	55	THR	3.0
1	C	166	GLY	3.0
1	A	94	SER	3.0
1	A	234	ARG	3.0
1	A	317	ALA	3.0
1	D	219	ALA	3.0
1	D	213	GLN	3.0
1	B	30	GLY	3.0
1	D	166	GLY	3.0
1	C	111	SER	3.0
1	B	76	PHE	3.0
1	D	15	LYS	3.0
1	D	85	ASP	3.0
1	C	49	PRO	3.0
1	D	56	PRO	3.0
1	A	177	ILE	2.9
1	A	308	LEU	2.9
1	B	92	LEU	2.9
1	C	265	TYR	2.9
1	A	40	ASN	2.9
1	D	273	ASP	2.9
1	A	62	ALA	2.9
1	A	80	ALA	2.9
1	A	252	PRO	2.9
1	C	43	ALA	2.9
1	C	146	GLU	2.9
1	A	48	LEU	2.9
1	A	114	GLY	2.9
1	B	260	GLY	2.9
1	C	287	ILE	2.9
1	A	281	TYR	2.9
1	C	79	TYR	2.9
1	B	301	ARG	2.9
1	C	199	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	2.9
1	D	251	HIS	2.9
1	A	56	PRO	2.9
1	D	238	PRO	2.9
1	C	197	THR	2.9
1	D	143	THR	2.9
1	B	302	LYS	2.9
1	C	67	LEU	2.9
1	C	257	ARG	2.9
1	D	68	ASN	2.9
1	D	281	TYR	2.9
1	D	82	HIS	2.9
1	C	53	VAL	2.9
1	D	63	VAL	2.9
1	D	322	VAL	2.9
1	A	26	PRO	2.9
1	A	37	PRO	2.9
1	C	62	ALA	2.9
1	D	317	ALA	2.9
1	C	318	GLY	2.9
1	C	292	LEU	2.9
1	A	87	ASN	2.9
1	B	71	ASN	2.9
1	A	282	GLU	2.8
1	C	156	GLY	2.8
1	A	168	LEU	2.8
1	B	61	ASN	2.8
1	D	59	ILE	2.8
1	A	72	GLN	2.8
1	D	194	TYR	2.8
1	D	268	ASP	2.8
1	D	245	GLU	2.8
1	D	283	LYS	2.8
1	D	319	CYS	2.8
1	A	158	GLY	2.8
1	D	288	THR	2.8
1	D	89	ILE	2.8
1	A	138	HIS	2.8
1	C	211	ASP	2.8
1	D	210	ASP	2.8
1	A	25	LYS	2.8
1	D	170	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	262	ILE	2.8
1	C	286	ASN	2.8
1	C	25	LYS	2.8
1	C	160	TYR	2.8
1	A	199	PHE	2.8
1	A	84	VAL	2.8
1	B	24	TRP	2.8
1	A	198	THR	2.8
1	B	192	THR	2.8
1	B	221	SER	2.7
1	D	253	MET	2.7
1	D	280	MET	2.7
1	A	211	ASP	2.7
1	D	236	PRO	2.7
1	A	69	PHE	2.7
1	B	205	VAL	2.7
1	B	250	ALA	2.7
1	C	198	THR	2.7
1	C	276	THR	2.7
1	D	147	GLN	2.7
1	A	61	ASN	2.7
1	A	239	ARG	2.7
1	A	109	PRO	2.7
1	B	31	ASP	2.7
1	D	124	ASP	2.7
1	B	225	PHE	2.7
1	A	186	VAL	2.7
1	B	315	VAL	2.7
1	C	47	TYR	2.7
1	D	312	PHE	2.7
1	C	84	VAL	2.7
1	D	125	ALA	2.7
1	B	64	GLN	2.7
1	D	58	GLN	2.7
1	C	102	THR	2.7
1	C	266	THR	2.7
1	A	68	ASN	2.7
1	B	307	ASN	2.7
1	D	153	ASN	2.7
1	A	173	ILE	2.7
1	C	177	ILE	2.7
1	B	280	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	252	PRO	2.7
1	A	223	PHE	2.7
1	B	75	VAL	2.7
1	A	119	GLY	2.7
1	C	158	GLY	2.7
1	C	256	GLY	2.7
1	D	171	LYS	2.7
1	A	144	LEU	2.7
1	B	279	LEU	2.7
1	A	11	ASN	2.7
1	C	136	ASN	2.7
1	D	202	ASN	2.7
1	B	238	PRO	2.7
1	C	19	ASP	2.7
1	B	53	VAL	2.7
1	B	186	VAL	2.7
1	C	222	PHE	2.7
1	D	76	PHE	2.7
1	C	171	LYS	2.7
1	D	189	ARG	2.6
1	D	141	ASN	2.6
1	B	262	ILE	2.6
1	D	176	SER	2.6
1	D	104	PRO	2.6
1	D	252	PRO	2.6
1	B	211	ASP	2.6
1	A	134	PHE	2.6
1	B	170	PHE	2.6
1	C	322	VAL	2.6
1	A	96	GLY	2.6
1	D	320	THR	2.6
1	B	60	ILE	2.6
1	B	26	PRO	2.6
1	D	35	PRO	2.6
1	C	309	ASP	2.6
1	A	147	GLN	2.6
1	A	33	ARG	2.6
1	A	312	PHE	2.6
1	B	17	VAL	2.6
1	B	121	PHE	2.6
1	D	289	VAL	2.6
1	A	201	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	103	GLY	2.6
1	C	21	ALA	2.6
1	D	314	GLY	2.6
1	A	297	THR	2.6
1	C	48	LEU	2.6
1	C	120	THR	2.6
1	C	143	THR	2.6
1	B	248	ILE	2.6
1	C	59	ILE	2.6
1	A	236	PRO	2.6
1	B	49	PRO	2.6
1	A	187	ASP	2.6
1	C	22	HIS	2.6
1	D	169	ARG	2.6
1	A	188	PHE	2.6
1	B	188	PHE	2.6
1	D	62	ALA	2.6
1	D	167	GLU	2.6
1	B	177	ILE	2.6
1	B	252	PRO	2.6
1	B	45	HIS	2.6
1	C	174	GLN	2.6
1	A	38	GLY	2.5
1	A	145	PHE	2.5
1	A	293	TYR	2.5
1	A	229	PRO	2.5
1	B	108	PRO	2.5
1	D	255	PRO	2.5
1	D	277	PRO	2.5
1	C	271	SER	2.5
1	B	149	VAL	2.5
1	D	244	VAL	2.5
1	D	247	VAL	2.5
1	C	93	LEU	2.5
1	C	283	LYS	2.5
1	C	281	TYR	2.5
1	B	138	HIS	2.5
1	B	28	ARG	2.5
1	B	220	ARG	2.5
1	C	209	ARG	2.5
1	D	33	ARG	2.5
1	D	173	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	152	SER	2.5
1	C	127	MET	2.5
1	B	69	PHE	2.5
1	C	69	PHE	2.5
1	C	75	VAL	2.5
1	D	84	VAL	2.5
1	D	83	LEU	2.5
1	B	266	THR	2.5
1	D	242	THR	2.5
1	B	56	PRO	2.5
1	C	239	ARG	2.5
1	D	181	PRO	2.5
1	B	146	GLU	2.5
1	A	241	GLY	2.5
1	B	62	ALA	2.5
1	B	155	PHE	2.5
1	B	218	ALA	2.5
1	C	323	PHE	2.5
1	B	93	LEU	2.5
1	B	144	LEU	2.5
1	A	120	THR	2.5
1	C	51	ASN	2.5
1	C	295[A]	ASN	2.5
1	D	276	THR	2.5
1	B	277	PRO	2.5
1	A	60	ILE	2.4
1	B	319	CYS	2.4
1	C	314	GLY	2.4
1	D	119	GLY	2.4
1	D	318	GLY	2.4
1	B	134	PHE	2.4
1	D	48	LEU	2.4
1	B	58	GLN	2.4
1	D	128	THR	2.4
1	C	60	ILE	2.4
1	D	60	ILE	2.4
1	C	150	ASP	2.4
1	C	118	HIS	2.4
1	C	251	HIS	2.4
1	A	76	PHE	2.4
1	B	83	LEU	2.4
1	A	129	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	100	ARG	2.4
1	A	180	ASN	2.4
1	A	191	PHE	2.4
1	C	164	VAL	2.4
1	C	247	VAL	2.4
1	C	267	VAL	2.4
1	C	41	THR	2.4
1	A	35	PRO	2.4
1	C	187	ASP	2.4
1	A	214	LEU	2.4
1	A	250	ALA	2.4
1	D	115	LEU	2.4
1	B	199	PHE	2.3
1	B	259	VAL	2.3
1	D	75	VAL	2.3
1	C	159	LYS	2.3
1	A	264	SER	2.3
1	B	231	ASP	2.3
1	D	175	ASP	2.3
1	A	79	TYR	2.3
1	A	151	TYR	2.3
1	B	118	HIS	2.3
1	C	227	ARG	2.3
1	A	260	GLY	2.3
1	C	34	GLY	2.3
1	A	203	LEU	2.3
1	B	162	LEU	2.3
1	C	115	LEU	2.3
1	D	162	LEU	2.3
1	A	178	ALA	2.3
1	C	73	ALA	2.3
1	A	276	THR	2.3
1	B	57	VAL	2.3
1	B	274	PHE	2.3
1	B	290	LYS	2.3
1	D	197	THR	2.3
1	B	296	PRO	2.3
1	A	150	ASP	2.3
1	B	135	GLY	2.3
1	C	46	GLY	2.3
1	B	87	ASN	2.3
1	D	117	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	161	ASN	2.3
1	A	204	PHE	2.3
1	C	223	PHE	2.3
1	D	29	PRO	2.3
1	C	90	THR	2.3
1	C	179	THR	2.3
1	D	191	PHE	2.3
1	C	208	ARG	2.3
1	B	59	ILE	2.3
1	D	72	GLN	2.3
1	B	166	GLY	2.3
1	C	216	MET	2.2
1	C	293	TYR	2.2
1	C	229	PRO	2.2
1	D	129	ARG	2.2
1	D	205	VAL	2.2
1	D	239	ARG	2.2
1	B	82	HIS	2.2
1	B	32	ILE	2.2
1	B	240	SER	2.2
1	C	273	ASP	2.2
1	B	212	GLY	2.2
1	B	292	LEU	2.2
1	C	182	ASN	2.2
1	B	209	ARG	2.2
1	A	242	THR	2.2
1	B	288	THR	2.2
1	A	267	VAL	2.2
1	A	231	ASP	2.2
1	C	215	ASP	2.2
1	C	52	GLY	2.2
1	D	293	TYR	2.2
1	C	54	ALA	2.2
1	C	109	PRO	2.2
1	C	316	ALA	2.2
1	D	285	VAL	2.2
1	B	171	LYS	2.2
1	C	206	ASP	2.2
1	B	173	ILE	2.2
1	C	280	MET	2.2
1	B	40	ASN	2.2
1	B	80	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	41	THR	2.2
1	C	192	THR	2.2
1	C	270	THR	2.2
1	B	164	VAL	2.2
1	B	247	VAL	2.2
1	C	244	VAL	2.2
1	D	315	VAL	2.2
1	A	139	ASP	2.2
1	D	211	ASP	2.2
1	A	146	GLU	2.1
1	A	97	ARG	2.1
1	A	305	ASN	2.1
1	D	203	LEU	2.1
1	D	118	HIS	2.1
1	B	229	PRO	2.1
1	A	77	ALA	2.1
1	B	74	ALA	2.1
1	B	219	ALA	2.1
1	C	77	ALA	2.1
1	D	316	ALA	2.1
1	B	163	THR	2.1
1	A	284	PHE	2.1
1	C	188	PHE	2.1
1	C	175	ASP	2.1
1	D	206	ASP	2.1
1	B	94	SER	2.1
1	B	195	GLY	2.1
1	D	103	GLY	2.1
1	D	126	SER	2.1
1	A	189	ARG	2.1
1	C	153	ASN	2.1
1	B	99	THR	2.1
1	C	99	THR	2.1
1	A	149	VAL	2.1
1	B	323	PHE	2.1
1	B	131	ASP	2.1
1	A	157	GLY	2.1
1	B	184	SER	2.1
1	B	291	SER	2.1
1	B	180	ASN	2.1
1	C	302	LYS	2.1
1	C	308	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	PRO	2.1
1	C	35	PRO	2.1
1	B	73	ALA	2.1
1	B	306	THR	2.1
1	D	297	THR	2.1
1	B	234	ARG	2.1
1	A	95	ILE	2.1
1	A	98	LYS	2.1
1	C	141	ASN	2.1
1	C	255	PRO	2.1
1	B	227	ARG	2.0
1	A	194	TYR	2.0
1	A	247	VAL	2.0
1	B	183	PHE	2.0
1	A	130	GLY	2.0
1	C	45	HIS	2.0
1	A	83	LEU	2.0
1	C	36	CYS	2.0
1	C	148	LEU	2.0
1	C	161	ASN	2.0
1	B	242	THR	2.0
1	C	132	ALA	2.0
1	D	198	THR	2.0
1	B	187	ASP	2.0
1	B	230	ASP	2.0
1	D	46	GLY	2.0
1	A	176	SER	2.0
1	A	261	LYS	2.0
1	B	111	SER	2.0
1	B	136	ASN	2.0
1	C	279	LEU	2.0
1	D	258	ASN	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, 95^{th} 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	NAG	N	2	14/15	-0.00	0.45	74,77,79,81	0
4	NAG	R	2	14/15	0.08	0.47	73,76,77,78	0
4	NAG	I	2	14/15	0.17	0.49	75,78,81,81	0
3	MAN	F	5	11/12	0.18	0.42	88,90,90,91	0
4	NAG	R	1	14/15	0.38	0.35	55,60,64,69	0
3	MAN	F	4	11/12	0.40	0.35	79,81,84,88	0
3	MAN	J	5	11/12	0.40	0.32	78,80,81,81	0
4	NAG	S	2	14/15	0.41	0.36	60,62,65,66	0
6	BMA	T	3	11/12	0.41	0.35	58,60,62,62	0
4	NAG	I	1	14/15	0.44	0.30	56,64,68,70	0
2	MAN	E	4	11/12	0.49	0.35	51,54,58,63	0
4	NAG	L	2	14/15	0.50	0.33	57,59,63,64	0
5	MAN	H	8	11/12	0.50	0.34	60,61,63,64	0
4	NAG	G	2	14/15	0.50	0.36	57,61,65,66	0
5	MAN	M	8	11/12	0.53	0.30	47,50,52,52	0
3	BMA	J	3	11/12	0.54	0.27	59,62,64,66	0
2	MAN	E	6	11/12	0.56	0.31	64,65,66,67	0
4	NAG	K	2	14/15	0.57	0.29	43,49,52,53	0
6	BMA	O	3	11/12	0.57	0.22	75,78,79,79	0
4	NAG	Q	2	14/15	0.57	0.30	56,60,63,65	0
4	NAG	P	2	14/15	0.58	0.32	47,53,55,58	0
2	MAN	E	5	11/12	0.60	0.27	66,68,70,71	0
6	NAG	T	2	14/15	0.61	0.28	48,52,58,58	0
5	MAN	H	7	11/12	0.62	0.28	52,53,54,55	0
3	NAG	F	2	14/15	0.62	0.29	37,42,46,52	0
3	BMA	F	3	11/12	0.63	0.23	56,58,68,74	0
2	BMA	E	3	11/12	0.63	0.32	49,54,59,62	0
6	NAG	T	1	14/15	0.65	0.23	26,34,39,43	0
2	NAG	E	2	14/15	0.65	0.27	40,46,53,56	0
5	MAN	H	6	11/12	0.65	0.23	46,49,55,59	0
4	NAG	G	1	14/15	0.66	0.24	39,43,47,54	0
4	NAG	N	1	14/15	0.67	0.32	51,57,62,69	0
4	NAG	L	1	14/15	0.68	0.23	39,42,46,53	0
5	NAG	H	1	14/15	0.68	0.19	34,39,42,43	0
5	MAN	H	4	11/12	0.68	0.25	55,59,60,62	0
5	MAN	H	5	11/12	0.68	0.28	58,64,65,65	0
3	MAN	J	4	11/12	0.68	0.22	67,69,72,75	0
4	NAG	S	1	14/15	0.68	0.32	50,54,56,59	0
5	MAN	M	5	11/12	0.69	0.27	52,55,57,58	0
5	NAG	H	2	14/15	0.70	0.30	42,45,47,47	0
4	NAG	Q	1	14/15	0.71	0.18	31,42,48,51	0

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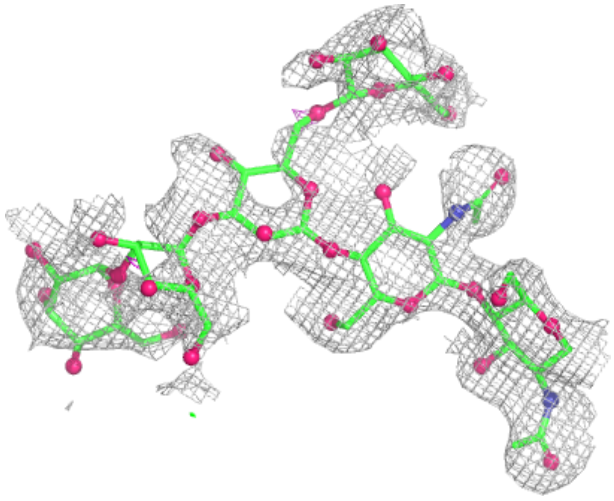
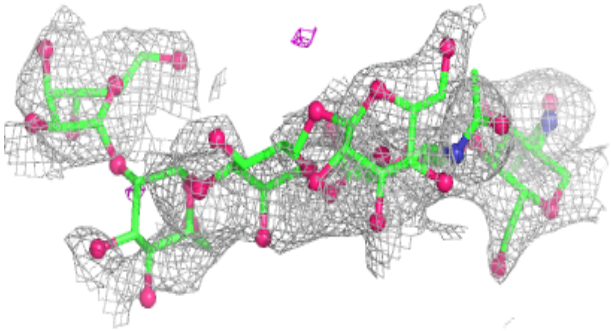
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	O	2	14/15	0.71	0.28	58,61,65,70	0
5	MAN	M	6	11/12	0.71	0.21	26,30,36,45	0
6	NAG	O	1	14/15	0.72	0.25	41,46,49,54	0
5	MAN	M	4	11/12	0.72	0.19	40,43,45,50	0
5	NAG	M	2	14/15	0.74	0.20	23,31,34,40	0
3	NAG	J	2	14/15	0.75	0.22	45,50,52,56	0
2	NAG	E	1	14/15	0.75	0.20	33,36,41,41	0
5	NAG	M	1	14/15	0.76	0.18	26,30,32,37	0
5	BMA	H	3	11/12	0.76	0.24	40,44,47,48	0
4	NAG	P	1	14/15	0.76	0.19	25,30,36,42	0
3	NAG	J	1	14/15	0.80	0.16	30,34,41,45	0
3	NAG	F	1	14/15	0.80	0.15	18,21,26,30	0
4	NAG	K	1	14/15	0.84	0.14	16,23,29,36	0
5	MAN	M	7	11/12	0.85	0.15	27,31,32,34	0
5	BMA	M	3	11/12	0.85	0.17	30,33,36,37	0

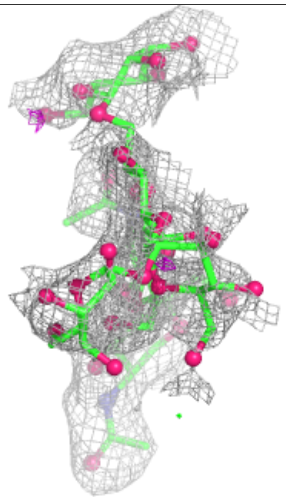
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

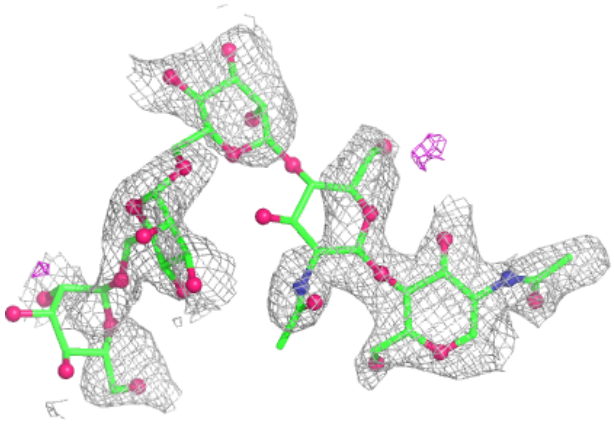


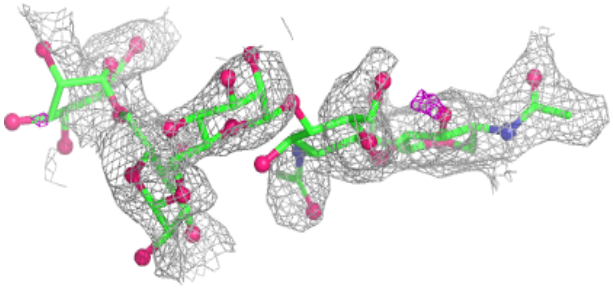


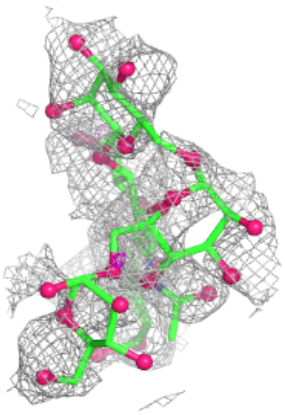


Electron density around Chain F:

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

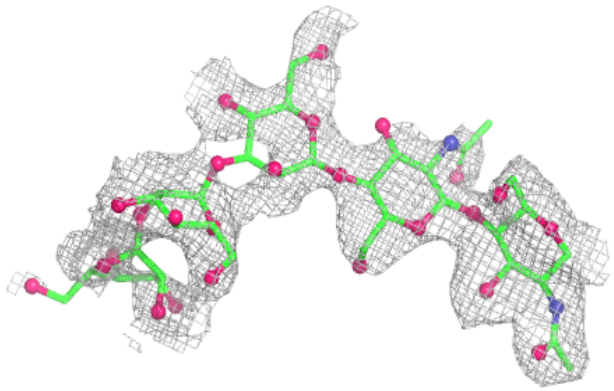


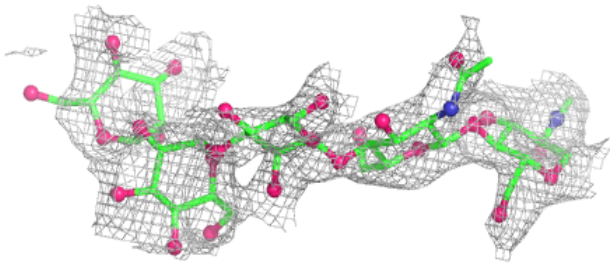


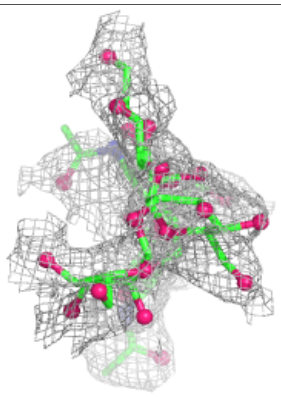


Electron density around Chain J:

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

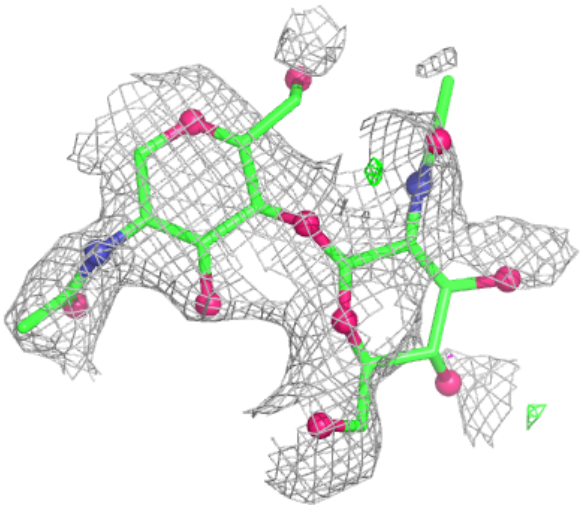


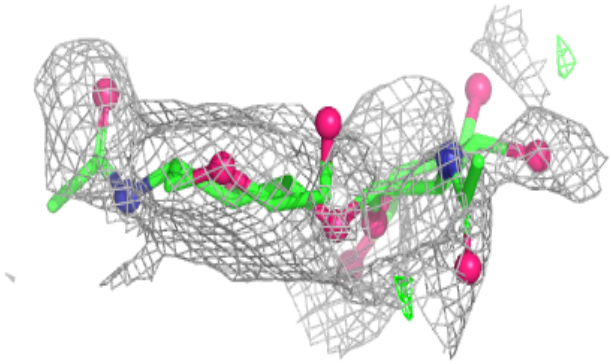


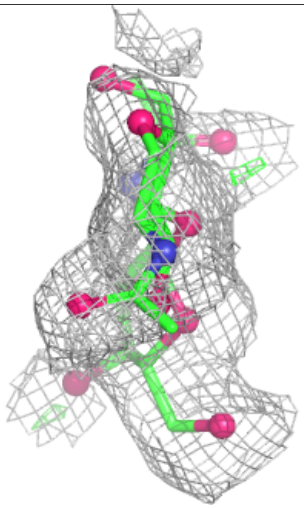


Electron density around Chain G:

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

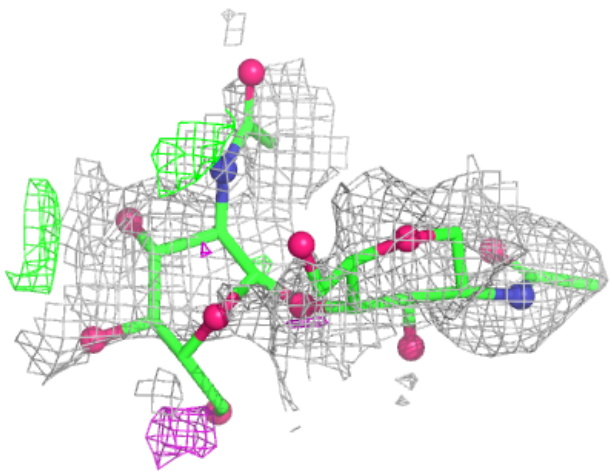


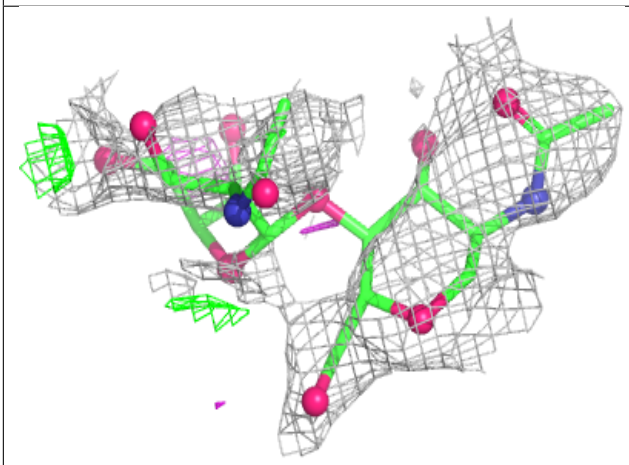


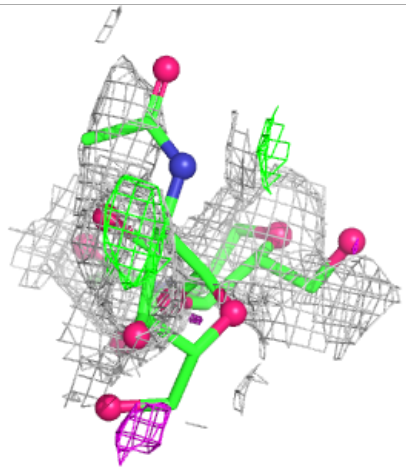


Electron density around Chain I:

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

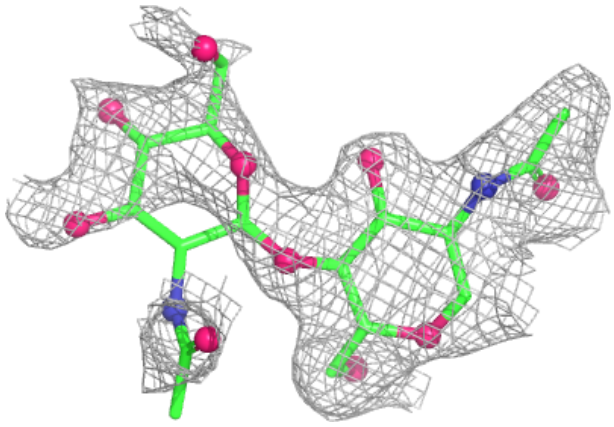


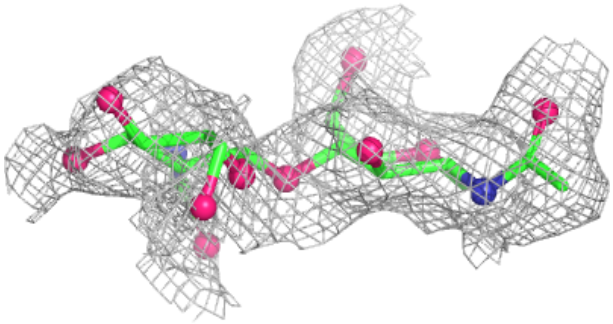


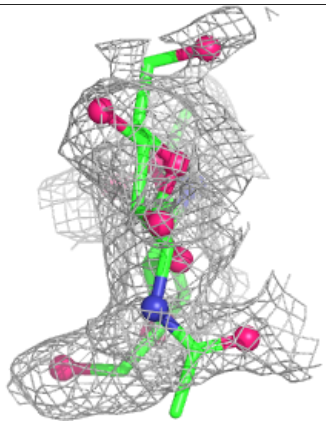


Electron density around Chain K:

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

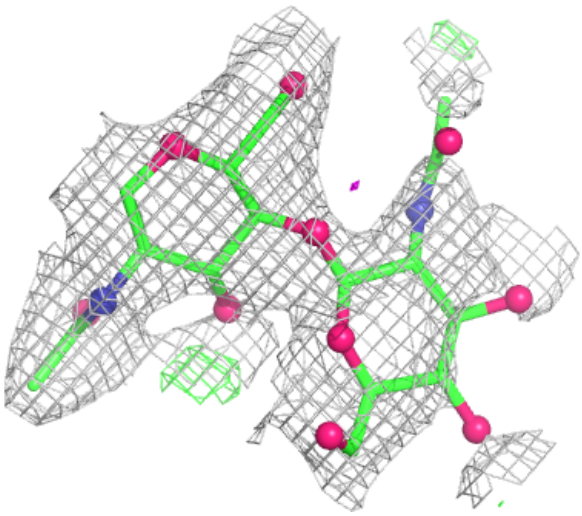


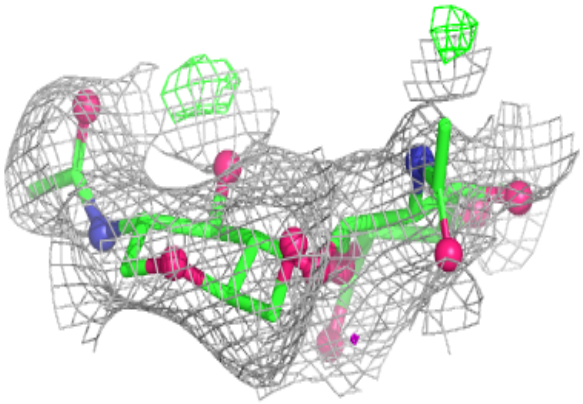


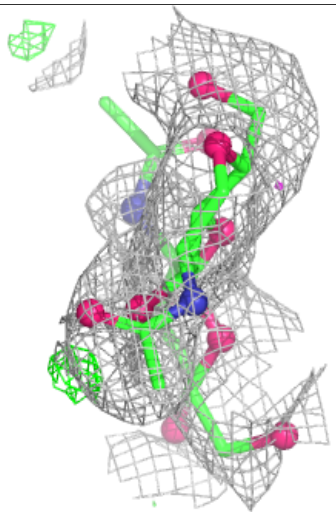


Electron density around Chain L:

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

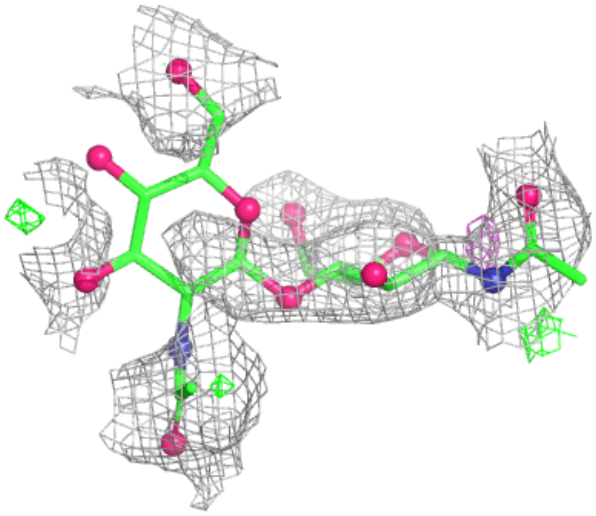


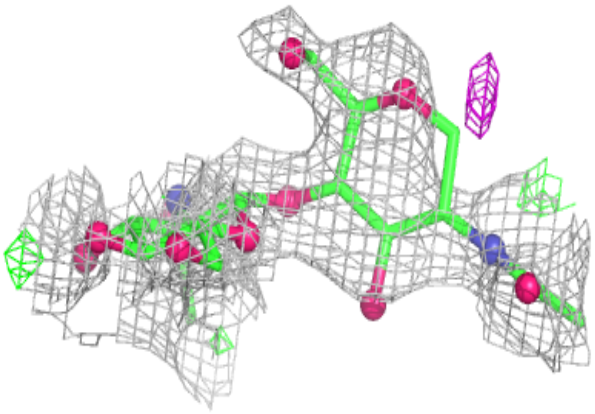


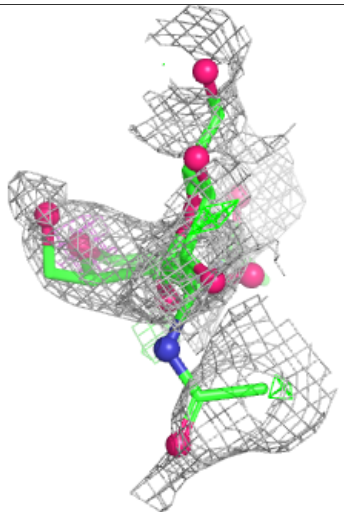


Electron density around Chain N:

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

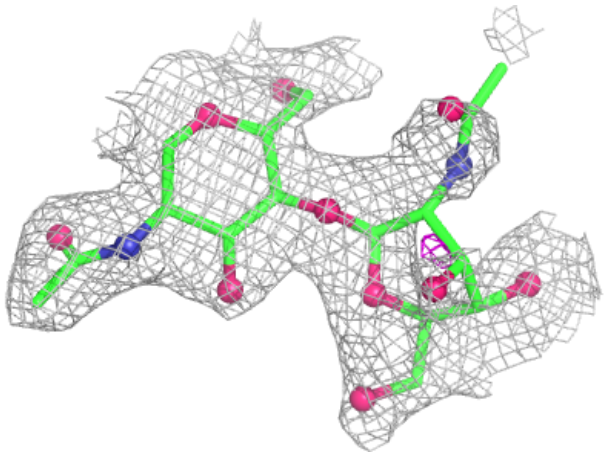


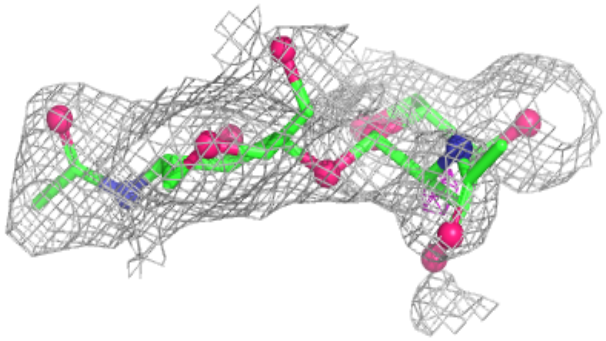


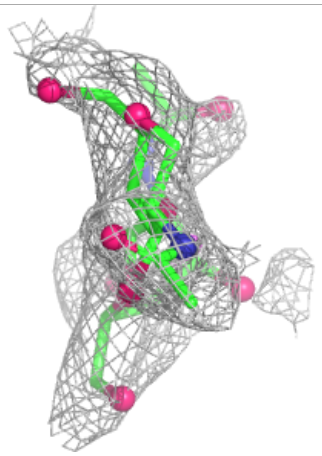


Electron density around Chain P:

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

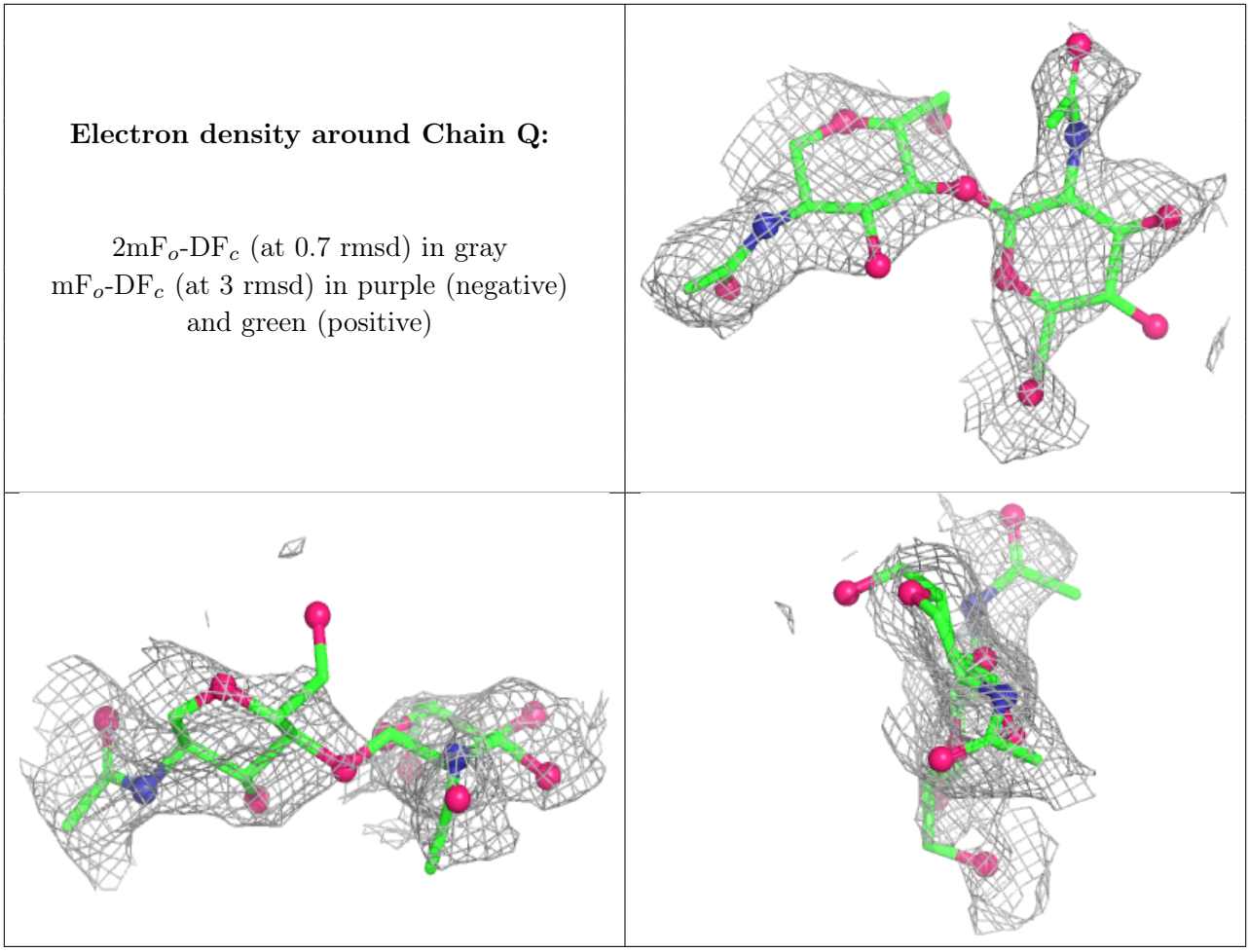






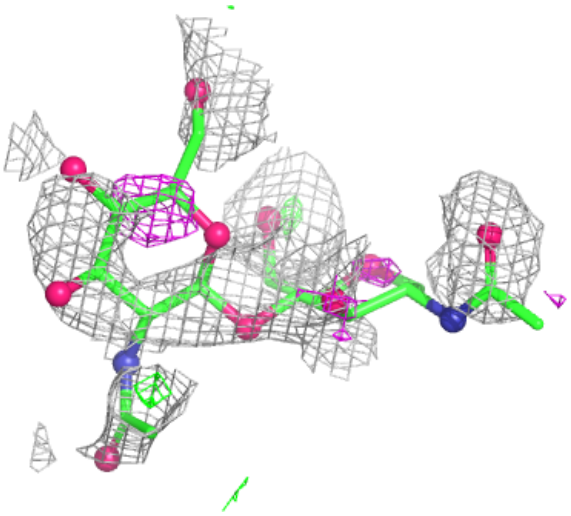
Electron density around Chain Q:

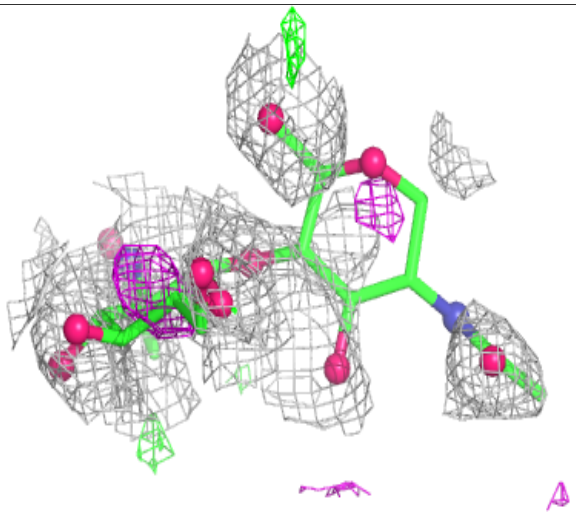
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

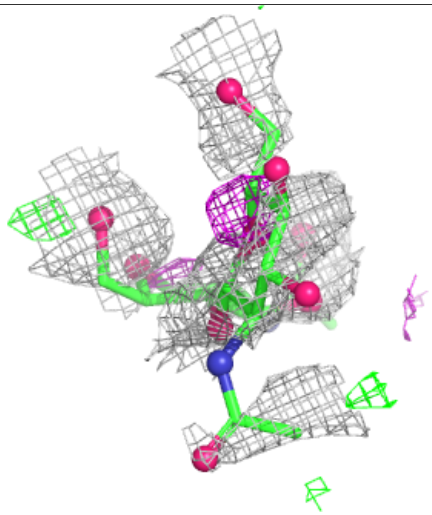


Electron density around Chain R:

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

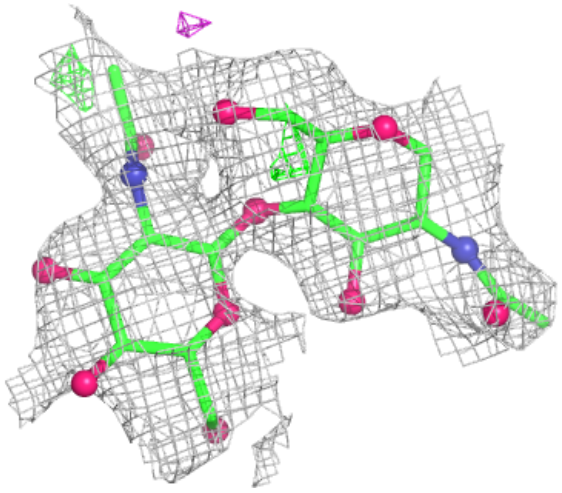


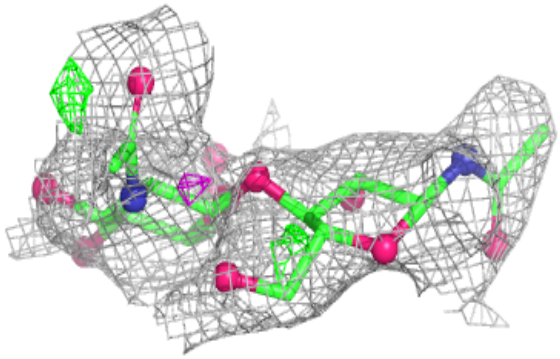


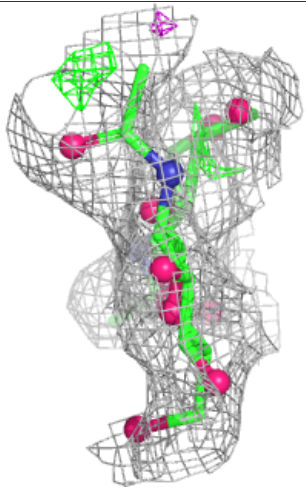


Electron density around Chain S:

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

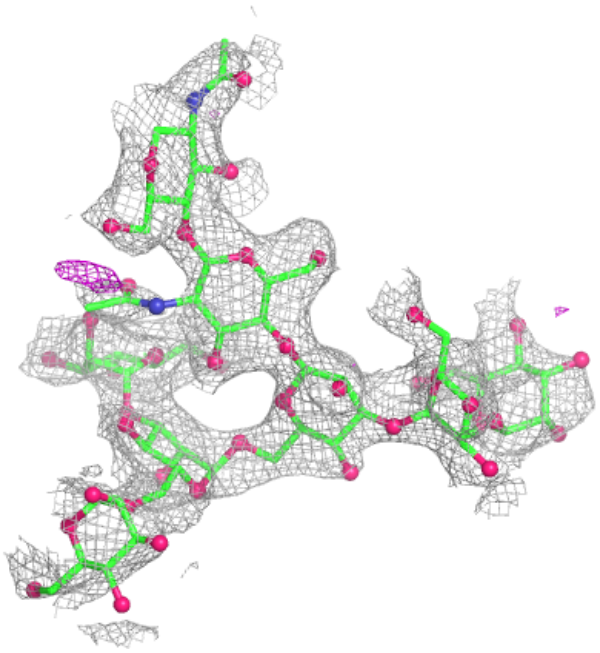


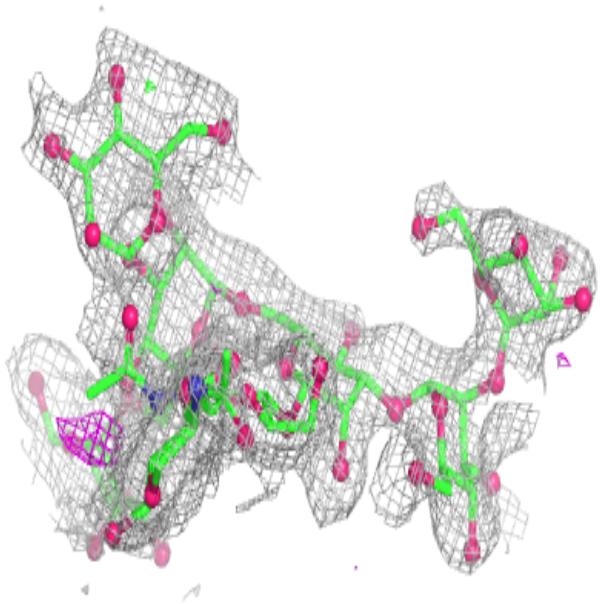


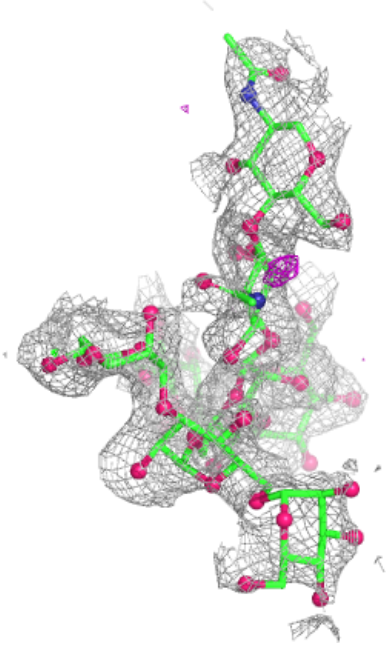


Electron density around Chain H:

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

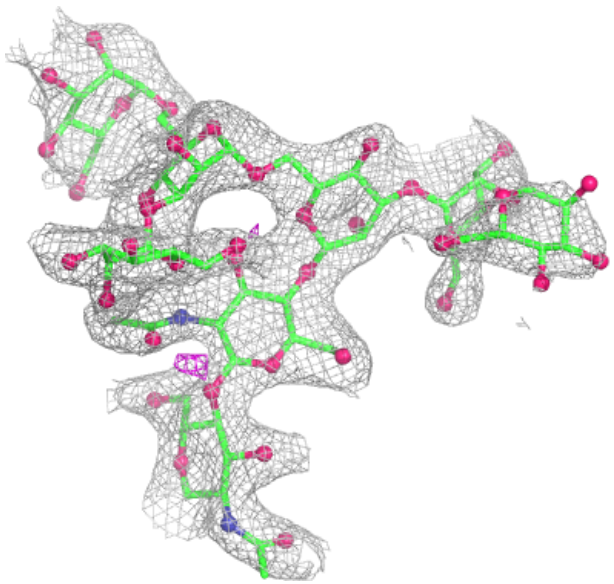


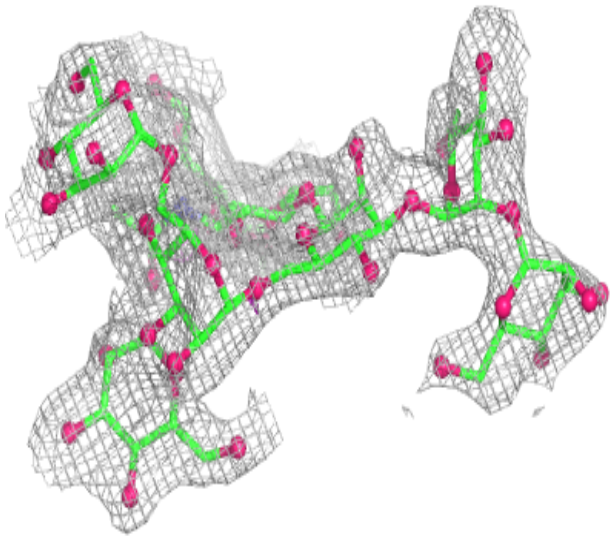


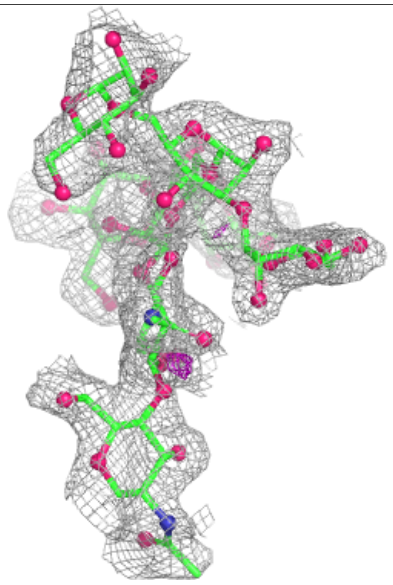


Electron density around Chain M:

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

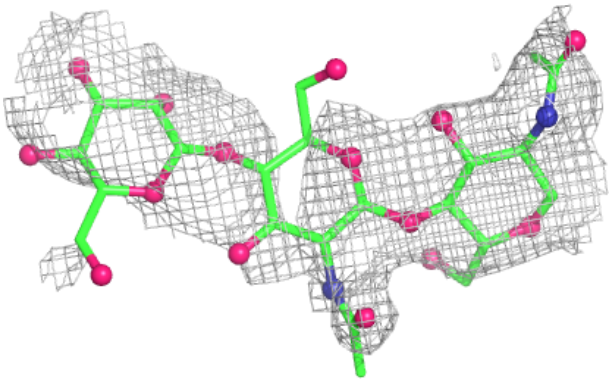


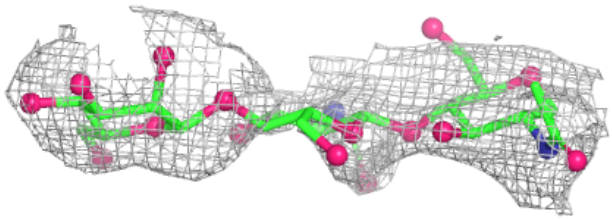


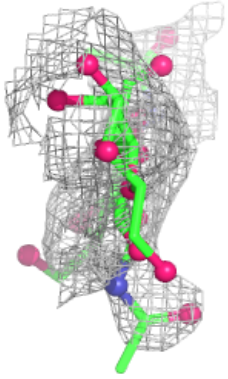


Electron density around Chain O:

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

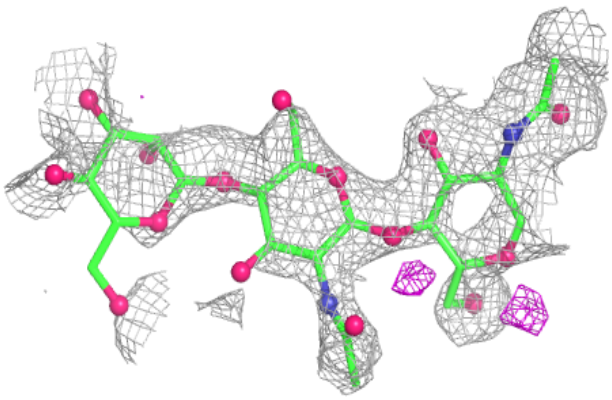


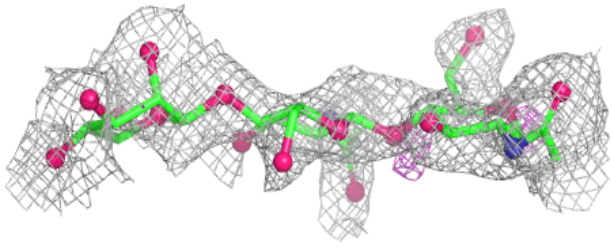


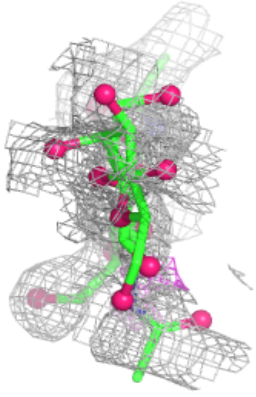


Electron density around Chain T:

$2mF_o$-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)

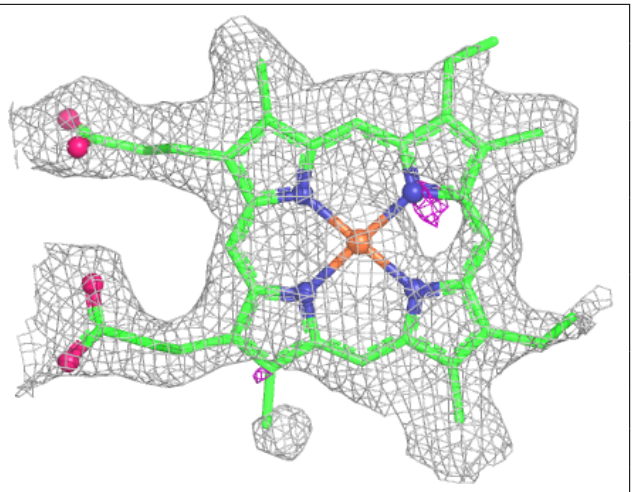
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

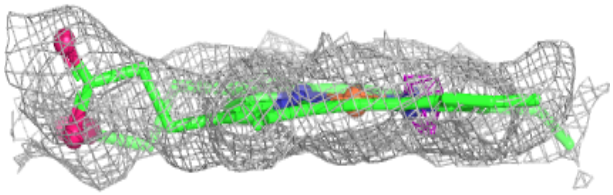
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	D	411	14/15	0.50	0.30	53,56,58,59	0
10	SO4	B	1330	5/5	0.60	0.29	65,65,65,66	0
11	NAG	D	391	14/15	0.65	0.24	46,48,51,53	0
9	ACT	D	1327	4/4	0.65	0.31	48,49,49,50	0
11	NAG	C	381	14/15	0.68	0.25	50,54,57,58	0
10	SO4	C	1333	5/5	0.69	0.28	74,75,75,75	0
10	SO4	C	1332	5/5	0.71	0.28	62,62,63,63	0
10	SO4	C	1331	5/5	0.72	0.44	87,88,88,89	0
10	SO4	A	1330	5/5	0.76	0.25	59,62,63,63	0
10	SO4	A	1331	5/5	0.76	0.34	60,60,61,63	0
9	ACT	C	1329	4/4	0.76	0.25	31,34,37,38	0
10	SO4	A	1329	5/5	0.78	0.17	70,71,71,72	0
10	SO4	B	1331	5/5	0.78	0.39	68,69,69,71	0
9	ACT	A	1327	4/4	0.79	0.21	30,32,32,32	0
11	NAG	D	381	14/15	0.79	0.18	54,57,61,62	0
10	SO4	A	1328	5/5	0.80	0.18	56,56,58,59	0
8	MG	A	353	1/1	0.81	0.12	18,18,18,18	0
10	SO4	D	1329	5/5	0.82	0.45	55,56,58,58	0
8	MG	D	353	1/1	0.84	0.15	26,26,26,26	0
7	HEM	D	350	43/43	0.84	0.17	18,23,28,33	0
10	SO4	D	1328	5/5	0.85	0.20	60,60,61,62	0
9	ACT	C	1334	4/4	0.87	0.44	24,27,29,30	0
7	HEM	C	350	43/43	0.88	0.15	13,17,22,26	0
9	ACT	B	1328	4/4	0.88	0.15	25,25,30,32	0
7	HEM	A	350	43/43	0.89	0.15	12,19,21,27	0
10	SO4	C	1330	5/5	0.91	0.12	61,62,63,63	0
7	HEM	B	350	43/43	0.91	0.13	6,13,16,22	0
8	MG	B	353	1/1	0.92	0.07	12,12,12,12	0
10	SO4	B	1329	5/5	0.93	0.14	57,58,61,62	0
8	MG	C	353	1/1	0.95	0.05	19,19,19,19	0

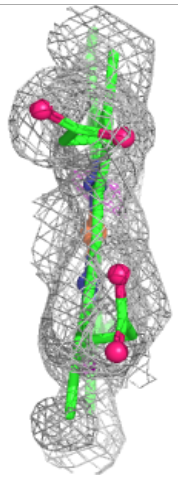
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM D 350:

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

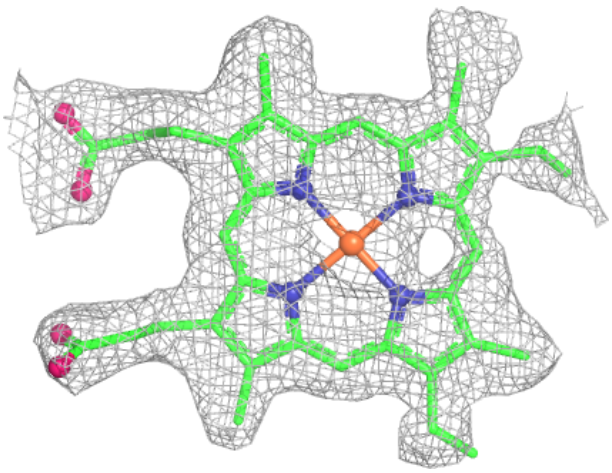


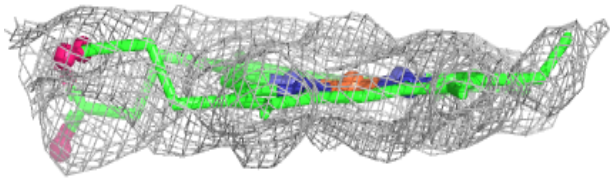


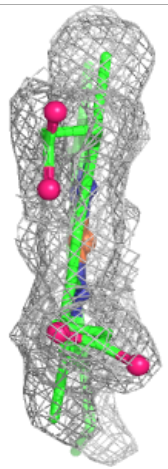


Electron density around HEM C 350:

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

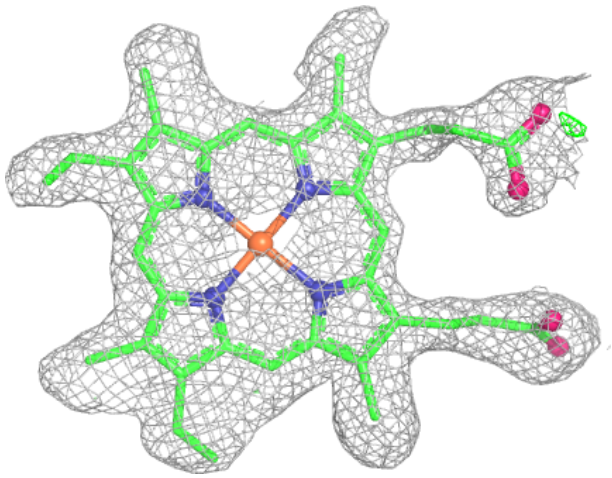


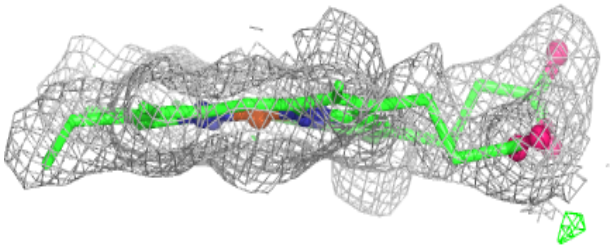


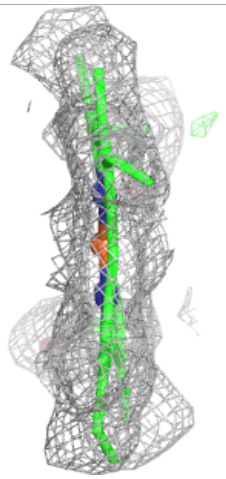


Electron density around HEM A 350:

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

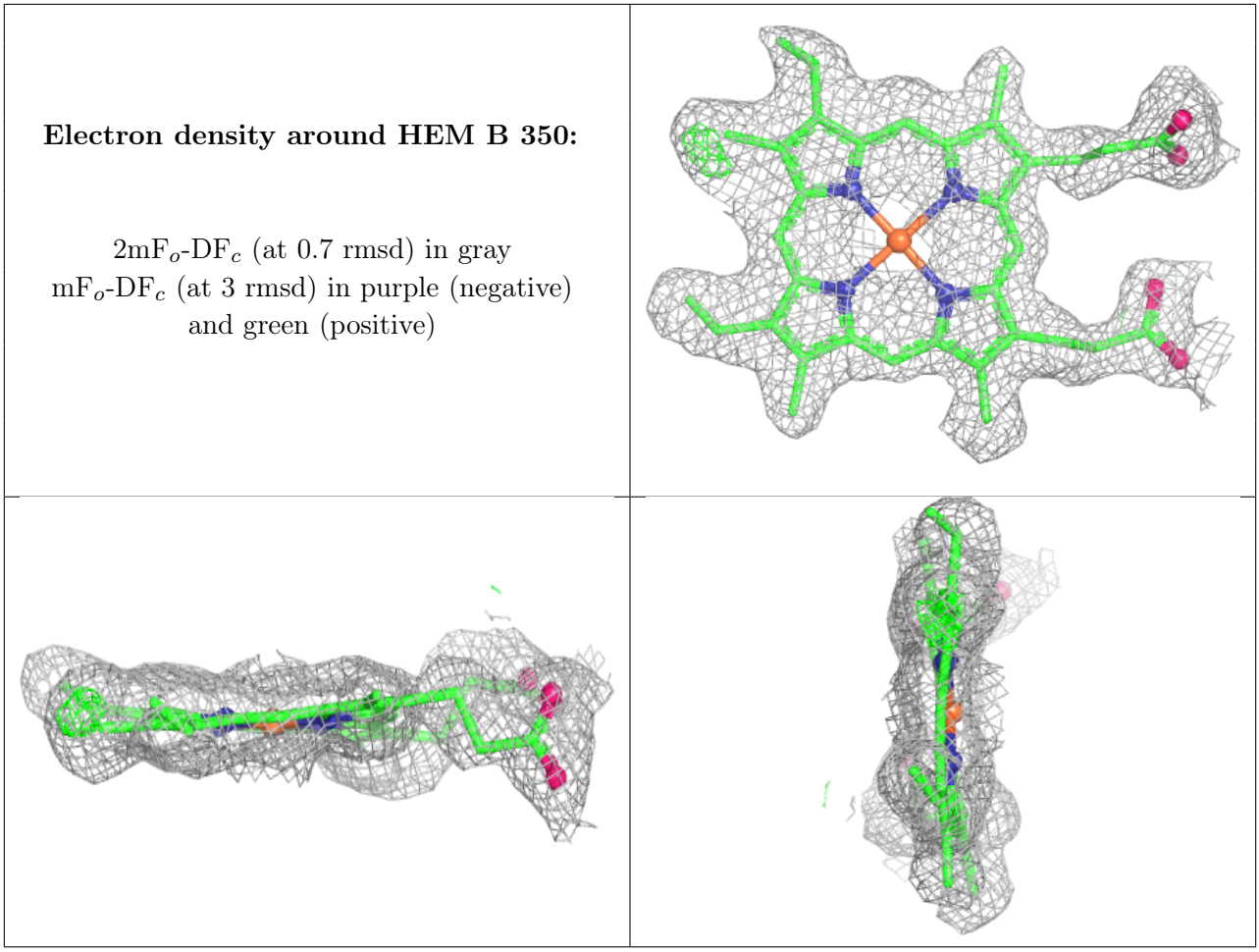






Electron density around HEM B 350:

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



6.5 Other polymers

There are no such residues in this entry.