



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:15 AM UTC

PDB ID : 4A5G / pdb_00004a5g
Title : Raphanus sativus anionic peroxidase.
Authors : Jimenez-Arroyo, N.; Valderrama, B.; Gil-Rodriguez, P.; Rojas-Trejo, S.P.;
Rudino-Pinera, E.
Deposited on : 2011-10-25
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

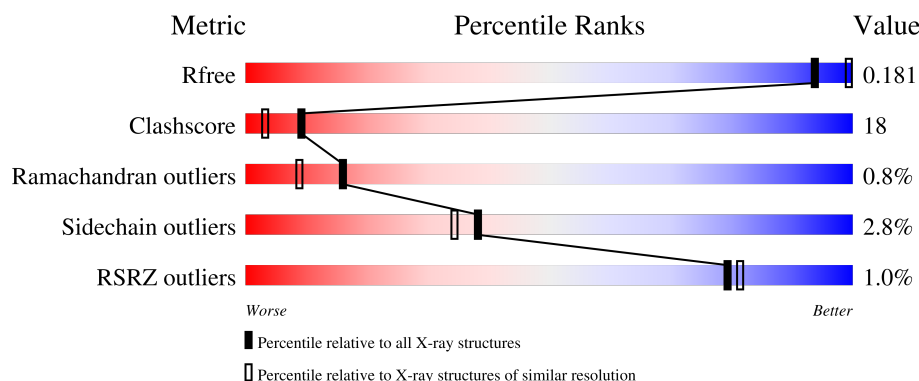
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



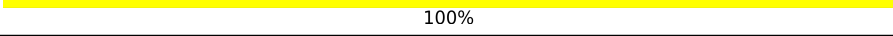
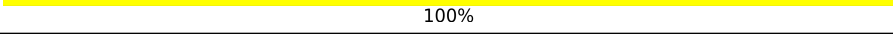
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	308	% 41% 50% 7% •
1	B	308	% 45% 48% 6% •
2	C	6	
2	I	6	
3	D	4	

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Mol	Chain	Length	Quality of chain
4	E	4	
5	F	4	
5	L	4	
6	G	6	
7	H	2	
8	J	4	
9	K	3	

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
12	NAG	B	1326	X	-	-	-
12	NAG	B	1328	X	-	-	-
13	1PE	B	1330	-	-	X	-
2	NAG	I	2	X	-	-	-
2	MAN	I	5	X	-	-	-
3	BMA	D	3	X	-	-	-
5	NAG	L	1	X	-	-	-
6	NAG	G	2	X	-	-	-

2 Entry composition [i](#)

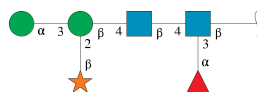
There are 15 unique types of molecules in this entry. The entry contains 5969 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANIONIC PEROXIDASE.

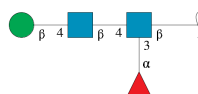
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	7	0
			2277	1395	400	467	15			
1	B	307	Total	C	N	O	S	0	5	0
			2258	1388	395	462	13			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			69	39	2	28			
2	I	6	Total	C	N	O	0	0	0
			69	39	2	28			

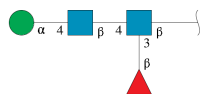
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

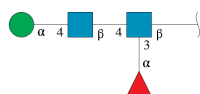
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



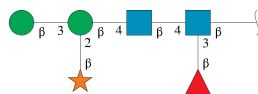
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	L	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



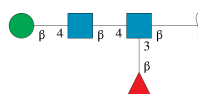
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	6	Total	C	N	O	0	0	0
			69	39	2	28			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



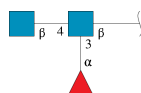
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



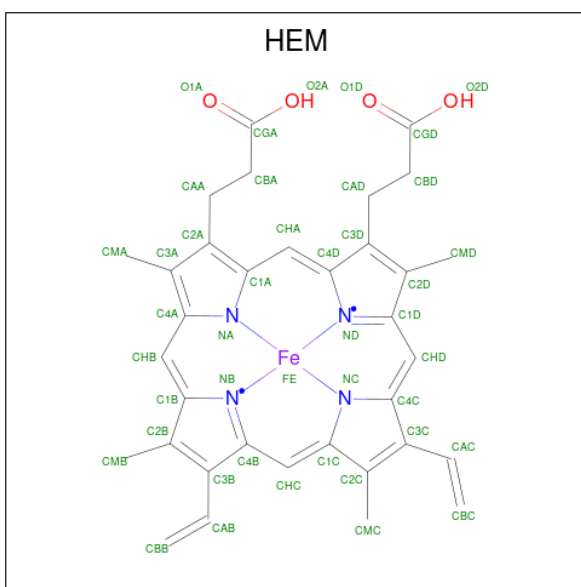
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 9 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

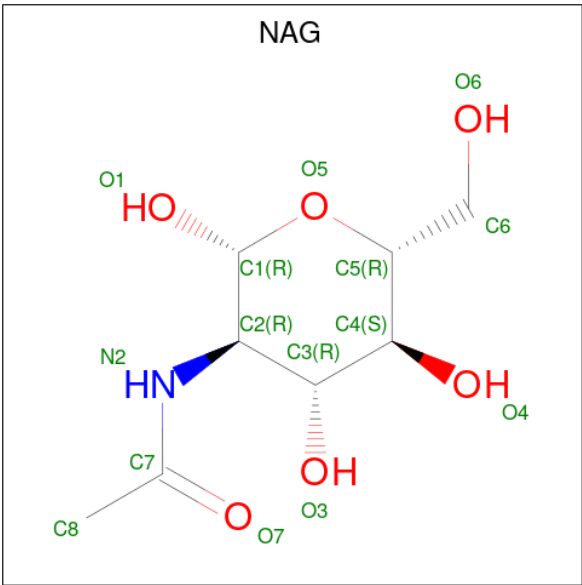


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

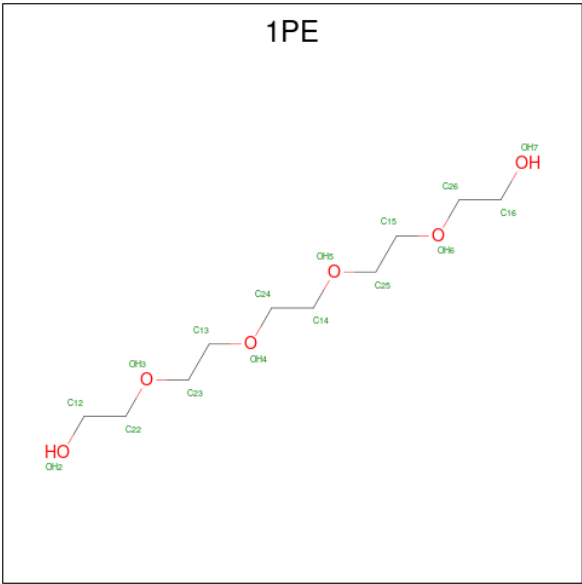
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total Ca 2 2	0	0
11	B	2	Total Ca 2 2	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



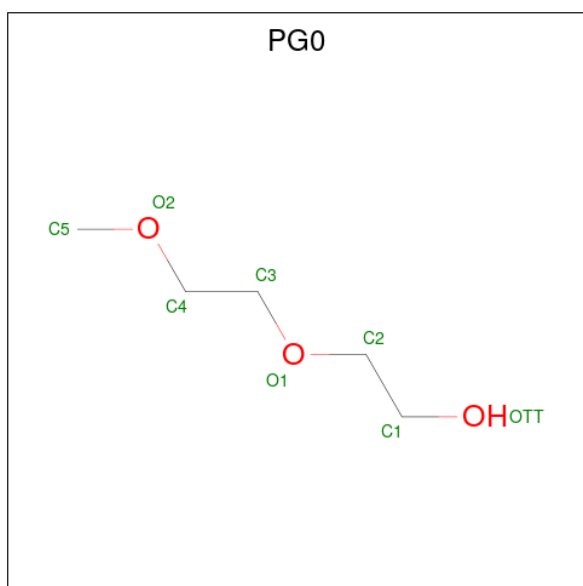
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			5	3	2		
13	A	1	Total	C	O	0	0
			10	6	4		
13	B	1	Total	C	O	0	0
			15	10	5		
13	B	1	Total	C	O	0	0
			16	10	6		
13	B	1	Total	C	O	0	0
			5	3	2		
13	B	1	Total	C	O	0	0
			6	4	2		
13	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 14 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	C	O	0	0
			8	5	3		

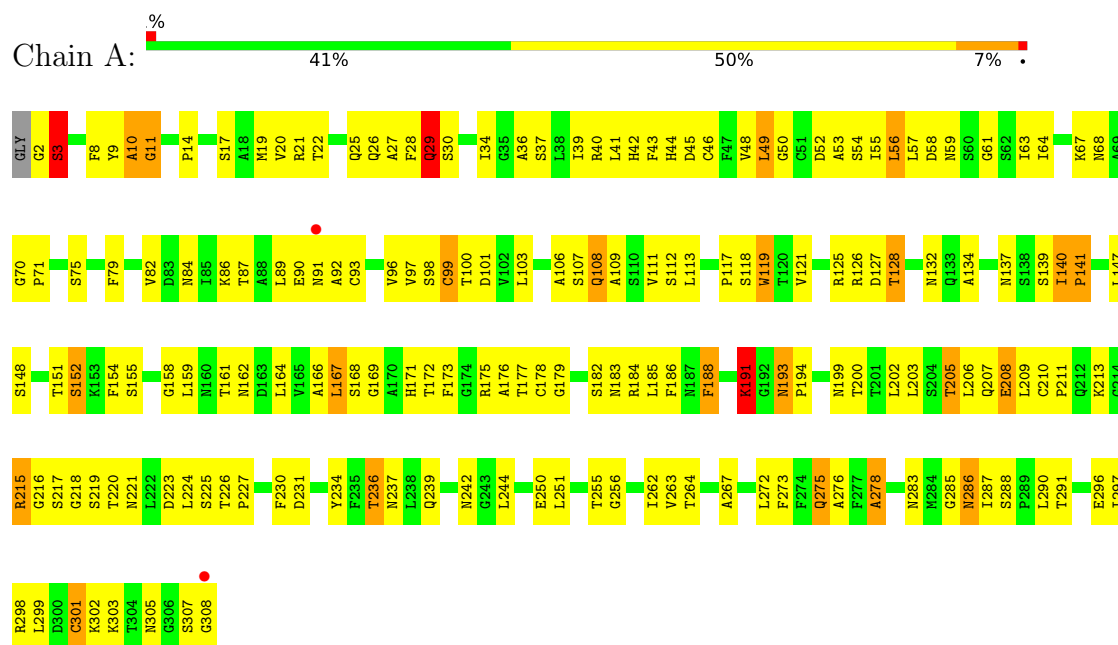
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	364	Total	O	0	0
			364	364		
15	B	336	Total	O	0	0
			336	336		

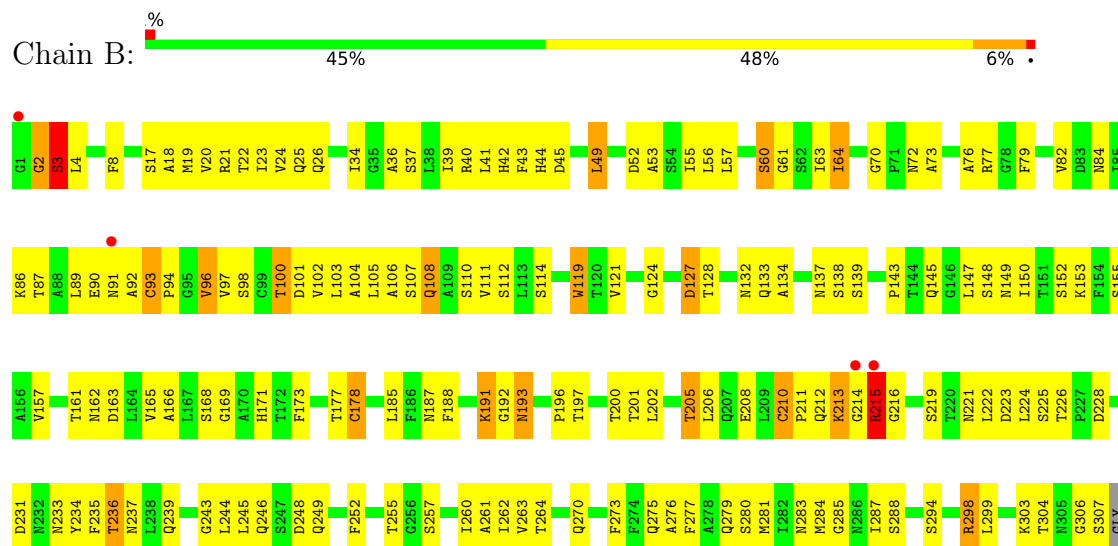
3 Residue-property plots

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

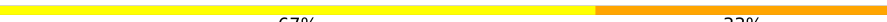
• Molecule 1: ANIONIC PEROXIDASE



• Molecule 1: ANIONIC PEROXIDASE

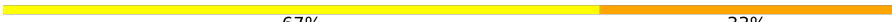


- Molecule 2: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  67% 33%

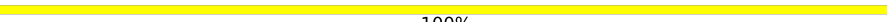
NAG1
NAG2
BMA3
XYP4
MAN5
FUC6

- Molecule 2: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  67% 33%

NAG1
NAG2
BMA3
XYP4
MAN5
FUC6

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

Chain D:  100%

NAG1
NAG2
BMA3
FUC4

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

Chain E:  25% 75%

NAG1
NAG2
MAN3
FUL4

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

Chain F:  100%

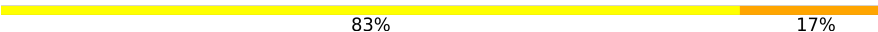
NAG1
NAG2
MAN3
FUC4

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

Chain L:  50% 50%

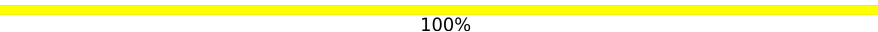
NAG1
NAG2
MAN3
FUC4

- Molecule 6: beta-D-xylopyranose-(1-2)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  83% 17%

NAG1
NAG2
BMA3
XYP4
BMA5
FUL6

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

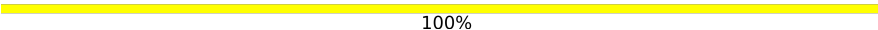
NAG1
NAG2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

NAG1
NAG2
BMA3
FUL4

- Molecule 9: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

NAG1
FUC2
NAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.15Å 41.19Å 137.80Å 90.00° 96.91° 90.00°	Depositor
Resolution (Å)	35.29 – 2.05 35.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.29-2.05) 99.5 (35.29-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.185 0.157 , 0.181	Depositor DCC
R_{free} test set	2634 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5969	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 12.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUL, BMA, 1PE, MAN, XYP, FUC, PG0, HEM, CA

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	2.27	148/2314 (6.4%)	1.15	9/3144 (0.3%)
1	B	2.29	136/2301 (5.9%)	1.21	18/3128 (0.6%)
All	All	2.28	284/4615 (6.2%)	1.18	27/6272 (0.4%)

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	A	0	4
1	B	0	3
All	All	0	7

All (284) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ASN	C-N	-18.39	1.08	1.33
1	B	90	GLU	C-N	-15.76	1.13	1.33
1	A	288	SER	C-O	-14.63	1.16	1.23
1	A	91	ASN	C-N	-14.25	1.14	1.33
1	A	226	THR	C-O	-9.58	1.13	1.24
1	A	90	GLU	C-N	-8.50	1.22	1.33
1	B	157[A]	VAL	CA-C	-8.34	1.43	1.53
1	B	157[B]	VAL	CA-C	-8.34	1.43	1.53
1	B	23	ILE	C-O	-8.26	1.14	1.24
1	B	171	HIS	CG-ND1	-8.16	1.29	1.38
1	B	44	HIS	CG-ND1	-8.09	1.29	1.38
1	B	236[A]	THR	N-CA	-7.60	1.36	1.46
1	B	236[B]	THR	N-CA	-7.60	1.36	1.46
1	B	42	HIS	CG-ND1	-7.58	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	ILE	C-O	-7.36	1.16	1.24
1	A	22	THR	C-O	-7.23	1.15	1.24
1	B	45	ASP	C-O	-7.21	1.15	1.24
1	A	285	GLY	C-O	-7.19	1.16	1.24
1	B	169	GLY	C-O	-7.11	1.16	1.24
1	B	41	LEU	C-O	-7.10	1.15	1.24
1	A	262	ILE	C-O	-7.02	1.15	1.24
1	B	70	GLY	C-O	-7.02	1.17	1.24
1	A	166	ALA	C-O	-6.96	1.16	1.24
1	A	34	ILE	C-O	-6.93	1.16	1.24
1	B	106	ALA	C-O	-6.89	1.16	1.24
1	A	121	VAL	C-O	-6.85	1.16	1.24
1	B	237	ASN	C-O	-6.78	1.16	1.24
1	B	40	ARG	C-O	-6.74	1.16	1.24
1	B	108	GLN	C-O	-6.71	1.16	1.24
1	B	8	PHE	C-O	-6.69	1.16	1.24
1	A	250	GLU	C-O	-6.64	1.15	1.24
1	B	171	HIS	CD2-NE2	-6.63	1.30	1.37
1	B	283	ASN	C-O	-6.63	1.16	1.24
1	A	127	ASP	C-O	-6.62	1.16	1.24
1	A	20	VAL	C-O	-6.61	1.16	1.24
1	B	243	GLY	C-O	-6.59	1.16	1.23
1	B	57	LEU	C-O	-6.59	1.16	1.23
1	B	201	THR	C-O	-6.56	1.16	1.24
1	A	162	ASN	C-O	-6.56	1.16	1.24
1	A	28	PHE	C-O	-6.54	1.16	1.24
1	B	248	ASP	C-O	-6.53	1.16	1.24
1	A	242	ASN	C-O	-6.51	1.15	1.24
1	B	228	ASP	C-O	-6.50	1.15	1.23
1	A	71	PRO	C-O	-6.50	1.15	1.24
1	A	210	CYS	C-O	-6.48	1.16	1.24
1	B	96	VAL	C-O	-6.44	1.16	1.23
1	A	255	THR	C-O	-6.42	1.16	1.23
1	A	42	HIS	CG-ND1	-6.40	1.31	1.38
1	A	167	LEU	C-O	-6.39	1.16	1.24
1	B	262	ILE	C-O	-6.39	1.17	1.24
1	A	193	ASN	C-O	-6.38	1.17	1.24
1	B	82	VAL	C-O	-6.38	1.16	1.24
1	A	96	VAL	C-O	-6.36	1.16	1.23
1	B	152	SER	C-O	-6.34	1.16	1.24
1	B	298	ARG	C-O	-6.34	1.16	1.23
1	A	98	SER	C-O	-6.31	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ALA	C-O	-6.31	1.16	1.24
1	B	107	SER	C-O	-6.31	1.16	1.24
1	B	112	SER	C-O	-6.29	1.16	1.24
1	B	219	SER	C-O	-6.29	1.16	1.23
1	B	264	THR	C-O	-6.28	1.16	1.24
1	A	158	GLY	C-O	-6.28	1.16	1.24
1	A	172	THR	C-O	-6.26	1.16	1.24
1	A	17	SER	C-O	-6.21	1.17	1.24
1	A	223	ASP	C-O	-6.21	1.16	1.24
1	A	86	LYS	C-O	-6.19	1.16	1.24
1	A	230	PHE	C-O	-6.19	1.16	1.24
1	A	42	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	225	SER	C-O	-6.16	1.16	1.24
1	A	57	LEU	C-O	-6.15	1.16	1.23
1	B	36	ALA	C-O	-6.15	1.17	1.24
1	B	111	VAL	C-O	-6.15	1.17	1.24
1	A	155	SER	C-O	-6.14	1.17	1.24
1	B	19	MET	C-O	-6.14	1.17	1.24
1	A	251	LEU	C-O	-6.13	1.17	1.24
1	A	264	THR	C-O	-6.13	1.17	1.24
1	A	48	VAL	C-O	-6.13	1.17	1.24
1	B	155	SER	C-O	-6.12	1.17	1.24
1	A	171	HIS	CD2-NE2	-6.11	1.31	1.37
1	B	275	GLN	C-O	-6.09	1.17	1.24
1	A	161	THR	C-O	-6.09	1.17	1.24
1	B	270	GLN	C-O	-6.09	1.16	1.24
1	B	87	THR	C-O	-6.07	1.17	1.24
1	A	286	ASN	C-O	-6.06	1.15	1.24
1	A	75	SER	C-O	-6.05	1.16	1.24
1	A	25	GLN	C-O	-6.04	1.17	1.24
1	B	303	LYS	C-O	-6.03	1.16	1.23
1	A	147	LEU	C-O	-6.03	1.17	1.24
1	B	39	ILE	C-O	-6.02	1.17	1.24
1	A	283	ASN	C-O	-6.02	1.17	1.24
1	A	176	ALA	C-O	-5.99	1.16	1.23
1	A	202	LEU	C-O	-5.98	1.17	1.24
1	B	222	LEU	C-O	-5.98	1.17	1.24
1	B	299	LEU	C-O	-5.97	1.17	1.24
1	A	272	LEU	C-O	-5.97	1.17	1.24
1	A	89	LEU	C-O	-5.97	1.17	1.24
1	B	55	ILE	C-O	-5.96	1.16	1.24
1	B	168	SER	C-O	-5.96	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	SER	C-O	-5.95	1.17	1.24
1	B	224	LEU	C-O	-5.95	1.16	1.24
1	A	164	LEU	C-O	-5.95	1.17	1.24
1	B	273	PHE	C-O	-5.94	1.17	1.24
1	B	221	ASN	C-O	-5.91	1.16	1.23
1	A	70	GLY	C-O	-5.90	1.16	1.24
1	B	225	SER	C-O	-5.88	1.17	1.24
1	B	261	ALA	C-O	-5.87	1.17	1.24
1	B	257	SER	C-O	-5.86	1.16	1.23
1	A	169	GLY	C-O	-5.85	1.17	1.24
1	A	148	SER	C-O	-5.83	1.17	1.24
1	A	125	ARG	C-O	-5.83	1.16	1.23
1	B	76	ALA	C-O	-5.81	1.17	1.23
1	A	267	ALA	C-O	-5.81	1.17	1.24
1	B	100	THR	C-O	-5.80	1.17	1.24
1	A	237	ASN	C-O	-5.80	1.17	1.24
1	B	255	THR	C-O	-5.80	1.17	1.23
1	A	39	ILE	C-O	-5.80	1.17	1.24
1	B	127	ASP	C-O	-5.79	1.16	1.23
1	A	27	ALA	C-O	-5.78	1.17	1.24
1	A	208	GLU	C-O	-5.78	1.17	1.24
1	B	90	GLU	C-O	-5.78	1.17	1.24
1	B	185	LEU	C-O	-5.78	1.17	1.24
1	A	97	VAL	C-O	-5.77	1.17	1.24
1	B	25	GLN	C-O	-5.76	1.17	1.24
1	A	159	LEU	C-O	-5.76	1.17	1.24
1	A	276	ALA	C-O	-5.76	1.17	1.24
1	A	209	LEU	C-O	-5.75	1.17	1.24
1	A	55	ILE	C-O	-5.75	1.17	1.24
1	B	210	CYS	C-O	-5.75	1.17	1.24
1	B	72	ASN	C-O	-5.74	1.16	1.24
1	B	285	GLY	C-O	-5.73	1.17	1.24
1	B	17	SER	C-O	-5.73	1.17	1.24
1	A	205	THR	C-O	-5.72	1.17	1.24
1	B	206	LEU	C-O	-5.72	1.17	1.24
1	B	260	ILE	C-O	-5.72	1.17	1.24
1	A	273	PHE	C-O	-5.71	1.17	1.24
1	A	137	ASN	C-O	-5.70	1.17	1.24
1	B	44	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	50	GLY	C-O	-5.67	1.15	1.23
1	B	98	SER	C-O	-5.67	1.16	1.23
1	A	37	SER	C-O	-5.67	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	VAL	C-O	-5.66	1.17	1.24
1	A	119	TRP	NE1-CE2	-5.66	1.31	1.37
1	A	128	THR	C-O	-5.66	1.16	1.23
1	A	287	ILE	C-O	-5.66	1.17	1.23
1	B	279	GLN	C-O	-5.66	1.17	1.24
1	A	113	LEU	C-O	-5.65	1.16	1.24
1	B	89	LEU	C-O	-5.65	1.17	1.24
1	A	117	PRO	C-O	-5.65	1.17	1.23
1	B	148	SER	C-O	-5.64	1.17	1.24
1	A	296	GLU	C-O	-5.63	1.16	1.23
1	A	41	LEU	C-O	-5.63	1.17	1.24
1	A	111	VAL	C-O	-5.62	1.17	1.24
1	A	8	PHE	C-O	-5.61	1.17	1.24
1	A	21	ARG	C-O	-5.60	1.17	1.24
1	B	110	SER	C-O	-5.60	1.17	1.24
1	A	154	PHE	C-O	-5.59	1.17	1.24
1	A	168	SER	C-O	-5.59	1.16	1.24
1	B	239	GLN	C-O	-5.58	1.16	1.24
1	B	22	THR	C-O	-5.58	1.17	1.24
1	B	42	HIS	CD2-NE2	-5.57	1.31	1.37
1	B	166	ALA	C-O	-5.57	1.17	1.24
1	A	109	ALA	C-O	-5.57	1.17	1.24
1	A	183	ASN	C-O	-5.56	1.17	1.24
1	B	105	LEU	C-O	-5.56	1.17	1.24
1	B	147	LEU	C-O	-5.55	1.17	1.24
1	B	162	ASN	C-O	-5.55	1.17	1.24
1	A	29	GLN	C-O	-5.55	1.17	1.24
1	A	278	ALA	C-O	-5.55	1.17	1.24
1	B	104	ALA	C-O	-5.55	1.17	1.24
1	B	124	GLY	C-O	-5.54	1.18	1.24
1	B	163	ASP	C-O	-5.54	1.17	1.24
1	B	223	ASP	C-O	-5.53	1.17	1.24
1	A	126	ARG	C-O	-5.53	1.16	1.23
1	A	220	THR	C-O	-5.53	1.17	1.23
1	A	256	GLY	C-O	-5.52	1.16	1.23
1	A	151	THR	C-O	-5.52	1.17	1.24
1	A	305	ASN	C-O	-5.52	1.17	1.23
1	A	299	LEU	C-O	-5.52	1.17	1.24
1	A	175	ARG	C-O	-5.52	1.16	1.23
1	B	226	THR	C-O	-5.51	1.17	1.24
1	A	67	LYS	C-O	-5.51	1.17	1.24
1	B	288	SER	C-O	-5.51	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	GLN	C-O	-5.50	1.17	1.24
1	A	84	ASN	C-O	-5.50	1.17	1.24
1	A	56	LEU	C-O	-5.50	1.17	1.24
1	B	244	LEU	C-O	-5.49	1.17	1.24
1	A	103	LEU	C-O	-5.48	1.17	1.24
1	A	46	CYS	C-O	-5.48	1.17	1.24
1	B	276	ALA	C-O	-5.48	1.17	1.24
1	B	86	LYS	C-O	-5.47	1.17	1.24
1	B	281	MET	C-O	-5.46	1.17	1.24
1	A	191	LYS	C-O	-5.46	1.16	1.24
1	B	91	ASN	C-O	-5.46	1.17	1.24
1	B	102	VAL	C-O	-5.46	1.18	1.24
1	B	245	LEU	C-O	-5.46	1.16	1.23
1	B	79	PHE	C-O	-5.45	1.17	1.24
1	A	14	PRO	C-O	-5.45	1.17	1.24
1	B	234	TYR	C-O	-5.45	1.17	1.24
1	A	26[A]	GLN	C-O	-5.44	1.17	1.24
1	A	26[B]	GLN	C-O	-5.44	1.17	1.24
1	A	19	MET	C-O	-5.44	1.17	1.24
1	A	10	ALA	C-O	-5.42	1.17	1.24
1	A	302	LYS	C-O	-5.41	1.17	1.24
1	A	263	VAL	C-O	-5.41	1.17	1.24
1	A	188	PHE	C-O	-5.41	1.17	1.24
1	A	200	THR	C-O	-5.41	1.17	1.24
1	B	121	VAL	C-O	-5.40	1.18	1.24
1	A	182	SER	C-O	-5.39	1.17	1.24
1	B	294	SER	C-O	-5.37	1.17	1.23
1	A	79	PHE	C-O	-5.37	1.17	1.24
1	A	43	PHE	C-O	-5.37	1.18	1.24
1	B	165	VAL	C-O	-5.37	1.17	1.24
1	B	202	LEU	C-O	-5.36	1.17	1.24
1	A	87	THR	C-O	-5.36	1.17	1.24
1	B	208	GLU	C-O	-5.36	1.17	1.24
1	A	59	ASN	C-O	-5.35	1.17	1.23
1	A	108	GLN	C-O	-5.35	1.17	1.24
1	A	231	ASP	C-O	-5.35	1.17	1.23
1	B	119	TRP	NE1-CE2	-5.35	1.31	1.37
1	A	141	PRO	C-O	-5.34	1.17	1.23
1	A	234	TYR	C-O	-5.34	1.17	1.24
1	B	43	PHE	C-O	-5.33	1.18	1.24
1	A	44	HIS	CG-ND1	-5.33	1.32	1.38
1	A	139	SER	C-O	-5.32	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	SER	C-O	-5.32	1.17	1.24
1	A	186	PHE	C-O	-5.31	1.17	1.24
1	A	199	ASN	C-O	-5.30	1.17	1.23
1	B	18	ALA	C-O	-5.30	1.18	1.24
1	A	107	SER	C-O	-5.29	1.18	1.24
1	B	284	MET	C-O	-5.29	1.18	1.24
1	A	184	ARG	C-O	-5.28	1.17	1.24
1	B	21	ARG	C-O	-5.28	1.18	1.24
1	B	56	LEU	C-O	-5.27	1.17	1.24
1	A	90	GLU	C-O	-5.26	1.18	1.24
1	A	30	SER	C-O	-5.26	1.17	1.24
1	B	137	ASN	C-O	-5.25	1.17	1.24
1	A	68	ASN	C-O	-5.24	1.17	1.24
1	B	252	PHE	C-O	-5.24	1.17	1.24
1	B	26	GLN	C-O	-5.24	1.18	1.24
1	A	179	GLY	C-O	-5.24	1.16	1.23
1	B	197	THR	C-O	-5.24	1.17	1.24
1	A	171	HIS	CG-ND1	-5.22	1.32	1.38
1	B	246	GLN	C-O	-5.22	1.18	1.24
1	B	143	PRO	C-O	-5.21	1.18	1.24
1	B	205	THR	C-O	-5.21	1.18	1.24
1	B	263	VAL	C-O	-5.20	1.18	1.24
1	A	298	ARG	C-O	-5.19	1.17	1.23
1	B	193	ASN	C-O	-5.19	1.18	1.24
1	B	134	ALA	C-O	-5.19	1.18	1.24
1	B	161	THR	C-O	-5.19	1.18	1.24
1	A	152	SER	C-O	-5.17	1.18	1.24
1	B	20	VAL	C-O	-5.16	1.18	1.24
1	B	49	LEU	C-O	-5.16	1.16	1.23
1	B	24	VAL	C-O	-5.15	1.18	1.24
1	B	97	VAL	C-O	-5.15	1.18	1.24
1	B	114	SER	C-O	-5.15	1.17	1.24
1	A	297	ILE	C-O	-5.14	1.18	1.24
1	A	44	HIS	CD2-NE2	-5.13	1.32	1.37
1	B	200	THR	C-O	-5.12	1.17	1.24
1	B	101	ASP	C-O	-5.12	1.18	1.24
1	B	128	THR	C-O	-5.10	1.17	1.23
1	A	101	ASP	C-O	-5.10	1.18	1.24
1	A	40	ARG	C-O	-5.09	1.18	1.24
1	B	277	PHE	C-O	-5.08	1.18	1.24
1	A	203	LEU	C-O	-5.08	1.18	1.24
1	B	103	LEU	C-O	-5.08	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	LYS	C-O	-5.07	1.18	1.24
1	A	244	LEU	C-O	-5.07	1.18	1.24
1	A	45	ASP	C-O	-5.06	1.18	1.24
1	A	58	ASP	C-O	-5.06	1.17	1.23
1	A	236	THR	C-O	-5.06	1.18	1.24
1	A	290	LEU	C-O	-5.05	1.17	1.24
1	A	207	GLN	C-O	-5.05	1.18	1.24
1	A	140	ILE	C-O	-5.05	1.17	1.24
1	B	233	ASN	C-O	-5.05	1.17	1.24
1	B	280	SER	C-O	-5.04	1.18	1.24
1	A	206	LEU	C-O	-5.03	1.18	1.24
1	B	150	ILE	C-O	-5.03	1.18	1.24
1	A	275	GLN	C-O	-5.03	1.18	1.24
1	A	106	ALA	C-O	-5.02	1.17	1.24
1	B	231	ASP	C-O	-5.02	1.17	1.23
1	B	73	ALA	C-O	-5.02	1.17	1.23
1	A	239	GLN	C-O	-5.00	1.17	1.24
1	A	219	SER	C-O	-5.00	1.17	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LEU	N-CA-C	9.54	121.75	111.36
1	B	185	LEU	N-CA-C	9.49	121.71	111.36
1	B	157[A]	VAL	CA-C-O	-8.68	110.71	120.26
1	B	157[B]	VAL	CA-C-O	-8.68	110.71	120.26
1	B	235	PHE	CA-C-N	8.56	131.75	120.28
1	B	235	PHE	C-N-CA	8.56	131.75	120.28
1	A	91	ASN	O-C-N	-8.19	113.25	122.09
1	A	139	SER	N-CA-C	7.89	119.96	111.36
1	A	96	VAL	N-CA-C	7.33	118.63	111.67
1	B	92	ALA	N-CA-C	7.25	120.00	111.59
1	B	139	SER	N-CA-C	7.13	120.09	111.82
1	B	2	GLY	N-CA-C	-6.66	97.39	113.18
1	A	92	ALA	N-CA-C	6.57	119.22	111.59
1	A	244	LEU	N-CA-C	6.57	119.41	111.40
1	B	90	GLU	O-C-N	-6.48	115.25	122.12
1	B	96	VAL	N-CA-C	6.28	117.64	111.67
1	B	90	GLU	CA-C-N	6.26	128.59	120.44
1	B	90	GLU	C-N-CA	6.26	128.59	120.44
1	B	236[A]	THR	CA-C-O	-6.02	114.12	120.63
1	B	236[B]	THR	CA-C-O	-6.02	114.12	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ILE	N-CA-C	5.63	115.97	107.80
1	B	3	SER	N-CA-C	5.41	117.21	108.34
1	B	34	ILE	N-CA-C	5.34	116.07	110.62
1	A	11	GLY	N-CA-C	5.24	120.39	113.37
1	B	63	ILE	N-CA-C	5.09	115.09	107.51
1	A	291	THR	N-CA-C	5.04	116.65	109.14
1	B	138	SER	N-CA-C	5.03	119.40	113.12

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3[B]	SER	Mainchain
1	A	301[B]	CYS	Mainchain
1	A	93[B]	CYS	Mainchain
1	A	99[B]	CYS	Mainchain
1	B	212	GLN	Peptide
1	B	236[A]	THR	Mainchain
1	B	236[B]	THR	Mainchain

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	2277	0	2185	76	0
1	B	2258	0	2177	78	1
2	C	69	0	51	5	0
2	I	69	0	51	5	0
3	D	49	0	43	0	0
4	E	49	0	43	2	0
5	F	49	0	43	2	1
5	L	49	0	43	1	0
6	G	69	0	51	1	0
7	H	28	0	25	0	0
8	J	49	0	43	4	0
9	K	38	0	34	0	0
10	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	43	0	30	2	0
11	A	2	0	0	0	0
11	B	2	0	0	0	0
12	A	14	0	13	2	0
12	B	42	0	39	2	0
13	A	15	0	17	6	0
13	B	47	0	55	13	0
14	B	8	0	12	1	0
15	A	364	0	0	32	9
15	B	336	0	0	29	2
All	All	5969	0	4985	184	11

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 18.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:THR:HG23	15:A:2200:HOH:O	1.22	1.31
1:A:99[B]:CYS:SG	1:A:301[B]:CYS:HB3	1.73	1.27
1:A:56:LEU:CD1	1:A:99[B]:CYS:SG	2.30	1.20
1:B:60:SER:HA	15:B:2089:HOH:O	1.02	1.20
1:A:308:GLY:O	15:A:2328:HOH:O	1.57	1.19
1:B:215:ARG:HB2	15:B:2228:HOH:O	1.37	1.19
1:A:56:LEU:HD13	1:A:99[B]:CYS:SG	1.91	1.09
13:B:1330:1PE:H142	15:B:2328:HOH:O	0.87	1.05
1:A:29:GLN:NE2	15:A:2037:HOH:O	1.89	1.04
15:A:2342:HOH:O	2:C:4:XYP:O4	1.74	1.03
1:A:29:GLN:OE1	15:A:2045:HOH:O	1.77	1.01
15:B:2322:HOH:O	8:J:3:BMA:O3	1.79	1.00
1:A:308:GLY:HA2	1:B:77:ARG:HE	1.26	0.99
1:A:56:LEU:HD12	1:A:99[B]:CYS:SG	2.03	0.98
1:A:99[B]:CYS:SG	1:A:301[B]:CYS:CB	2.51	0.98
15:B:2319:HOH:O	8:J:2:NAG:O7	1.82	0.97
1:B:307:SER:N	15:B:2303:HOH:O	1.99	0.94
1:B:213:LYS:HD2	1:B:214:GLY:HA2	1.47	0.93
1:B:216:GLY:O	15:B:2207:HOH:O	1.87	0.91
13:B:1330:1PE:H132	15:B:2317:HOH:O	1.71	0.91
12:A:1336:NAG:H83	15:A:2169:HOH:O	1.71	0.90
1:A:205:THR:HG21	15:A:2229:HOH:O	1.72	0.89
1:B:191:LYS:NZ	1:B:196:PRO:HD3	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLU:OE1	15:A:2235:HOH:O	1.92	0.88
1:B:177:THR:OG1	15:B:2204:HOH:O	1.80	0.86
1:B:215:ARG:HE	1:B:216:GLY:H	1.22	0.86
13:B:1334:1PE:C22	15:B:2328:HOH:O	2.22	0.86
1:B:213:LYS:HZ2	1:B:215:ARG:H	1.24	0.85
1:B:214:GLY:C	1:B:215:ARG:HD3	2.03	0.83
15:A:2359:HOH:O	6:G:5:BMA:O4	1.96	0.82
1:B:215:ARG:NE	1:B:216:GLY:H	1.78	0.81
1:A:52:ASP:HA	1:A:100:THR:HG21	1.63	0.80
1:B:52:ASP:C	1:B:100:THR:HG22	2.06	0.80
1:B:213:LYS:HD2	1:B:214:GLY:CA	2.12	0.79
1:A:308:GLY:C	15:A:2322:HOH:O	2.25	0.79
1:A:52:ASP:C	1:A:100:THR:CG2	2.57	0.78
1:A:53:ALA:N	1:A:100:THR:HG22	1.99	0.77
14:B:1331:PG0:H12	15:B:2333:HOH:O	1.83	0.77
1:B:211:PRO:HA	15:B:2225:HOH:O	1.84	0.76
1:B:214:GLY:O	1:B:215:ARG:HB3	1.85	0.76
1:B:52:ASP:C	1:B:100:THR:CG2	2.59	0.75
1:A:177:THR:CG2	15:A:2200:HOH:O	1.99	0.75
1:B:53:ALA:N	1:B:100:THR:HG22	2.02	0.75
1:B:191:LYS:HZ3	1:B:196:PRO:HD3	1.49	0.74
1:B:191:LYS:HG2	1:B:193:ASN:H	1.52	0.74
13:B:1330:1PE:H241	15:B:2317:HOH:O	1.87	0.74
1:B:191:LYS:CG	1:B:193:ASN:H	1.99	0.73
1:B:211:PRO:HD2	1:B:215:ARG:HD2	1.71	0.73
1:A:152:SER:N	15:A:2171:HOH:O	2.21	0.72
1:A:49:LEU:HD11	1:A:132:ASN:HD22	1.54	0.72
1:B:215:ARG:HG2	1:B:216:GLY:H	1.55	0.72
1:A:211:PRO:HD2	1:A:215:ARG:HH22	1.54	0.71
13:B:1330:1PE:H242	13:B:1330:1PE:OH6	1.90	0.71
13:B:1334:1PE:C22	2:I:2:NAG:H62	2.20	0.71
1:A:11:GLY:N	15:A:2019:HOH:O	2.24	0.71
1:A:191:LYS:NZ	15:A:2213:HOH:O	2.23	0.70
1:A:275:GLN:NE2	15:A:2291:HOH:O	2.13	0.70
1:B:213:LYS:NZ	1:B:215:ARG:H	1.89	0.70
1:B:215:ARG:CG	1:B:216:GLY:H	2.04	0.70
1:A:52:ASP:C	1:A:100:THR:HG22	2.17	0.70
15:A:2346:HOH:O	4:E:3:MAN:O6	2.10	0.70
12:A:1336:NAG:O4	12:A:1336:NAG:N2	2.25	0.70
1:B:191:LYS:CE	1:B:193:ASN:HB2	2.22	0.69
1:B:52:ASP:HA	1:B:100:THR:HG21	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLY:O	1:B:307:SER:C	2.37	0.68
15:B:2315:HOH:O	2:I:5:MAN:O5	2.11	0.68
1:B:3:SER:HA	13:B:1333:1PE:H132	1.75	0.68
1:B:191:LYS:HE2	1:B:193:ASN:HB2	1.77	0.67
15:A:2341:HOH:O	2:C:4:XYP:O3	2.11	0.67
1:A:191:LYS:HD3	1:A:193:ASN:O	1.94	0.67
15:B:2315:HOH:O	2:I:5:MAN:C5	2.42	0.67
1:B:133:GLN:OE1	12:B:1326:NAG:N2	2.23	0.67
15:A:2332:HOH:O	2:C:4:XYP:O2	2.14	0.66
15:B:2316:HOH:O	2:I:5:MAN:O6	2.13	0.66
1:A:49:LEU:CD1	1:A:132:ASN:HD22	2.09	0.66
1:B:306:GLY:C	15:B:2303:HOH:O	2.35	0.65
1:B:191:LYS:HD3	1:B:193:ASN:O	1.95	0.65
1:A:188:PHE:HB3	1:A:191:LYS:HD3	1.78	0.65
1:A:215:ARG:NH2	15:A:2201:HOH:O	2.30	0.65
1:B:145:GLN:HA	12:B:1327:NAG:H83	1.78	0.65
1:A:308:GLY:HA2	1:B:77:ARG:NE	2.06	0.64
1:B:191:LYS:HE2	1:B:193:ASN:CB	2.27	0.64
1:A:215:ARG:HE	1:A:217:SER:H	1.45	0.64
1:B:49:LEU:HD12	15:B:2082:HOH:O	1.97	0.64
1:A:213:LYS:HE3	15:A:2240:HOH:O	1.97	0.63
1:B:215:ARG:HE	1:B:216:GLY:N	1.94	0.63
1:A:191:LYS:CG	1:A:193:ASN:H	2.12	0.62
1:B:215:ARG:HG2	1:B:216:GLY:N	2.13	0.62
1:B:4:LEU:H	13:B:1333:1PE:H132	1.63	0.62
15:A:2354:HOH:O	5:F:3:MAN:O3	2.16	0.62
1:A:2:GLY:N	15:A:2001:HOH:O	2.33	0.62
1:B:214:GLY:O	1:B:215:ARG:HD3	2.00	0.62
1:A:3[B]:SER:HA	13:A:1337:1PE:C22	2.31	0.61
1:A:213:LYS:CE	15:A:2240:HOH:O	2.49	0.61
1:A:215:ARG:HE	1:A:216:GLY:N	1.98	0.60
1:A:191:LYS:HG2	1:A:193:ASN:H	1.64	0.60
1:A:64:ILE:HG21	15:A:2159:HOH:O	2.02	0.59
1:B:205:THR:HG21	15:B:2107:HOH:O	2.02	0.59
1:B:93[B]:CYS:O	1:B:96:VAL:HG23	2.04	0.57
13:B:1330:1PE:H252	2:I:5:MAN:O2	2.05	0.57
1:B:3:SER:N	15:B:2003:HOH:O	2.26	0.57
1:B:52:ASP:HA	1:B:100:THR:CG2	2.33	0.56
2:C:4:XYP:O5	2:C:5:MAN:H5	2.06	0.56
15:B:2324:HOH:O	8:J:3:BMA:H2	2.05	0.56
1:A:108:GLN:HE21	1:A:118:SER:HA	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:2:NAG:O7	8:J:2:NAG:H3	2.07	0.55
1:B:188:PHE:HB3	1:B:191:LYS:HD3	1.89	0.54
1:A:191:LYS:HE2	1:A:194:PRO:O	2.06	0.54
1:A:3[B]:SER:OG	13:A:1337:1PE:C22	2.55	0.54
1:A:52:ASP:CA	1:A:100:THR:HG21	2.36	0.54
1:B:64:ILE:CG2	1:B:133:GLN:NE2	2.71	0.54
1:A:36:ALA:HB1	10:A:1307:HEM:HMD1	1.90	0.53
1:B:214:GLY:O	1:B:215:ARG:CB	2.55	0.53
1:A:215:ARG:NE	1:A:216:GLY:N	2.57	0.53
1:A:2:GLY:CA	15:A:2001:HOH:O	2.57	0.52
1:A:52:ASP:HA	1:A:100:THR:CG2	2.36	0.52
1:A:236:THR:HG21	15:A:2259:HOH:O	2.09	0.52
13:B:1330:1PE:H251	15:B:2330:HOH:O	2.09	0.52
1:A:308:GLY:CA	15:A:2322:HOH:O	2.57	0.52
1:A:52:ASP:CA	1:A:100:THR:CG2	2.87	0.52
10:B:1306:HEM:HBB2	10:B:1306:HEM:HHC	1.91	0.52
1:A:167:LEU:HB3	10:A:1307:HEM:HMC3	1.92	0.52
1:B:49:LEU:HD21	1:B:132:ASN:HD22	1.73	0.52
10:B:1306:HEM:HMC2	10:B:1306:HEM:HBC2	1.91	0.52
1:A:61:GLY:HA3	1:B:84:ASN:ND2	2.25	0.52
1:B:108:GLN:HE21	1:B:119:TRP:H	1.57	0.51
15:A:2341:HOH:O	2:C:4:XYP:C3	2.59	0.51
1:A:56:LEU:CD1	1:A:99[B]:CYS:HG	2.21	0.51
1:B:191:LYS:HG2	1:B:192:GLY:N	2.25	0.51
1:B:213:LYS:NZ	1:B:215:ARG:N	2.56	0.51
1:A:215:ARG:NH2	1:A:216:GLY:H	2.08	0.50
1:A:49:LEU:HD23	15:A:2072:HOH:O	2.11	0.50
1:A:3[B]:SER:HA	13:A:1337:1PE:OH3	2.11	0.50
1:B:178[B]:CYS:CB	1:B:210:CYS:SG	3.00	0.50
13:B:1330:1PE:C14	15:B:2328:HOH:O	1.74	0.50
1:A:215:ARG:CZ	1:A:215:ARG:H	2.24	0.49
1:B:215:ARG:HG2	15:B:2206:HOH:O	2.11	0.49
1:B:215:ARG:NE	1:B:216:GLY:N	2.55	0.49
1:B:211:PRO:CD	1:B:215:ARG:HD2	2.39	0.49
1:A:215:ARG:CZ	1:A:215:ARG:N	2.76	0.49
1:B:187:ASN:OD1	1:B:192:GLY:N	2.45	0.48
1:B:64:ILE:HG21	1:B:133:GLN:HE22	1.78	0.48
1:B:215:ARG:CD	1:B:216:GLY:H	2.27	0.48
1:B:52:ASP:CA	1:B:100:THR:CG2	2.91	0.48
1:B:191:LYS:HG3	1:B:193:ASN:H	1.77	0.48
1:B:307:SER:CA	15:B:2303:HOH:O	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:THR:HG23	1:B:127:ASP:OD1	2.15	0.47
1:B:215:ARG:CG	15:B:2206:HOH:O	2.62	0.47
1:A:10:ALA:N	15:A:2019:HOH:O	2.48	0.47
1:A:308:GLY:HA3	15:A:2322:HOH:O	2.14	0.46
1:A:178[B]:CYS:SG	1:A:218:GLY:CA	3.03	0.46
1:A:303:LYS:HB3	1:A:307:SER:OG	2.16	0.45
1:B:191:LYS:HZ1	1:B:196:PRO:HD3	1.77	0.45
1:A:9:TYR:C	15:A:2019:HOH:O	2.60	0.45
1:A:108:GLN:HE21	1:A:118:SER:CA	2.28	0.45
1:A:286:ASN:OD1	13:A:1337:1PE:H231	2.16	0.44
1:A:54:SER:HB3	1:A:128:THR:HG21	1.99	0.44
1:A:215:ARG:HH21	1:A:216:GLY:H	1.66	0.44
1:A:286:ASN:CG	13:A:1337:1PE:H231	2.43	0.44
1:B:64:ILE:HG21	1:B:133:GLN:NE2	2.33	0.44
1:B:177:THR:O	1:B:178[B]:CYS:C	2.60	0.44
1:B:52:ASP:CA	1:B:100:THR:HG22	2.48	0.43
1:A:177:THR:O	1:A:178[B]:CYS:C	2.61	0.43
1:A:177:THR:HG22	1:A:178[B]:CYS:N	2.33	0.43
1:B:61:GLY:N	15:B:2089:HOH:O	2.51	0.43
13:B:1330:1PE:H141	13:B:1334:1PE:C22	2.49	0.43
1:A:191:LYS:HG3	1:A:193:ASN:H	1.83	0.42
1:A:221:ASN:CG	1:A:227:PRO:HB3	2.44	0.42
5:L:2:NAG:C8	5:L:4:FUC:H61	2.49	0.42
5:F:1:NAG:H61	5:F:2:NAG:C1	2.48	0.42
1:B:298:ARG:HG3	15:B:2166:HOH:O	2.18	0.42
1:B:2:GLY:HA2	15:B:2003:HOH:O	2.18	0.42
1:B:213:LYS:HD2	1:B:213:LYS:HA	1.42	0.42
1:A:119:TRP:HB3	1:A:278:ALA:HB1	2.01	0.42
1:B:145:GLN:HE21	1:B:149:ASN:HB3	1.85	0.42
1:A:178[B]:CYS:SG	1:A:218:GLY:HA3	2.60	0.42
1:B:3:SER:HA	13:B:1333:1PE:C13	2.47	0.42
4:E:1:NAG:O3	4:E:4:FUL:H63	2.20	0.41
1:B:213:LYS:HA	1:B:214:GLY:HA2	1.65	0.41
1:A:3[A]:SER:HA	13:A:1337:1PE:C22	2.51	0.41
1:B:93[B]:CYS:O	1:B:96:VAL:CG2	2.68	0.41
1:B:191:LYS:CD	1:B:193:ASN:O	2.68	0.40
1:A:140:ILE:HA	1:A:141:PRO:HD3	1.98	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:4:FUC:C6	15:B:2137:HOH:O[1_445]	1.72	0.48
15:A:2194:HOH:O	15:A:2212:HOH:O[2_556]	1.95	0.25
1:B:93[B]:CYS:O	15:A:2353:HOH:O[1_665]	2.00	0.20
15:A:2076:HOH:O	15:A:2122:HOH:O[2_556]	2.02	0.18
15:A:2159:HOH:O	15:A:2358:HOH:O[2_656]	2.03	0.17
15:A:2025:HOH:O	15:A:2310:HOH:O[1_545]	2.05	0.15
15:A:2044:HOH:O	15:A:2149:HOH:O[1_545]	2.07	0.13
15:B:2188:HOH:O	15:B:2261:HOH:O[2_655]	2.09	0.11
15:A:2103:HOH:O	15:A:2283:HOH:O[2_546]	2.11	0.09
15:A:2179:HOH:O	15:A:2275:HOH:O[2_556]	2.12	0.08
15:A:2076:HOH:O	15:A:2104:HOH:O[1_565]	2.16	0.04

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	312/308 (101%)	305 (98%)	5 (2%)	2 (1%)	21	13
1	B	310/308 (101%)	297 (96%)	7 (2%)	6 (2%)	6	2
All	All	622/616 (101%)	602 (97%)	12 (2%)	8 (1%)	16	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	ARG
1	A	3[A]	SER
1	A	3[B]	SER
1	B	94	PRO
1	B	178[A]	CYS
1	B	178[B]	CYS
1	B	93[A]	CYS
1	B	93[B]	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/250 (103%)	251 (98%)	6 (2%)	44	42
1	B	255/250 (102%)	247 (97%)	8 (3%)	35	30
All	All	512/500 (102%)	498 (97%)	14 (3%)	38	36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	49	LEU
1	A	173	PHE
1	A	191	LYS
1	A	215	ARG
1	A	224	LEU
1	B	3	SER
1	B	60	SER
1	B	64	ILE
1	B	173	PHE
1	B	191	LYS
1	B	213	LYS
1	B	215	ARG
1	B	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	68	ASN
1	A	108	GLN
1	A	132	ASN
1	A	162	ASN
1	A	221	ASN
1	B	162	ASN
1	B	183	ASN

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Mol	Chain	Res	Type
1	B	221	ASN
1	B	246	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

43 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	C	1	2,1	14,14,15	1.97	4 (28%)	17,19,21	1.17	2 (11%)
2	NAG	C	2	2	14,14,15	2.02	5 (35%)	17,19,21	1.35	2 (11%)
2	BMA	C	3	2	11,11,12	1.94	2 (18%)	15,15,17	0.84	0
2	XYP	C	4	2	9,9,10	2.20	3 (33%)	10,12,14	1.06	1 (10%)
2	MAN	C	5	2	11,11,12	1.84	2 (18%)	15,15,17	0.82	0
2	FUC	C	6	2	10,10,11	1.91	2 (20%)	14,14,16	0.88	0
3	NAG	D	1	1,3	14,14,15	1.90	4 (28%)	17,19,21	1.13	0
3	NAG	D	2	3	14,14,15	1.96	5 (35%)	17,19,21	1.09	0
3	BMA	D	3	3	11,11,12	1.79	2 (18%)	15,15,17	1.07	0
3	FUC	D	4	3	10,10,11	1.85	2 (20%)	14,14,16	0.76	0
4	NAG	E	1	1,4	14,14,15	2.02	4 (28%)	17,19,21	1.78	3 (17%)
4	NAG	E	2	4	14,14,15	2.09	4 (28%)	17,19,21	1.11	2 (11%)
4	MAN	E	3	4	11,11,12	2.02	2 (18%)	15,15,17	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUL	E	4	4	10,10,11	2.00	2 (20%)	14,14,16	0.96	1 (7%)
5	NAG	F	1	1,5	14,14,15	1.89	4 (28%)	17,19,21	0.97	1 (5%)
5	NAG	F	2	5	14,14,15	1.95	5 (35%)	17,19,21	1.47	3 (17%)
5	MAN	F	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.97	1 (6%)
5	FUC	F	4	5	10,10,11	1.91	2 (20%)	14,14,16	1.16	2 (14%)
6	NAG	G	1	6,1	14,14,15	1.99	4 (28%)	17,19,21	1.48	4 (23%)
6	NAG	G	2	6	14,14,15	2.01	4 (28%)	17,19,21	1.18	2 (11%)
6	BMA	G	3	6	11,11,12	1.81	2 (18%)	15,15,17	0.76	0
6	XYP	G	4	6	9,9,10	2.20	3 (33%)	10,12,14	0.92	1 (10%)
6	BMA	G	5	6	11,11,12	1.72	2 (18%)	15,15,17	0.88	1 (6%)
6	FUL	G	6	6	10,10,11	1.92	2 (20%)	14,14,16	1.01	0
7	NAG	H	1	7,1	14,14,15	2.04	4 (28%)	17,19,21	1.05	1 (5%)
7	NAG	H	2	7	14,14,15	1.97	5 (35%)	17,19,21	1.20	3 (17%)
2	NAG	I	1	2,1	14,14,15	1.98	4 (28%)	17,19,21	1.17	2 (11%)
2	NAG	I	2	2	14,14,15	1.95	5 (35%)	17,19,21	1.62	5 (29%)
2	BMA	I	3	2	11,11,12	1.85	2 (18%)	15,15,17	0.75	0
2	XYP	I	4	2	9,9,10	2.27	3 (33%)	10,12,14	1.21	2 (20%)
2	MAN	I	5	2	11,11,12	1.77	2 (18%)	15,15,17	0.88	0
2	FUC	I	6	2	10,10,11	1.87	2 (20%)	14,14,16	1.08	0
8	NAG	J	1	1,8	14,14,15	1.99	4 (28%)	17,19,21	1.22	2 (11%)
8	NAG	J	2	8	14,14,15	2.00	4 (28%)	17,19,21	1.42	2 (11%)
8	BMA	J	3	8	11,11,12	1.77	2 (18%)	15,15,17	0.96	1 (6%)
8	FUL	J	4	8	10,10,11	2.00	2 (20%)	14,14,16	0.85	1 (7%)
9	NAG	K	1	9,1	14,14,15	1.98	4 (28%)	17,19,21	1.40	2 (11%)
9	FUC	K	2	9	10,10,11	1.95	2 (20%)	14,14,16	0.71	0
9	NAG	K	3	9	14,14,15	2.00	4 (28%)	17,19,21	1.23	2 (11%)
5	NAG	L	1	1,5	14,14,15	1.96	4 (28%)	17,19,21	1.69	5 (29%)
5	NAG	L	2	5	14,14,15	1.99	6 (42%)	17,19,21	1.28	2 (11%)
5	MAN	L	3	5	11,11,12	1.78	2 (18%)	15,15,17	1.24	2 (13%)
5	FUC	L	4	5	10,10,11	1.85	2 (20%)	14,14,16	0.96	1 (7%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	XYP	C	4	2	-	-	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
2	FUC	C	6	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	MAN	E	3	4	-	2/2/19/22	0/1/1/1
4	FUL	E	4	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	MAN	F	3	5	-	0/2/19/22	0/1/1/1
5	FUC	F	4	5	-	-	0/1/1/1
6	NAG	G	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	1/1/5/7	2/6/23/26	0/1/1/1
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	XYP	G	4	6	-	-	0/1/1/1
6	BMA	G	5	6	-	0/2/19/22	1/1/1/1
6	FUL	G	6	6	-	-	0/1/1/1
7	NAG	H	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	1/1/5/7	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	XYP	I	4	2	-	-	0/1/1/1
2	MAN	I	5	2	1/1/4/5	2/2/19/22	1/1/1/1
2	FUC	I	6	2	-	-	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
8	BMA	J	3	8	-	2/2/19/22	0/1/1/1
8	FUL	J	4	8	-	-	0/1/1/1
9	NAG	K	1	9,1	-	0/6/23/26	0/1/1/1
9	FUC	K	2	9	-	-	0/1/1/1
9	NAG	K	3	9	-	0/6/23/26	0/1/1/1
5	NAG	L	1	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	L	3	5	-	2/2/19/22	0/1/1/1
5	FUC	L	4	5	-	-	0/1/1/1

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	MAN	C2-C3	-5.47	1.44	1.52
2	C	3	BMA	C2-C3	-5.37	1.44	1.52
4	E	4	FUL	C2-C3	-5.26	1.44	1.52
8	J	4	FUL	C2-C3	-5.21	1.44	1.52
6	G	6	FUL	C2-C3	-5.08	1.44	1.52
2	C	6	FUC	C2-C3	-5.07	1.44	1.52
2	I	3	BMA	C2-C3	-5.06	1.44	1.52
9	K	2	FUC	C2-C3	-4.99	1.44	1.52
2	C	5	MAN	C2-C3	-4.94	1.44	1.52
5	L	3	MAN	C2-C3	-4.85	1.45	1.52
2	I	5	MAN	C2-C3	-4.80	1.45	1.52
6	G	3	BMA	C2-C3	-4.78	1.45	1.52
8	J	3	BMA	C2-C3	-4.77	1.45	1.52
3	D	3	BMA	C2-C3	-4.76	1.45	1.52
5	L	4	FUC	C2-C3	-4.76	1.45	1.52
3	D	4	FUC	C2-C3	-4.76	1.45	1.52
2	I	6	FUC	C2-C3	-4.74	1.45	1.52
5	F	4	FUC	C2-C3	-4.69	1.45	1.52
5	F	3	MAN	C2-C3	-4.69	1.45	1.52
6	G	4	XYP	O5-C1	4.59	1.51	1.43
6	G	5	BMA	C2-C3	-4.59	1.45	1.52
2	I	4	XYP	O5-C1	4.48	1.51	1.43
7	H	1	NAG	C7-N2	4.46	1.48	1.34
4	E	2	NAG	C7-N2	4.44	1.48	1.34
8	J	2	NAG	C7-N2	4.36	1.48	1.34
6	G	2	NAG	C7-N2	4.30	1.48	1.34
9	K	3	NAG	C7-N2	4.26	1.48	1.34
2	I	2	NAG	C7-N2	4.26	1.48	1.34
7	H	2	NAG	C7-N2	4.25	1.48	1.34
3	D	2	NAG	C7-N2	4.24	1.48	1.34
5	L	2	NAG	C7-N2	4.21	1.47	1.34
2	C	4	XYP	C2-C3	-4.18	1.46	1.52
6	G	1	NAG	C7-N2	4.16	1.47	1.34
5	L	1	NAG	C7-N2	4.13	1.47	1.34
9	K	1	NAG	C7-N2	4.12	1.47	1.34
8	J	1	NAG	C7-N2	4.12	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C7-N2	4.11	1.47	1.34
5	F	1	NAG	C7-N2	4.07	1.47	1.34
2	C	1	NAG	C7-N2	4.03	1.47	1.34
3	D	1	NAG	C7-N2	4.03	1.47	1.34
4	E	2	NAG	C3-C2	-4.01	1.44	1.52
2	C	4	XYP	O5-C1	4.01	1.50	1.43
2	I	1	NAG	C7-N2	4.01	1.47	1.34
2	C	2	NAG	C7-N2	4.01	1.47	1.34
5	F	2	NAG	C7-N2	3.97	1.47	1.34
2	I	4	XYP	C2-C3	-3.96	1.46	1.52
2	C	2	NAG	C3-C2	-3.94	1.44	1.52
4	E	1	NAG	C3-C2	-3.91	1.44	1.52
5	L	1	NAG	C3-C2	-3.86	1.44	1.52
6	G	1	NAG	C3-C2	-3.82	1.44	1.52
5	F	2	NAG	C3-C2	-3.81	1.44	1.52
2	I	1	NAG	C3-C2	-3.80	1.44	1.52
6	G	2	NAG	C3-C2	-3.79	1.44	1.52
2	C	1	NAG	C3-C2	-3.78	1.44	1.52
5	F	1	NAG	C3-C2	-3.76	1.44	1.52
6	G	4	XYP	C2-C3	-3.73	1.46	1.52
9	K	1	NAG	C3-C2	-3.72	1.44	1.52
9	K	3	NAG	C3-C2	-3.71	1.44	1.52
8	J	2	NAG	C3-C2	-3.70	1.44	1.52
7	H	1	NAG	C3-C2	-3.68	1.44	1.52
5	L	2	NAG	C3-C2	-3.66	1.44	1.52
8	J	1	NAG	C3-C2	-3.63	1.44	1.52
3	D	1	NAG	C3-C2	-3.60	1.45	1.52
7	H	2	NAG	C3-C2	-3.60	1.45	1.52
3	D	2	NAG	C3-C2	-3.56	1.45	1.52
2	I	2	NAG	C3-C2	-3.41	1.45	1.52
7	H	1	NAG	C2-N2	3.22	1.51	1.46
4	E	3	MAN	C4-C3	-3.04	1.44	1.52
5	F	4	FUC	C4-C3	-3.03	1.44	1.52
4	E	2	NAG	C2-N2	3.03	1.51	1.46
4	E	1	NAG	C4-C3	-3.02	1.44	1.52
8	J	4	FUL	C4-C3	-2.99	1.44	1.52
4	E	4	FUL	C4-C3	-2.96	1.44	1.52
9	K	2	FUC	C4-C3	-2.92	1.44	1.52
8	J	1	NAG	C4-C3	-2.92	1.44	1.52
2	I	2	NAG	C2-N2	2.91	1.51	1.46
8	J	2	NAG	C4-C3	-2.89	1.44	1.52
9	K	3	NAG	C2-N2	2.89	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	C2-N2	2.88	1.51	1.46
7	H	2	NAG	C2-N2	2.87	1.51	1.46
6	G	1	NAG	C4-C3	-2.84	1.45	1.52
6	G	1	NAG	C2-N2	2.82	1.50	1.46
2	I	6	FUC	C4-C3	-2.82	1.45	1.52
2	C	1	NAG	C4-C3	-2.81	1.45	1.52
8	J	1	NAG	C2-N2	2.79	1.50	1.46
3	D	2	NAG	C2-N2	2.79	1.50	1.46
9	K	3	NAG	C4-C3	-2.79	1.45	1.52
3	D	1	NAG	C4-C3	-2.79	1.45	1.52
3	D	3	BMA	C4-C3	-2.79	1.45	1.52
2	C	1	NAG	C2-N2	2.77	1.50	1.46
5	F	1	NAG	C4-C3	-2.77	1.45	1.52
9	K	1	NAG	C4-C3	-2.76	1.45	1.52
5	F	2	NAG	C4-C3	-2.76	1.45	1.52
5	L	1	NAG	C4-C3	-2.75	1.45	1.52
2	C	5	MAN	C4-C3	-2.75	1.45	1.52
6	G	3	BMA	C4-C3	-2.73	1.45	1.52
2	I	1	NAG	C4-C3	-2.72	1.45	1.52
6	G	2	NAG	C2-N2	2.72	1.50	1.46
9	K	1	NAG	C2-N2	2.72	1.50	1.46
4	E	2	NAG	C4-C3	-2.71	1.45	1.52
3	D	2	NAG	C4-C3	-2.71	1.45	1.52
4	E	1	NAG	C2-N2	2.70	1.50	1.46
5	F	3	MAN	C4-C3	-2.69	1.45	1.52
7	H	2	NAG	C4-C3	-2.68	1.45	1.52
6	G	5	BMA	C4-C3	-2.68	1.45	1.52
2	C	3	BMA	C4-C3	-2.66	1.45	1.52
5	L	3	MAN	C4-C3	-2.66	1.45	1.52
5	L	1	NAG	C2-N2	2.66	1.50	1.46
6	G	6	FUL	C4-C3	-2.66	1.45	1.52
2	C	6	FUC	C4-C3	-2.65	1.45	1.52
3	D	4	FUC	C4-C3	-2.65	1.45	1.52
5	L	4	FUC	C4-C3	-2.65	1.45	1.52
2	C	2	NAG	C4-C3	-2.65	1.45	1.52
2	I	3	BMA	C4-C3	-2.61	1.45	1.52
6	G	2	NAG	C4-C3	-2.61	1.45	1.52
7	H	1	NAG	C4-C3	-2.60	1.45	1.52
8	J	3	BMA	C4-C3	-2.58	1.45	1.52
2	C	2	NAG	C2-N2	2.55	1.50	1.46
2	I	2	NAG	C4-C3	-2.55	1.45	1.52
5	F	2	NAG	C2-N2	2.54	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2	NAG	C2-N2	2.53	1.50	1.46
5	L	2	NAG	C4-C3	-2.53	1.45	1.52
8	J	2	NAG	C2-N2	2.52	1.50	1.46
2	I	5	MAN	C4-C3	-2.42	1.46	1.52
2	I	4	XYP	C4-C3	-2.41	1.48	1.52
2	C	2	NAG	C1-C2	-2.24	1.49	1.52
3	D	1	NAG	C2-N2	2.20	1.49	1.46
2	C	4	XYP	C4-C3	-2.17	1.49	1.52
6	G	4	XYP	C4-C3	-2.16	1.49	1.52
5	L	2	NAG	O3-C3	2.15	1.48	1.43
5	F	1	NAG	C2-N2	2.10	1.49	1.46
5	L	2	NAG	C1-C2	-2.08	1.49	1.52
5	F	2	NAG	O3-C3	2.08	1.48	1.43
2	I	2	NAG	O3-C3	2.03	1.48	1.43
7	H	2	NAG	O3-C3	2.03	1.48	1.43
3	D	2	NAG	O3-C3	2.00	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C2-N2-C7	-4.06	117.46	122.90
4	E	1	NAG	C1-O5-C5	-3.80	107.09	112.19
2	C	2	NAG	C2-N2-C7	-3.78	117.83	122.90
8	J	2	NAG	C2-N2-C7	-3.64	118.02	122.90
5	F	2	NAG	C2-N2-C7	-3.62	118.05	122.90
5	L	1	NAG	C2-N2-C7	-3.59	118.09	122.90
9	K	1	NAG	C2-N2-C7	-3.49	118.22	122.90
2	I	2	NAG	C4-C3-C2	3.29	115.84	111.02
4	E	1	NAG	C8-C7-N2	3.18	121.39	116.12
5	L	1	NAG	C1-O5-C5	3.06	116.29	112.19
9	K	3	NAG	C2-N2-C7	-2.93	118.98	122.90
2	I	2	NAG	C8-C7-N2	2.91	120.94	116.12
2	C	1	NAG	C2-N2-C7	-2.86	119.07	122.90
5	F	4	FUC	C6-C5-C4	-2.75	108.04	113.08
5	F	2	NAG	C1-O5-C5	-2.70	108.57	112.19
5	L	3	MAN	C1-C2-C3	2.68	113.54	109.64
8	J	2	NAG	C8-C7-N2	2.66	120.53	116.12
6	G	1	NAG	C2-N2-C7	-2.64	119.36	122.90
4	E	4	FUL	O5-C5-C6	2.63	113.11	107.40
4	E	2	NAG	C8-C7-N2	2.54	120.33	116.12
9	K	1	NAG	C8-C7-N2	2.54	120.33	116.12
2	I	2	NAG	C2-N2-C7	-2.53	119.51	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	2	NAG	C3-C4-C5	2.50	114.76	110.23
2	C	2	NAG	C8-C7-N2	2.47	120.21	116.12
7	H	1	NAG	C8-C7-N2	2.43	120.15	116.12
2	I	4	XYP	C5-C4-C3	2.41	113.15	109.64
8	J	1	NAG	C8-C7-N2	2.39	120.08	116.12
9	K	3	NAG	C8-C7-N2	2.36	120.03	116.12
8	J	4	FUL	O5-C5-C6	2.35	112.50	107.40
8	J	1	NAG	C1-O5-C5	-2.33	109.06	112.19
5	L	1	NAG	C8-C7-N2	2.33	119.98	116.12
5	L	1	NAG	O6-C6-C5	2.32	119.22	111.33
2	C	4	XYP	C5-C4-C3	2.32	113.02	109.64
6	G	4	XYP	C1-C2-C3	2.31	113.01	109.64
2	I	1	NAG	O5-C5-C6	2.31	112.15	107.66
6	G	1	NAG	C4-C3-C2	2.29	114.38	111.02
6	G	2	NAG	C2-N2-C7	-2.26	119.87	122.90
5	F	1	NAG	C8-C7-N2	2.26	119.87	116.12
7	H	2	NAG	C8-C7-N2	2.20	119.76	116.12
2	I	4	XYP	C4-C3-C2	2.18	113.51	110.92
5	L	2	NAG	C1-C2-N2	-2.18	106.99	110.43
2	I	2	NAG	O6-C6-C5	2.17	118.73	111.33
5	L	1	NAG	O5-C1-C2	2.17	114.65	111.29
6	G	1	NAG	C3-C4-C5	2.16	114.15	110.23
6	G	1	NAG	C8-C7-N2	2.16	119.70	116.12
5	F	4	FUC	C1-C2-C3	2.15	112.77	109.64
6	G	2	NAG	C8-C7-N2	2.15	119.68	116.12
5	F	2	NAG	C8-C7-N2	2.14	119.67	116.12
5	L	3	MAN	O6-C6-C5	2.12	118.54	111.33
4	E	2	NAG	C2-N2-C7	-2.11	120.07	122.90
7	H	2	NAG	O6-C6-C5	2.10	118.50	111.33
2	I	1	NAG	C8-C7-N2	2.10	119.60	116.12
6	G	5	BMA	C1-C2-C3	2.09	112.69	109.64
2	C	1	NAG	C8-C7-N2	2.09	119.59	116.12
8	J	3	BMA	C1-C2-C3	2.07	112.66	109.64
7	H	2	NAG	C4-C3-C2	2.06	114.04	111.02
5	F	3	MAN	C1-C2-C3	2.05	112.63	109.64
2	I	2	NAG	O7-C7-N2	-2.04	118.38	121.98
5	L	4	FUC	C6-C5-C4	-2.03	109.36	113.08

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	2	NAG	C1

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Mol	Chain	Res	Type	Atom
2	I	5	MAN	C1
3	D	3	BMA	C1
5	L	1	NAG	C1
6	G	2	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	3	MAN	C4-C5-C6-O6
5	L	3	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
4	E	3	MAN	O5-C5-C6-O6
6	G	3	BMA	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
8	J	3	BMA	C4-C5-C6-O6
6	G	3	BMA	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
8	J	3	BMA	O5-C5-C6-O6
2	I	5	MAN	O5-C5-C6-O6
4	E	3	MAN	C4-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
8	J	2	NAG	C3-C2-N2-C7
2	I	5	MAN	C4-C5-C6-O6
8	J	2	NAG	C1-C2-N2-C7

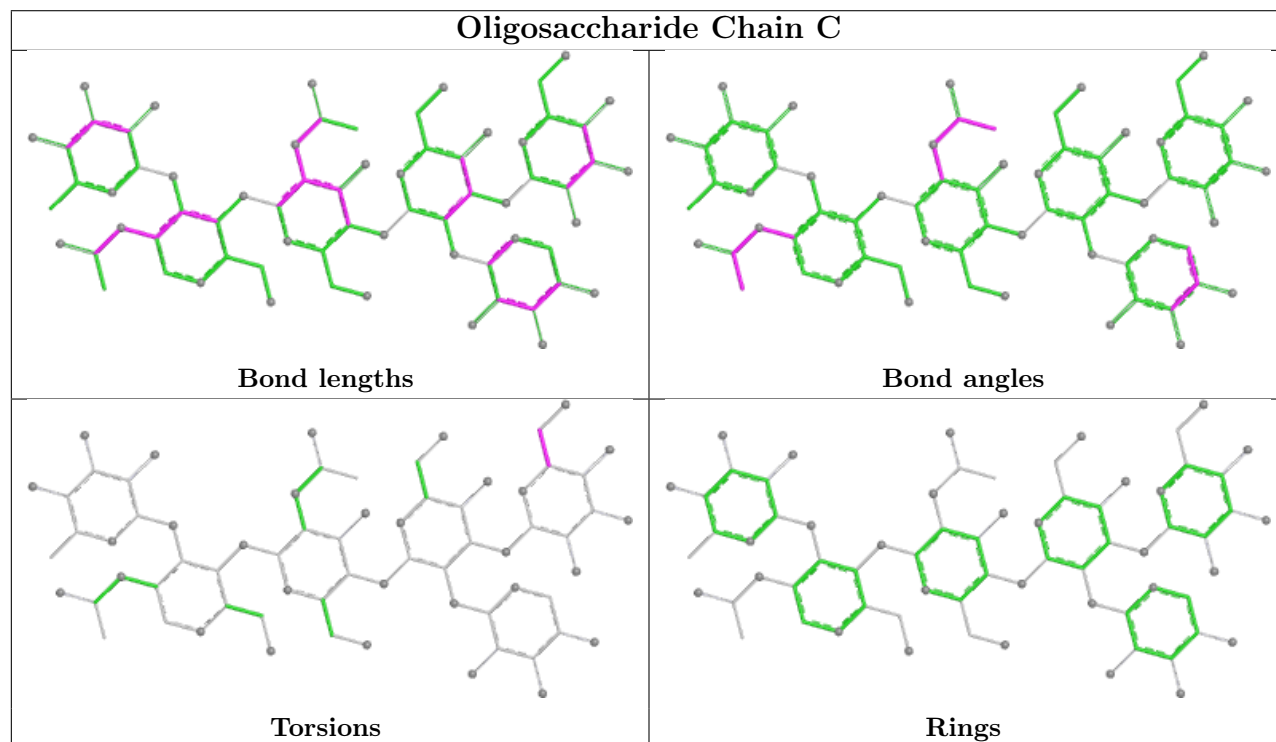
All (2) ring outliers are listed below:

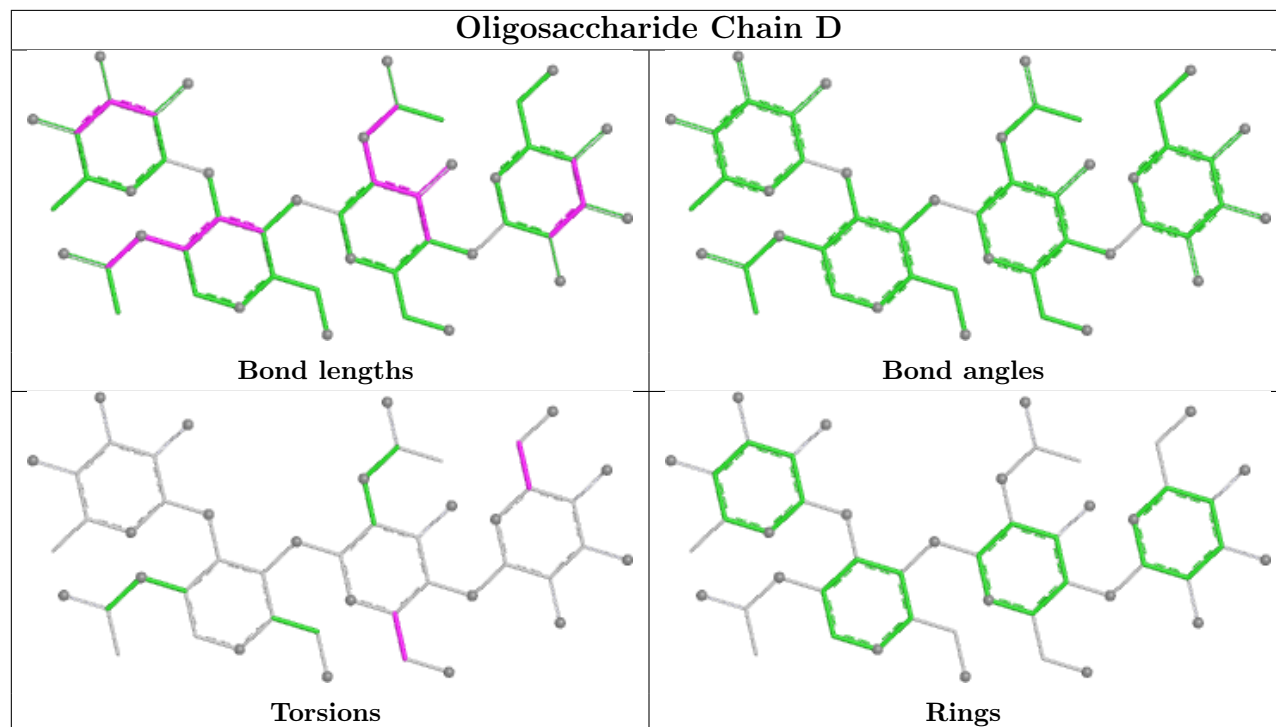
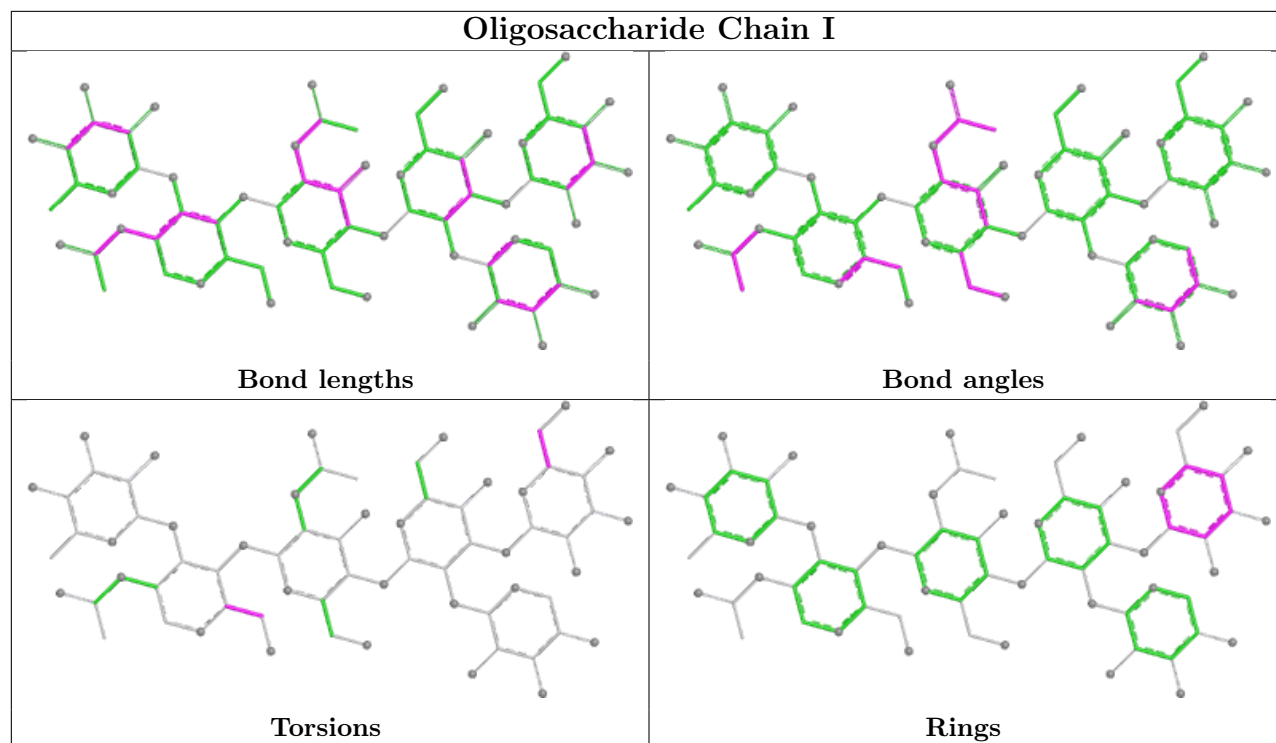
Mol	Chain	Res	Type	Atoms
6	G	5	BMA	C1-C2-C3-C4-C5-O5
2	I	5	MAN	C1-C2-C3-C4-C5-O5

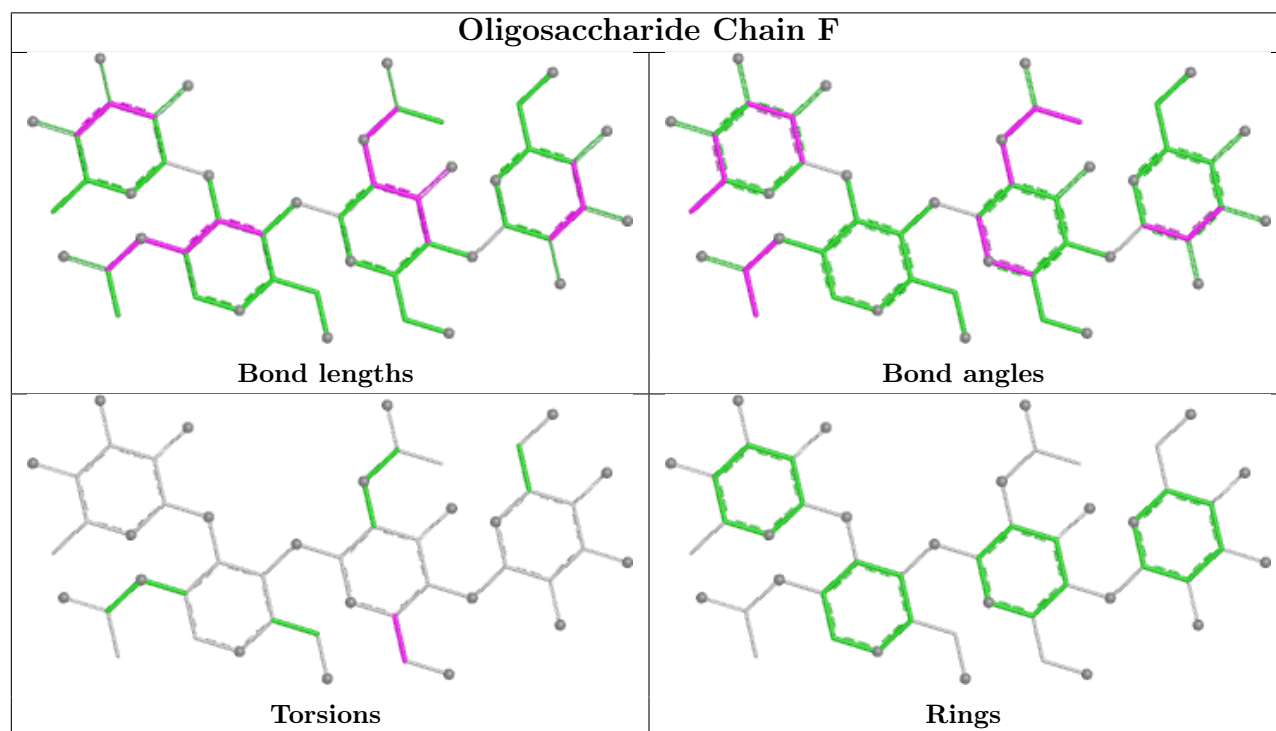
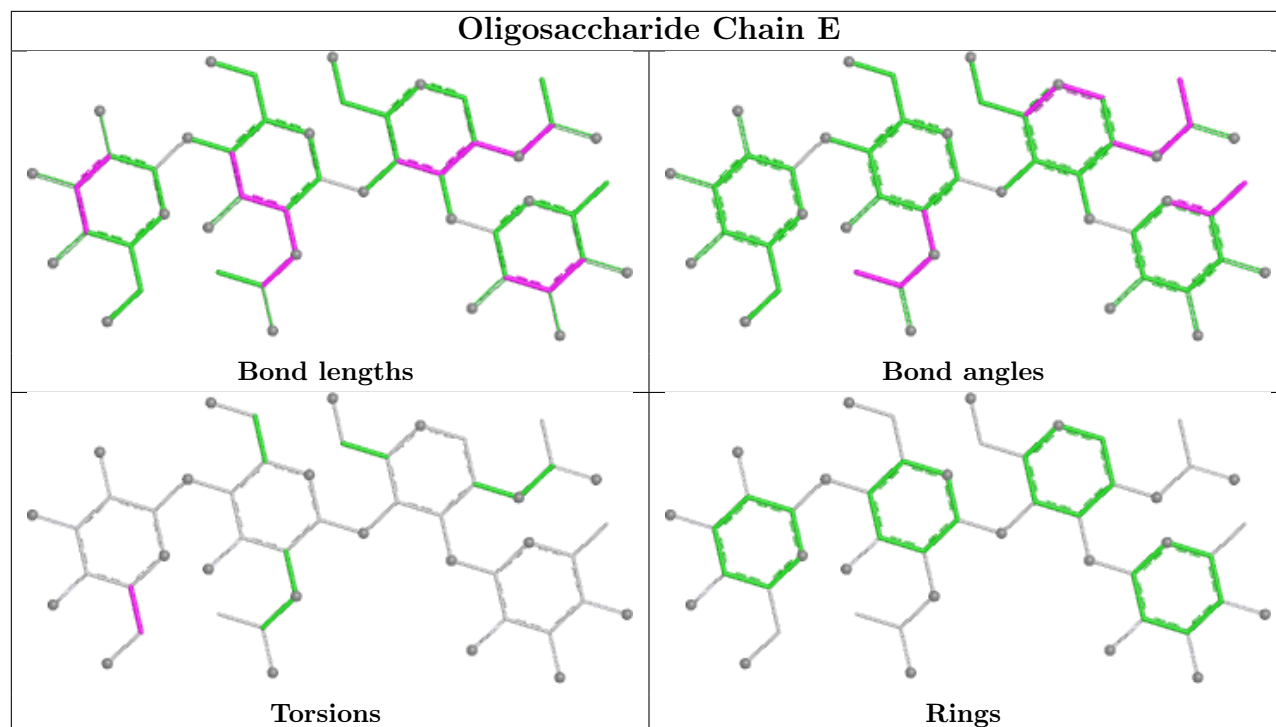
16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	5	BMA	1	0
2	C	4	XYP	5	0
5	F	2	NAG	1	0
5	F	4	FUC	0	1
4	E	3	MAN	1	0
2	I	5	MAN	4	0
4	E	1	NAG	1	0
4	E	4	FUL	1	0
2	I	2	NAG	1	0
5	L	4	FUC	1	0
5	F	1	NAG	1	0
5	F	3	MAN	1	0
5	L	2	NAG	1	0
8	J	2	NAG	2	0
8	J	3	BMA	2	0
2	C	5	MAN	1	0

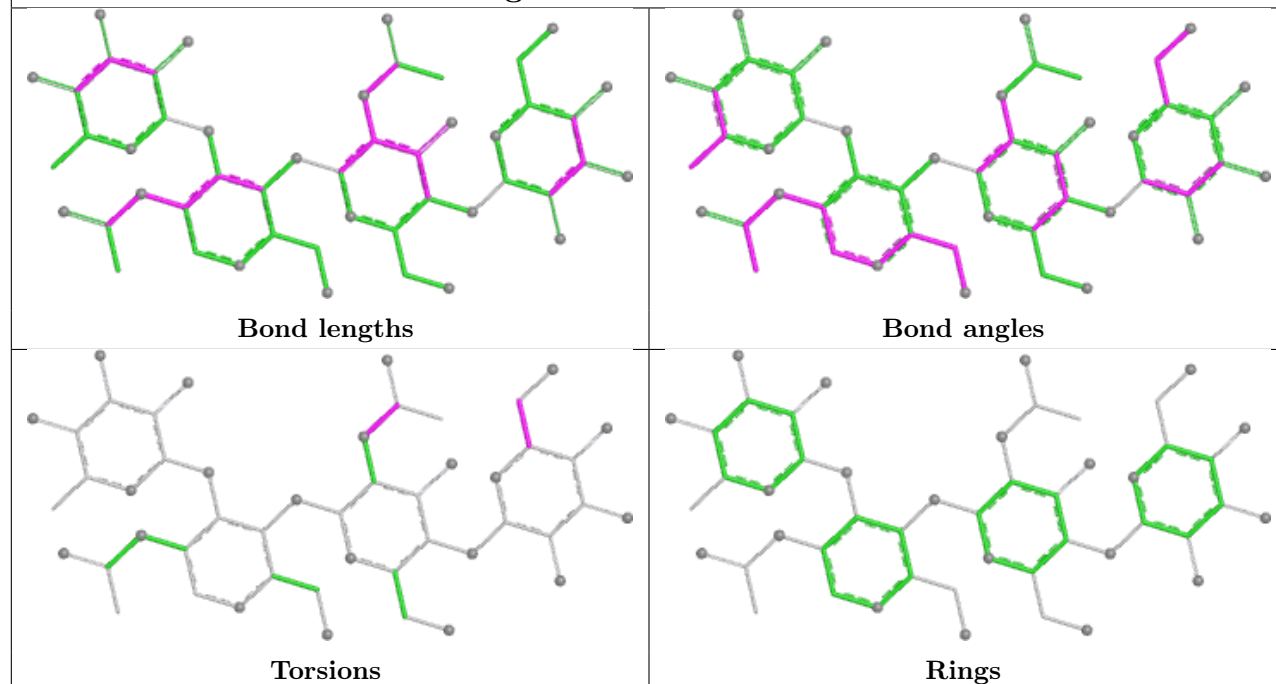
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



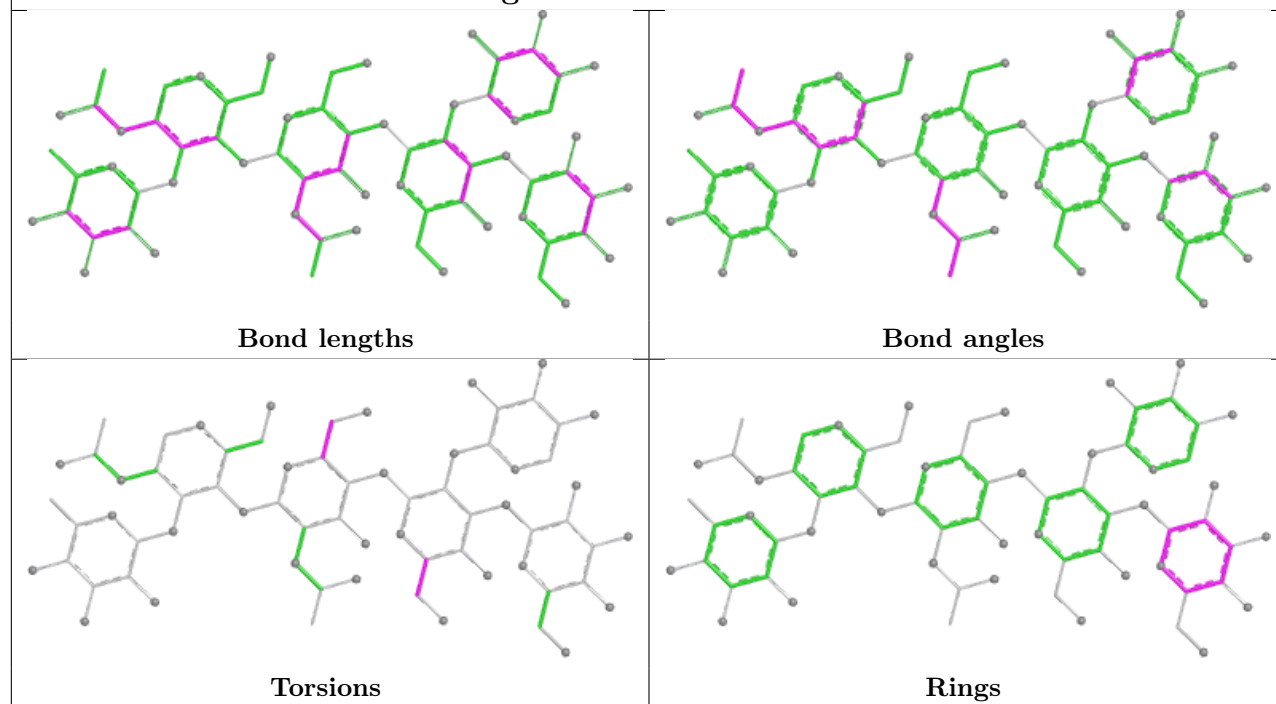


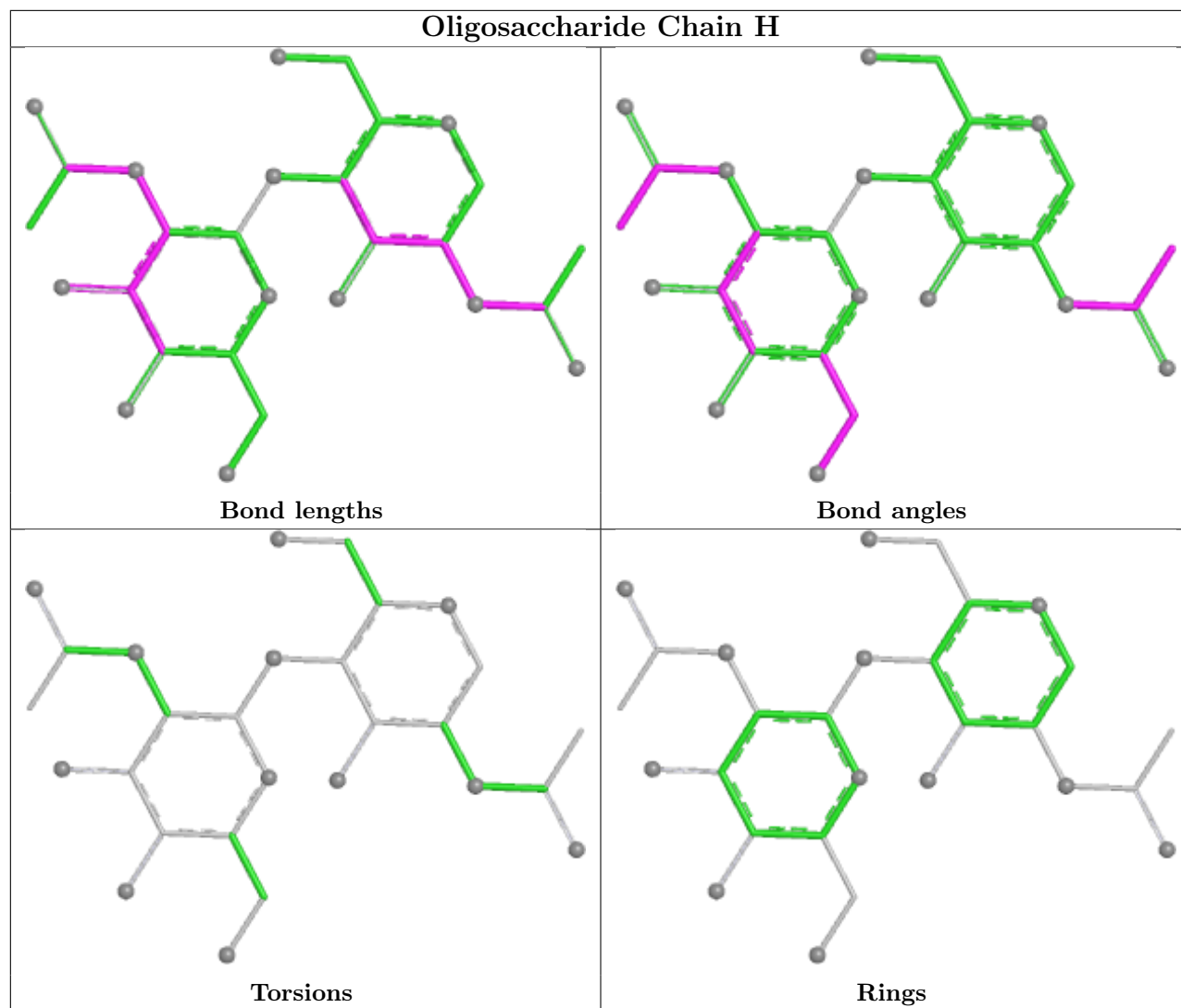


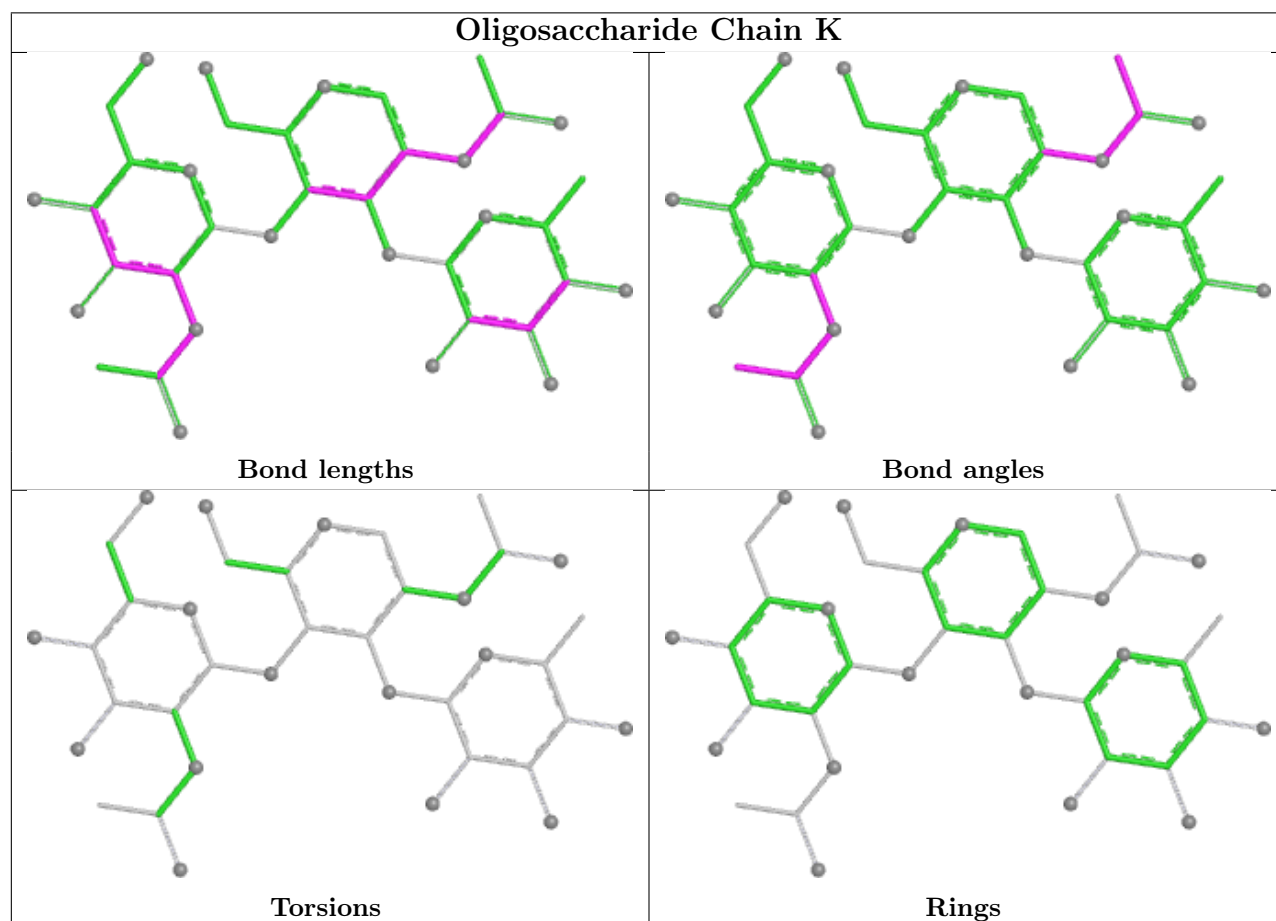
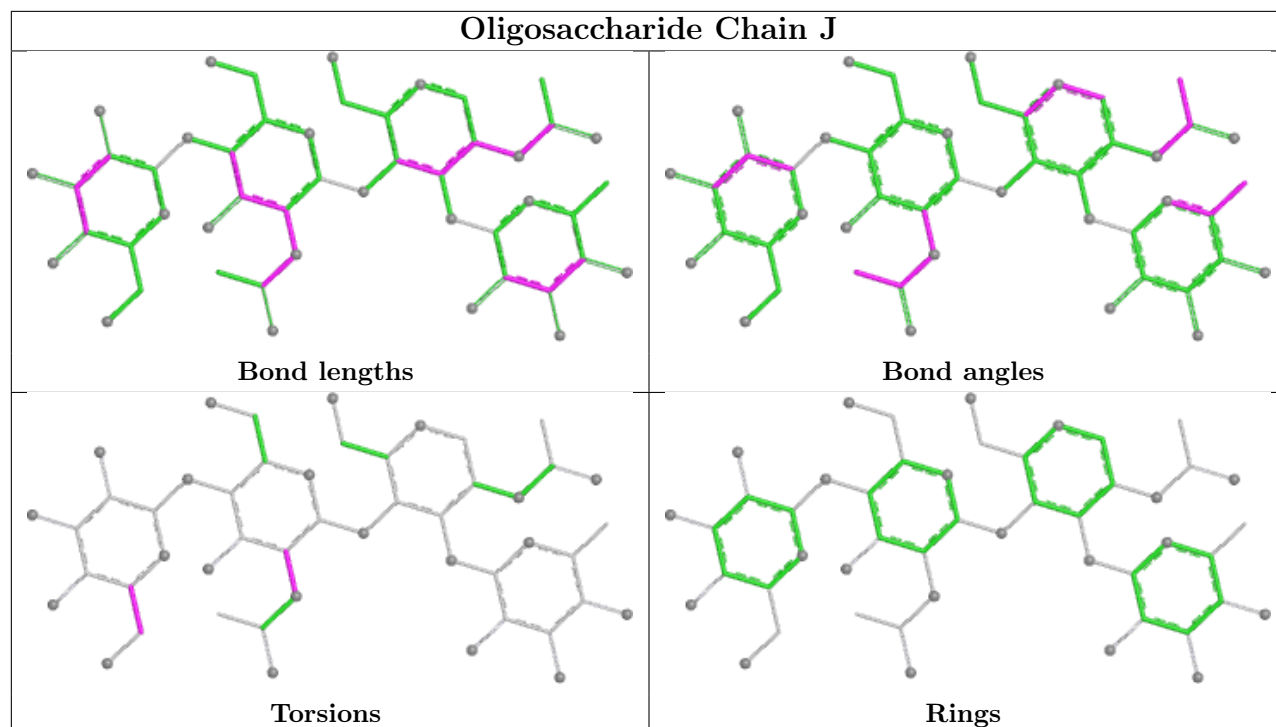
Oligosaccharide Chain L



Oligosaccharide Chain G







5.6 Ligand geometry

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	HEM	B	1306	1	50,50,50	1.95	7 (14%)	67,82,82	1.45	7 (10%)
12	NAG	B	1327	1	14,14,15	1.99	4 (28%)	17,19,21	1.34	3 (17%)
13	1PE	A	1338	-	9,9,15	0.65	0	8,8,14	1.47	0
13	1PE	B	1332	-	4,4,15	0.53	0	3,3,14	0.88	0
13	1PE	B	1333	-	5,5,15	0.56	0	4,4,14	1.23	0
13	1PE	A	1337	-	4,4,15	0.55	0	3,3,14	0.79	0
13	1PE	B	1334	-	4,4,15	0.58	0	3,3,14	0.72	0
12	NAG	B	1326	1	14,14,15	1.97	5 (35%)	17,19,21	1.30	3 (17%)
13	1PE	B	1329	-	14,14,15	0.64	0	13,13,14	1.60	1 (7%)
14	PG0	B	1331	-	7,7,7	0.35	0	6,6,6	0.60	0
12	NAG	B	1328	1	14,14,15	1.98	4 (28%)	17,19,21	1.36	2 (11%)
10	HEM	A	1307	1	50,50,50	2.00	9 (18%)	67,82,82	1.43	5 (7%)
13	1PE	B	1330	-	15,15,15	0.67	0	14,14,14	1.60	1 (7%)
12	NAG	A	1336	-	14,14,15	2.15	5 (35%)	17,19,21	1.26	1 (5%)

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
10	HEM	B	1306	1	-	1/14/54/54	-
12	NAG	B	1327	1	-	3/6/23/26	0/1/1/1
13	1PE	A	1338	-	-	1/7/7/13	-
13	1PE	B	1332	-	-	1/2/2/13	-
13	1PE	B	1333	-	-	2/3/3/13	-
13	1PE	A	1337	-	-	2/2/2/13	-
13	1PE	B	1334	-	-	1/2/2/13	-
12	NAG	B	1326	1	1/1/5/7	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	1PE	B	1329	-	-	7/12/12/13	-
14	PG0	B	1331	-	-	4/5/5/5	-
12	NAG	B	1328	1	1/1/5/7	2/6/23/26	0/1/1/1
10	HEM	A	1307	1	-	2/14/54/54	-
13	1PE	B	1330	-	-	6/13/13/13	-
12	NAG	A	1336	-	-	2/6/23/26	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1307	HEM	C3D-C2D	7.81	1.53	1.36
10	B	1306	HEM	C3D-C2D	7.68	1.53	1.36
10	A	1307	HEM	FE-NB	5.97	2.13	1.94
10	B	1306	HEM	FE-NB	5.31	2.11	1.94
10	A	1307	HEM	FE-NC	4.51	2.10	1.95
12	B	1327	NAG	C7-N2	4.44	1.48	1.34
12	A	1336	NAG	C7-N2	4.43	1.48	1.34
12	B	1326	NAG	C7-N2	4.30	1.48	1.34
10	B	1306	HEM	FE-NA	4.21	2.09	1.95
12	B	1328	NAG	C7-N2	4.18	1.47	1.34
10	B	1306	HEM	FE-ND	4.17	2.07	1.94
10	A	1307	HEM	FE-ND	4.11	2.07	1.94
12	A	1336	NAG	C3-C2	-4.06	1.44	1.52
12	B	1328	NAG	C3-C2	-3.84	1.44	1.52
12	B	1326	NAG	C3-C2	-3.49	1.45	1.52
12	B	1327	NAG	C3-C2	-3.48	1.45	1.52
12	B	1327	NAG	C2-N2	3.15	1.51	1.46
10	B	1306	HEM	FE-NC	3.13	2.05	1.95
10	B	1306	HEM	CAC-C3C	3.13	1.55	1.47
10	B	1306	HEM	CAB-C3B	2.98	1.55	1.47
10	A	1307	HEM	CAC-C3C	2.97	1.55	1.47
12	A	1336	NAG	C4-C3	-2.97	1.44	1.52
12	B	1326	NAG	C2-N2	2.93	1.51	1.46
12	A	1336	NAG	C2-N2	2.93	1.51	1.46
10	A	1307	HEM	FE-NA	2.88	2.04	1.95
12	B	1328	NAG	C4-C3	-2.84	1.45	1.52
12	B	1326	NAG	C4-C3	-2.71	1.45	1.52
10	A	1307	HEM	CAB-C3B	2.60	1.54	1.47
12	B	1328	NAG	C2-N2	2.55	1.50	1.46
12	B	1327	NAG	C4-C3	-2.50	1.45	1.52
10	A	1307	HEM	CMA-C3A	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1326	NAG	O3-C3	2.10	1.48	1.43
12	A	1336	NAG	O3-C3	2.09	1.48	1.43
10	A	1307	HEM	CMC-C2C	2.00	1.54	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1307	HEM	C4D-ND-C1D	5.48	111.70	105.21
10	B	1306	HEM	C4D-ND-C1D	5.27	111.44	105.21
10	A	1307	HEM	CBD-CAD-C3D	-4.13	101.11	112.53
10	B	1306	HEM	CBD-CAD-C3D	-4.06	101.32	112.53
12	B	1328	NAG	C2-N2-C7	-3.54	118.15	122.90
12	A	1336	NAG	C8-C7-N2	3.29	121.58	116.12
12	B	1327	NAG	C4-C3-C2	2.87	115.23	111.02
10	B	1306	HEM	C1B-NB-C4B	2.72	108.43	105.21
10	B	1306	HEM	C3B-C2B-C1B	2.67	108.42	106.41
10	B	1306	HEM	C3B-C4B-NB	-2.67	107.55	109.47
12	B	1328	NAG	C8-C7-N2	2.50	120.26	116.12
12	B	1326	NAG	C8-C7-N2	2.49	120.25	116.12
10	A	1307	HEM	C1B-NB-C4B	2.45	108.11	105.21
12	B	1326	NAG	C2-N2-C7	-2.40	119.69	122.90
10	A	1307	HEM	C3B-C2B-C1B	2.30	108.14	106.41
10	A	1307	HEM	C3B-C4B-NB	-2.26	107.85	109.47
13	B	1329	1PE	C22-OH3-C23	2.22	120.86	113.06
12	B	1327	NAG	C3-C4-C5	2.18	114.19	110.23
10	B	1306	HEM	CHD-C1D-ND	2.16	126.74	124.42
10	B	1306	HEM	C2A-C1A-NA	-2.13	107.79	110.15
12	B	1326	NAG	C4-C3-C2	2.06	114.03	111.02
12	B	1327	NAG	C8-C7-N2	2.01	119.45	116.12
13	B	1330	1PE	OH5-C14-C24	2.00	119.47	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	1326	NAG	C1
12	B	1328	NAG	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	1327	NAG	C1-C2-N2-C7
12	B	1327	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	B	1327	NAG	C4-C5-C6-O6
12	B	1328	NAG	O5-C5-C6-O6
14	B	1331	PG0	O1-C3-C4-O2
13	B	1329	1PE	OH5-C14-C24-OH4
13	B	1329	1PE	OH6-C15-C25-OH5
13	B	1334	1PE	OH4-C13-C23-OH3
13	A	1338	1PE	C23-C13-OH4-C24
12	A	1336	NAG	C8-C7-N2-C2
12	A	1336	NAG	O7-C7-N2-C2
13	B	1330	1PE	OH2-C12-C22-OH3
12	B	1328	NAG	C4-C5-C6-O6
14	B	1331	PG0	OTT-C1-C2-O1
12	B	1326	NAG	O5-C5-C6-O6
13	B	1329	1PE	OH7-C16-C26-OH6
13	B	1329	1PE	OH4-C13-C23-OH3
13	B	1330	1PE	OH7-C16-C26-OH6
13	B	1329	1PE	C12-C22-OH3-C23
13	B	1329	1PE	C16-C26-OH6-C15
14	B	1331	PG0	C3-C4-O2-C5
14	B	1331	PG0	C1-C2-O1-C3
13	B	1333	1PE	C13-C23-OH3-C22
13	B	1333	1PE	OH4-C13-C23-OH3
13	A	1337	1PE	C13-C23-OH3-C22
13	B	1329	1PE	C25-C15-OH6-C26
13	B	1330	1PE	C23-C13-OH4-C24
13	B	1330	1PE	C15-C25-OH5-C14
10	A	1307	HEM	CAD-CBD-CGD-O2D
13	B	1332	1PE	C13-C23-OH3-C22
10	A	1307	HEM	CAD-CBD-CGD-O1D
13	A	1337	1PE	OH4-C13-C23-OH3
13	B	1330	1PE	C13-C23-OH3-C22
13	B	1330	1PE	OH5-C14-C24-OH4
10	B	1306	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1306	HEM	2	0
12	B	1327	NAG	1	0
13	B	1333	1PE	3	0
13	A	1337	1PE	6	0

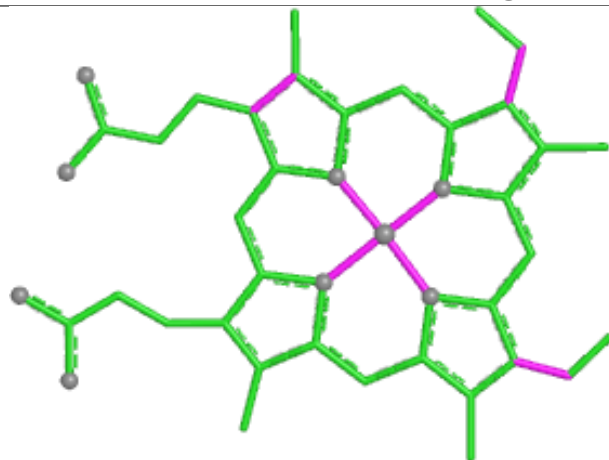
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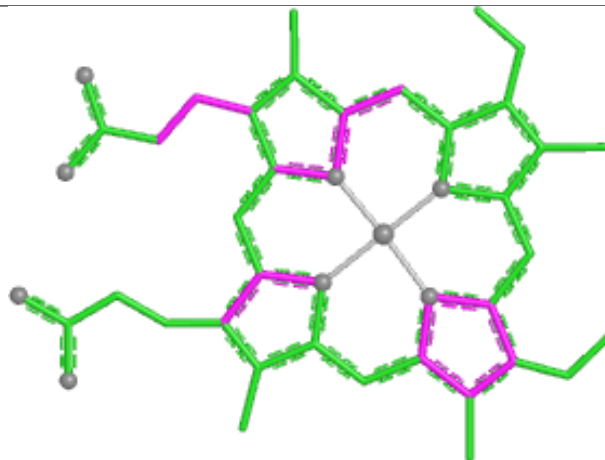
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1334	1PE	3	0
12	B	1326	NAG	1	0
14	B	1331	PG0	1	0
10	A	1307	HEM	2	0
13	B	1330	1PE	8	0
12	A	1336	NAG	2	0

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 than 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.

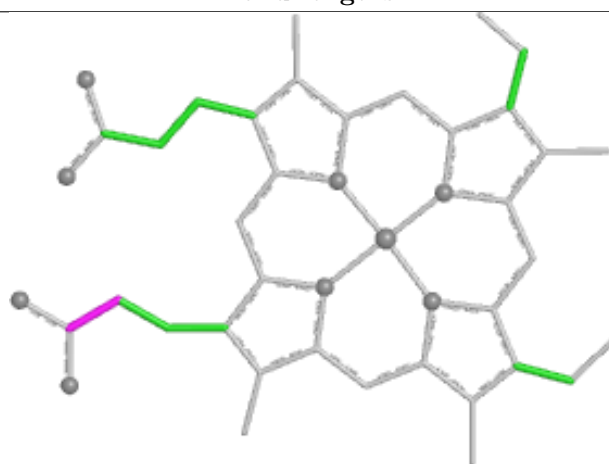
Ligand HEM B 1306



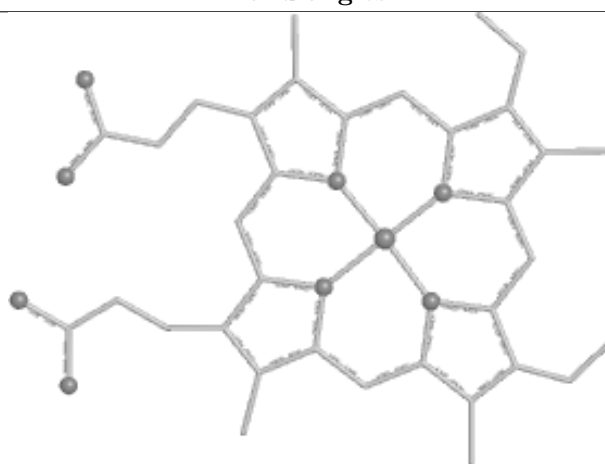
Bond lengths



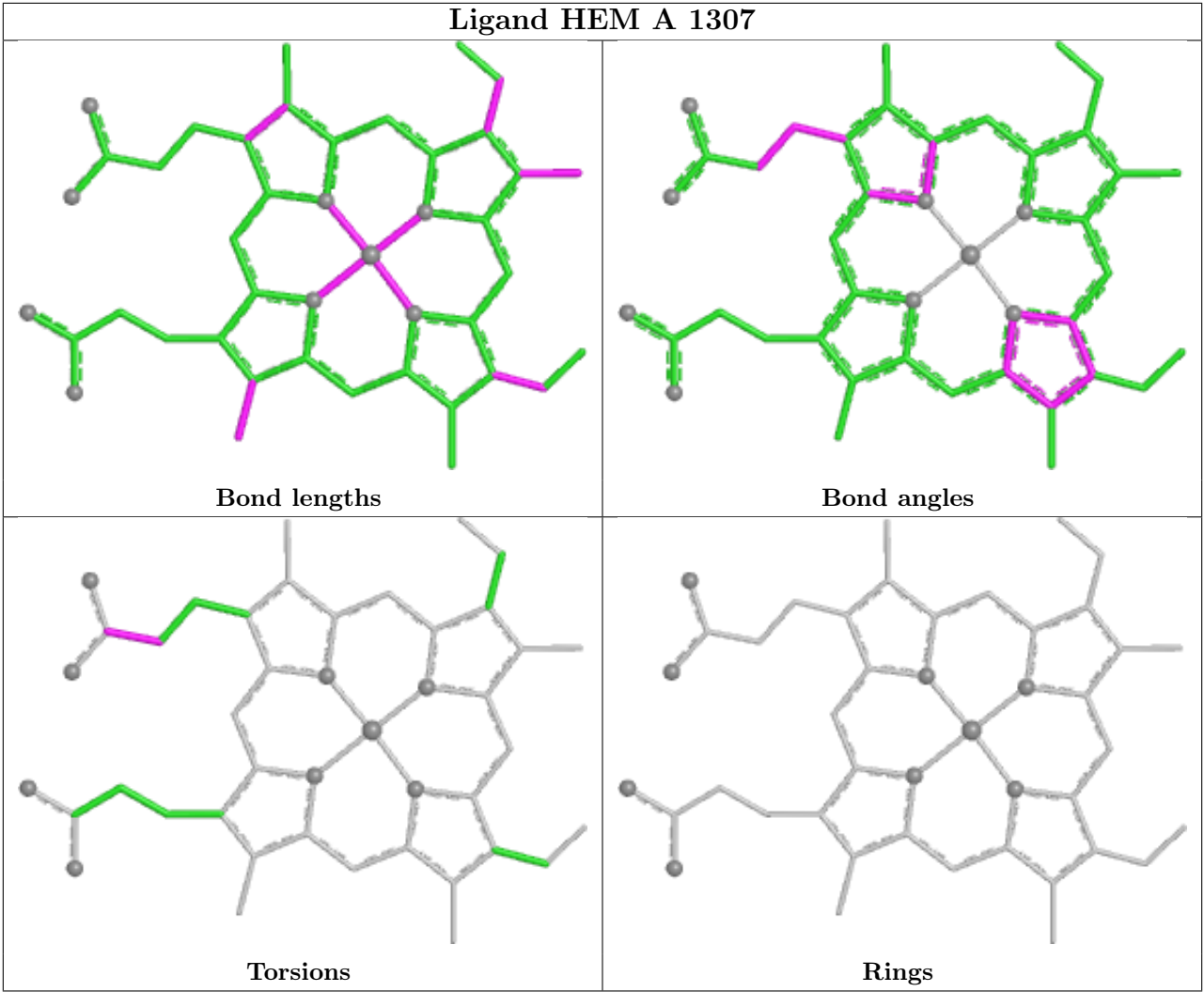
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	91:ASN	C	92:ALA	N	1.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	90:GLU	C	91:ASN	N	1.13
1	B	91:ASN	C	92:ALA	N	1.08

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	307/308 (99%)	-0.58	2 (0%) 84 85	10, 23, 35, 50	7 (2%)
1	B	307/308 (99%)	-0.52	4 (1%) 75 76	14, 25, 41, 67	5 (1%)
All	All	614/616 (99%)	-0.55	6 (0%) 79 81	10, 24, 38, 67	12 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	ASN	3.1
1	A	308	GLY	2.8
1	B	1	GLY	2.6
1	B	91	ASN	2.5
1	B	214	GLY	2.5
1	B	215	ARG	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	L	3	11/12	0.39	0.15	73,77,80,86	0
9	FUC	K	2	10/11	0.53	0.14	66,71,77,82	0
7	NAG	H	1	14/15	0.64	0.13	52,61,67,72	0

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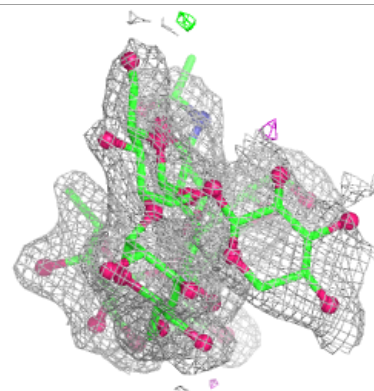
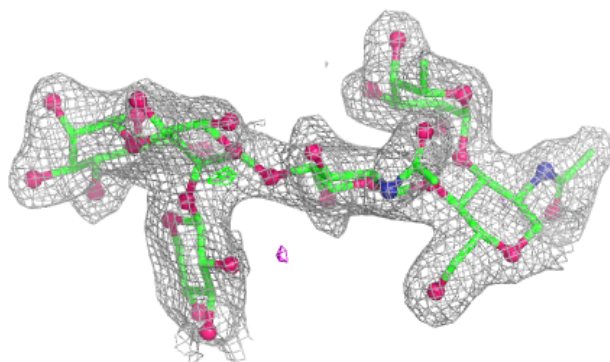
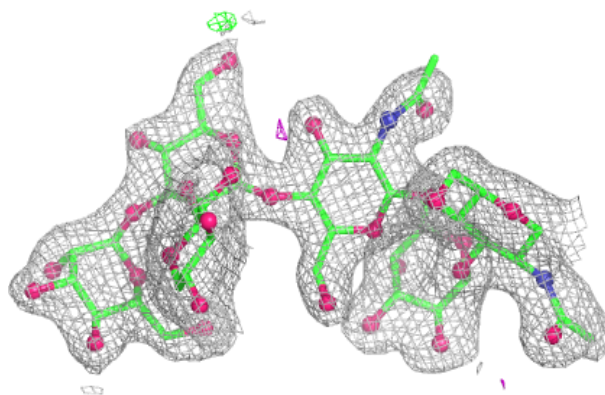
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	E	3	11/12	0.64	0.13	55,63,71,72	0
8	BMA	J	3	11/12	0.71	0.11	52,63,67,68	0
6	FUL	G	6	10/11	0.72	0.13	59,63,68,69	0
7	NAG	H	2	14/15	0.72	0.11	57,72,88,88	0
6	BMA	G	5	11/12	0.73	0.12	55,60,65,70	0
9	NAG	K	3	14/15	0.73	0.11	60,71,82,86	0
3	BMA	D	3	11/12	0.74	0.12	61,70,75,78	0
8	FUL	J	4	10/11	0.75	0.14	30,41,53,55	0
6	XYP	G	4	9/10	0.75	0.10	56,64,70,70	0
5	FUC	L	4	10/11	0.75	0.12	56,64,71,77	0
5	MAN	F	3	11/12	0.79	0.10	47,56,60,61	0
2	MAN	I	5	11/12	0.80	0.13	43,50,61,63	0
4	FUL	E	4	10/11	0.80	0.14	30,43,51,57	0
6	NAG	G	1	14/15	0.81	0.11	47,53,60,62	0
2	BMA	I	3	11/12	0.81	0.11	52,60,67,70	0
2	NAG	I	2	14/15	0.82	0.11	29,52,59,61	0
6	NAG	G	2	14/15	0.82	0.11	52,60,66,68	0
6	BMA	G	3	11/12	0.82	0.10	58,61,64,64	0
5	NAG	L	1	14/15	0.83	0.11	37,50,58,60	0
2	XYP	I	4	9/10	0.84	0.11	41,47,52,56	0
9	NAG	K	1	14/15	0.84	0.09	46,56,64,66	0
8	NAG	J	2	14/15	0.86	0.12	32,48,53,60	0
5	NAG	L	2	14/15	0.87	0.10	36,50,60,63	0
3	NAG	D	2	14/15	0.89	0.10	36,51,63,75	0
2	XYP	C	4	9/10	0.89	0.09	35,44,49,49	0
3	FUC	D	4	10/11	0.89	0.10	39,48,50,52	0
4	NAG	E	2	14/15	0.90	0.09	32,42,49,53	0
5	FUC	F	4	10/11	0.90	0.08	28,37,41,49	0
2	FUC	I	6	10/11	0.91	0.09	30,37,42,43	0
2	BMA	C	3	11/12	0.91	0.07	42,44,49,56	0
2	NAG	I	1	14/15	0.91	0.10	23,32,49,51	0
2	NAG	C	2	14/15	0.92	0.09	31,38,41,44	0
5	NAG	F	2	14/15	0.92	0.08	31,37,46,49	0
3	NAG	D	1	14/15	0.94	0.07	29,36,40,48	0
4	NAG	E	1	14/15	0.94	0.07	21,28,33,38	0
8	NAG	J	1	14/15	0.94	0.07	23,30,35,37	0
2	MAN	C	5	11/12	0.95	0.06	32,36,39,44	0
5	NAG	F	1	14/15	0.95	0.07	25,30,35,40	0
2	FUC	C	6	10/11	0.96	0.06	26,31,33,35	0
2	NAG	C	1	14/15	0.96	0.06	25,27,32,37	0

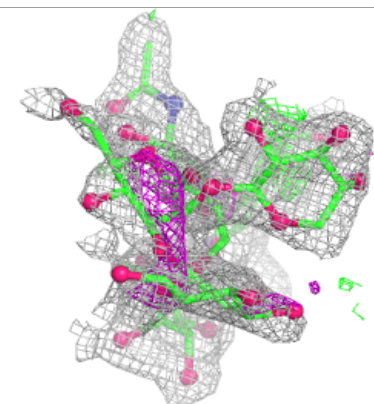
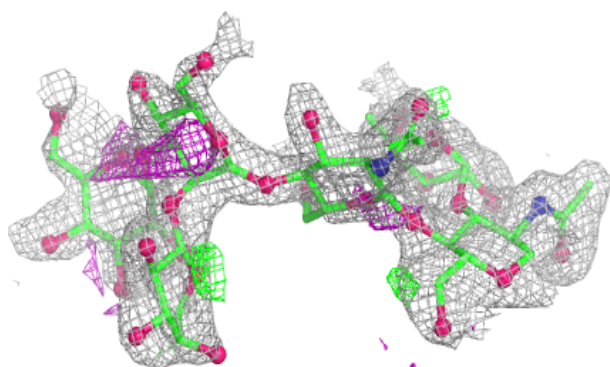
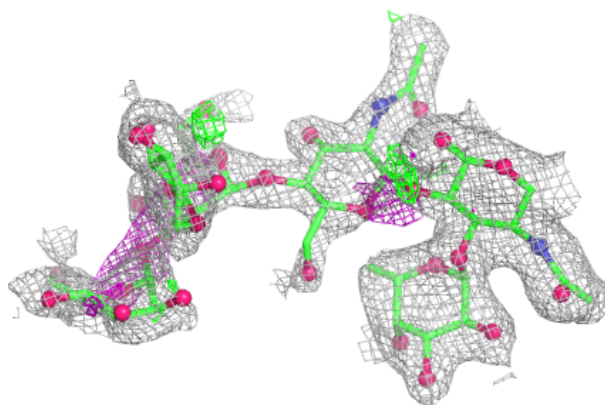
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

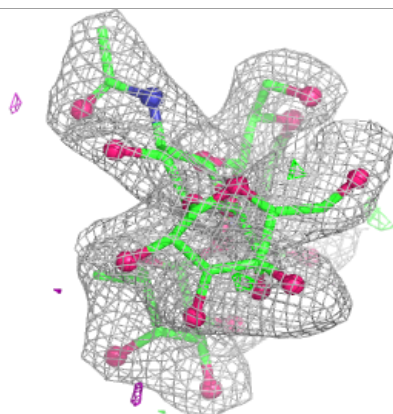
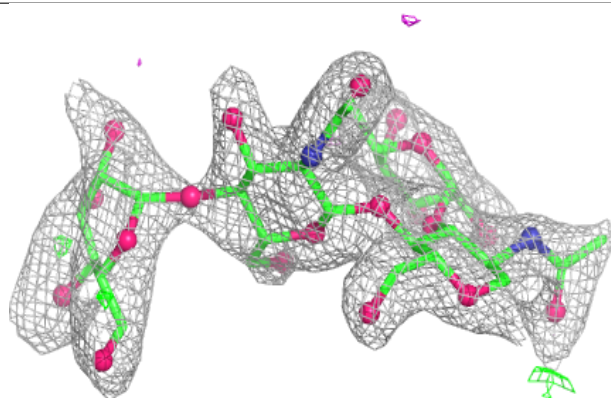
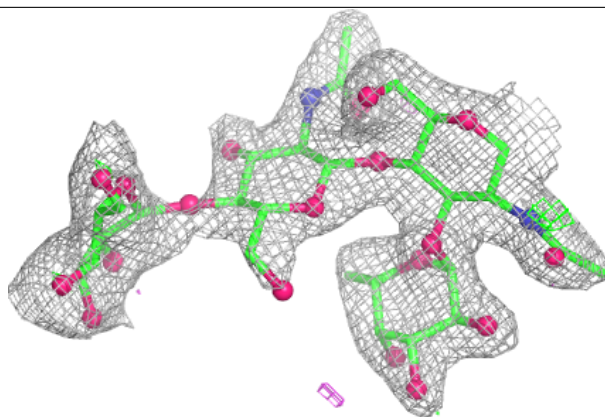
**Electron density around Chain I:**

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

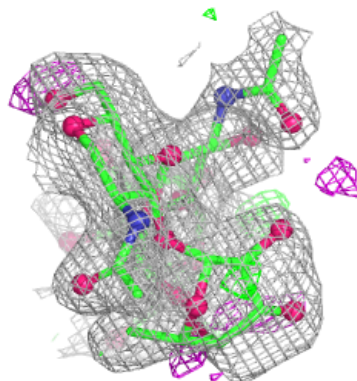
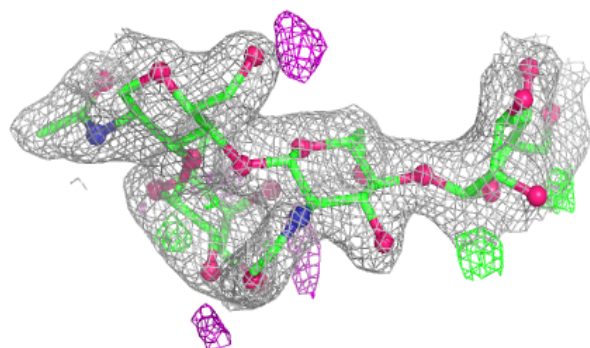
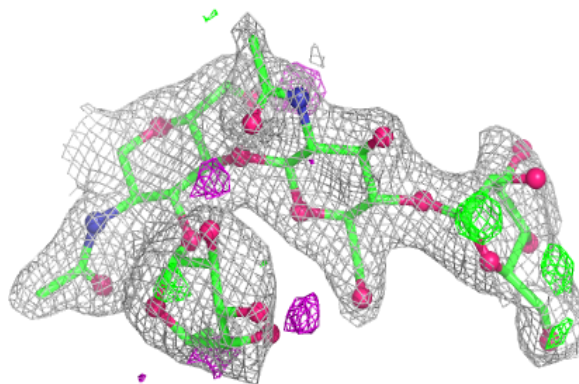


Electron density around Chain D:

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

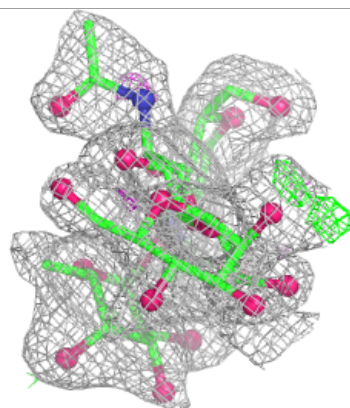
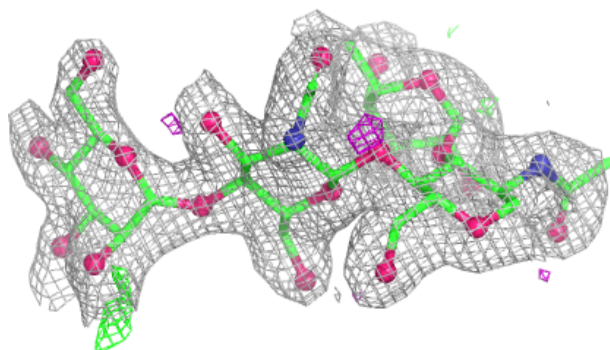
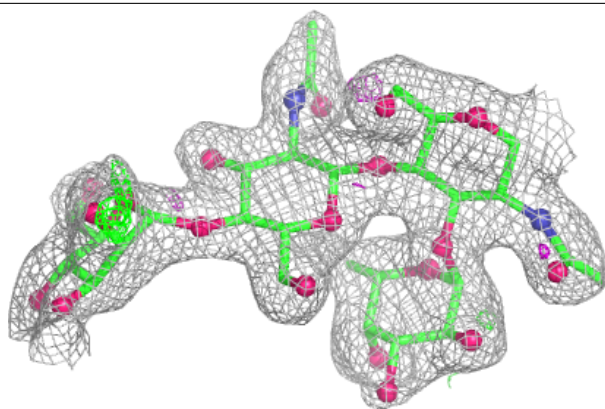
**Electron density around Chain E:**

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

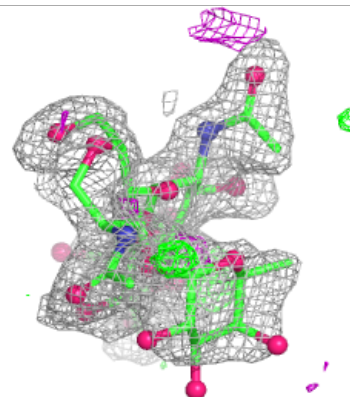
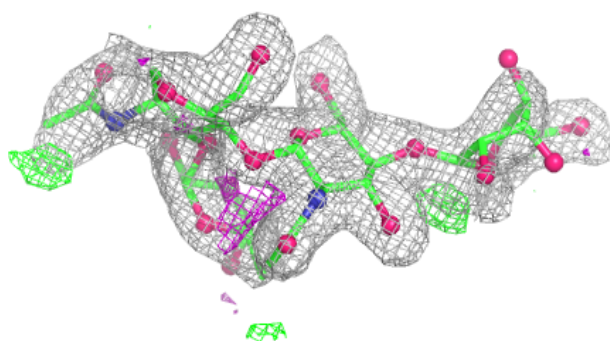
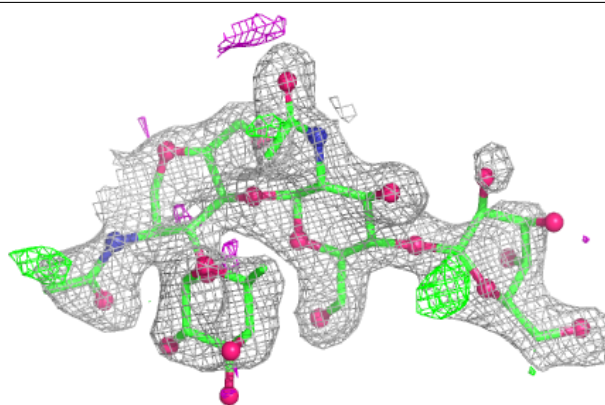


Electron density around Chain F:

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

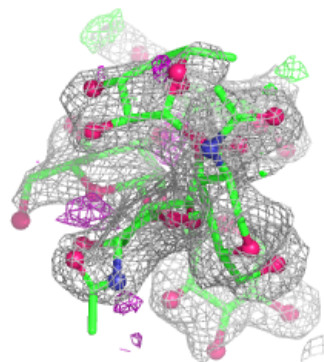
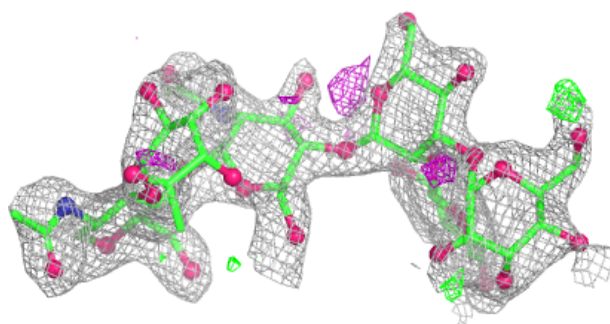
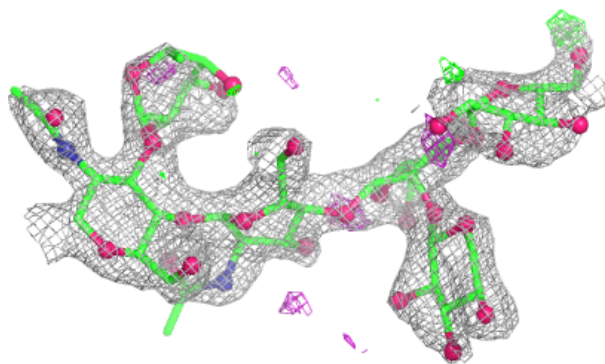
**Electron density around Chain L:**

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

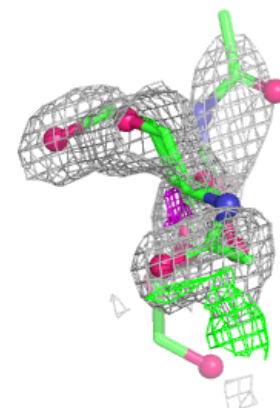
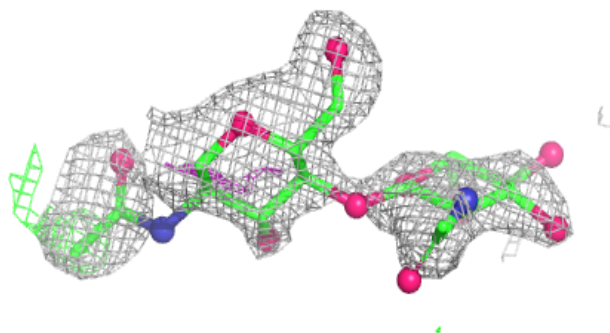
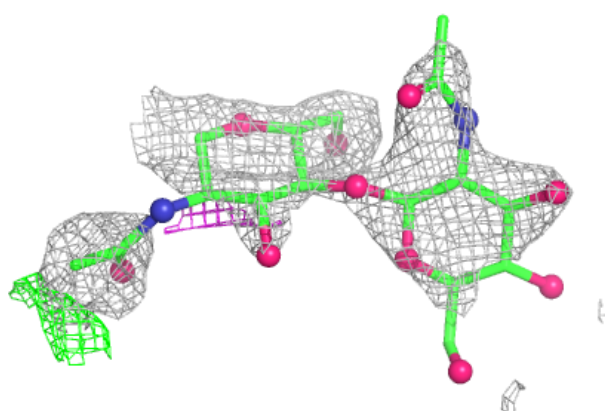


Electron density around Chain G:

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and green (positive)

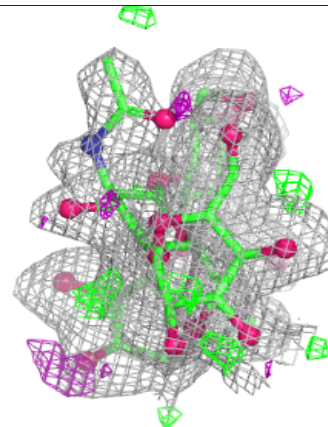
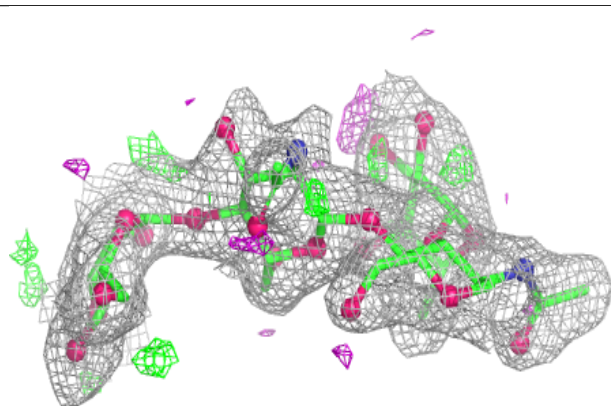
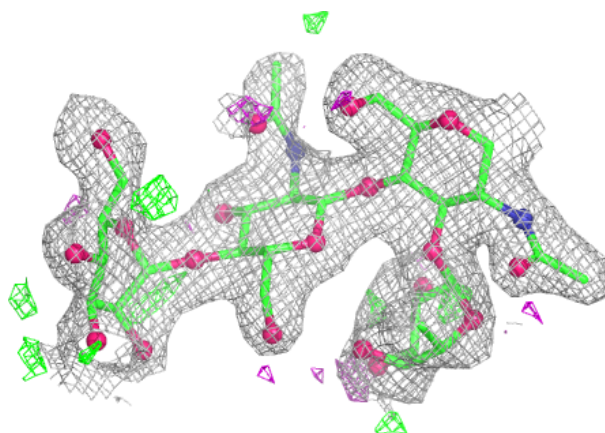
**Electron density around Chain H:**

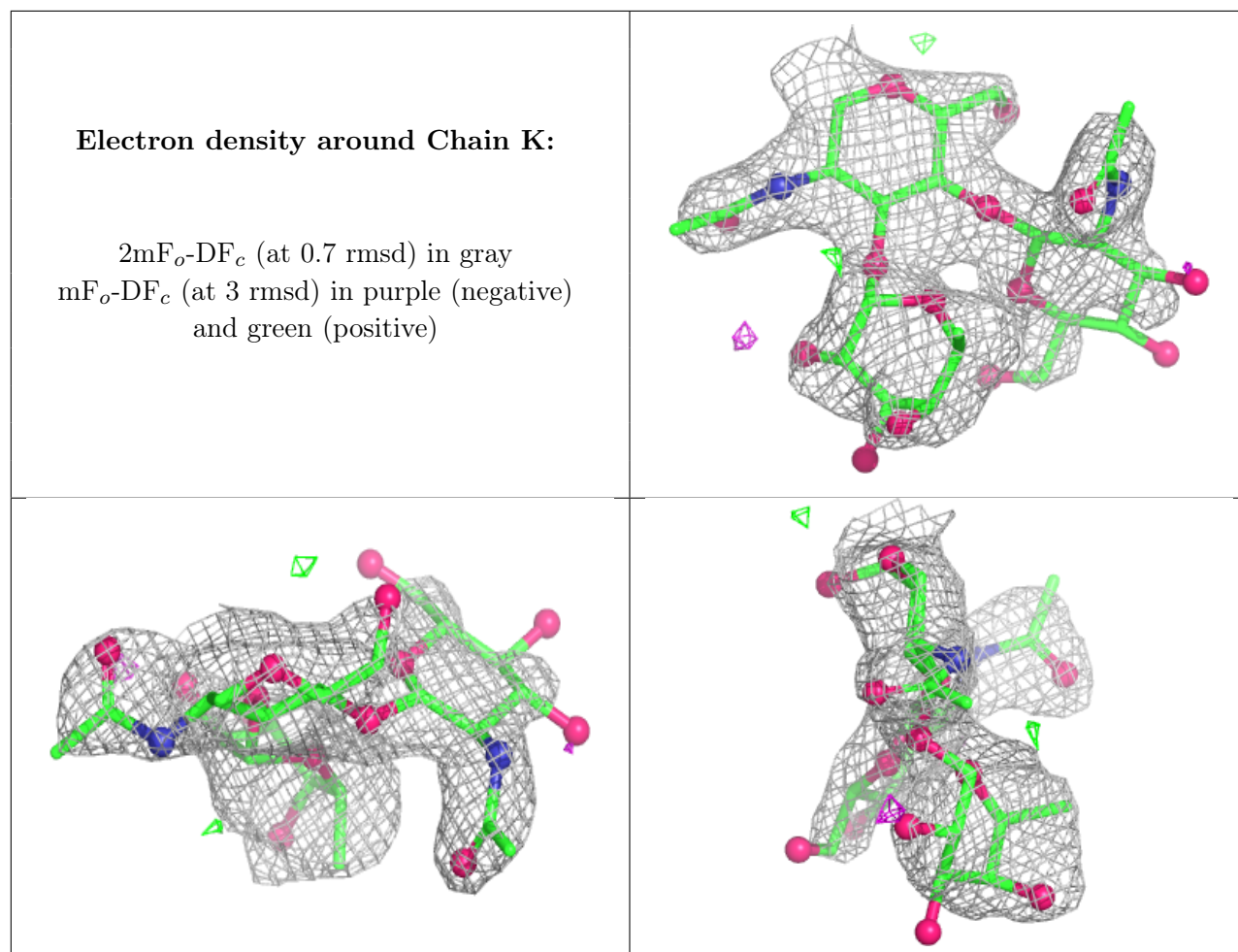
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	NAG	B	1326	14/15	0.62	0.13	57,65,72,75	0
12	NAG	B	1328	14/15	0.62	0.12	59,74,80,85	0
12	NAG	B	1327	14/15	0.71	0.13	49,66,75,78	0
12	NAG	A	1336	14/15	0.77	0.12	48,61,67,86	0
13	1PE	B	1330	16/16	0.84	0.12	41,49,57,57	0
13	1PE	B	1332	5/16	0.84	0.13	40,48,50,59	0
13	1PE	B	1334	5/16	0.84	0.13	49,50,57,60	0
14	PG0	B	1331	8/8	0.86	0.11	41,52,54,55	0
13	1PE	B	1329	15/16	0.88	0.11	32,42,54,61	0
13	1PE	B	1333	6/16	0.88	0.12	30,43,51,55	0
13	1PE	A	1337	5/16	0.91	0.09	31,31,42,48	0

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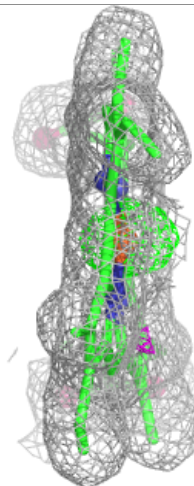
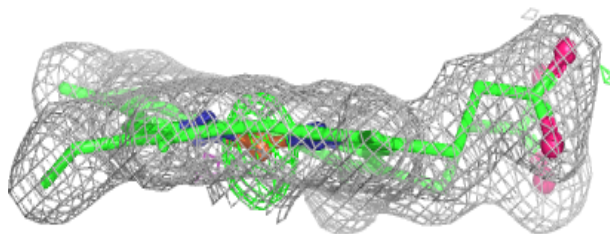
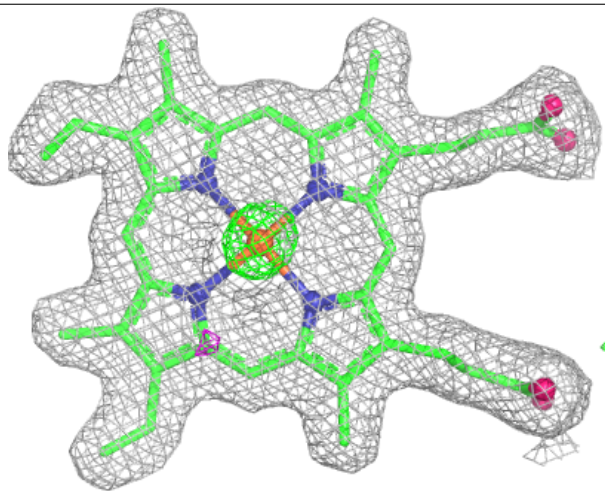
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	1PE	A	1338	10/16	0.93	0.07	32,37,46,47	0
10	HEM	A	1307	43/43	0.97	0.05	14,18,24,29	0
10	HEM	B	1306	43/43	0.97	0.06	15,21,26,35	0
11	CA	B	1307	1/1	0.98	0.03	25,25,25,25	0
11	CA	A	1309	1/1	0.99	0.02	20,20,20,20	0
11	CA	A	1308	1/1	0.99	0.03	22,22,22,22	0
11	CA	B	1308	1/1	1.00	0.01	22,22,22,22	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.

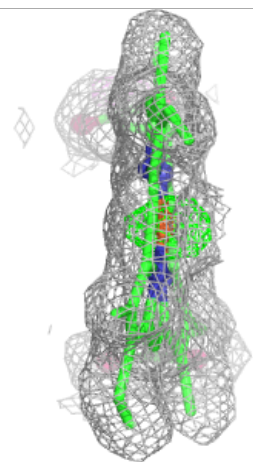
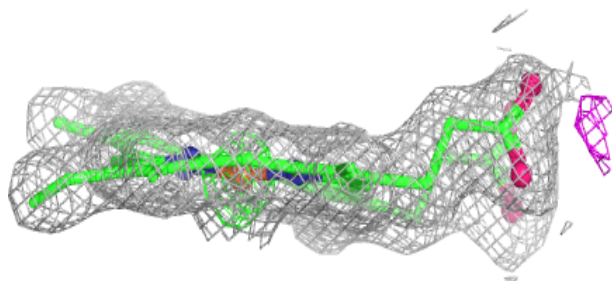
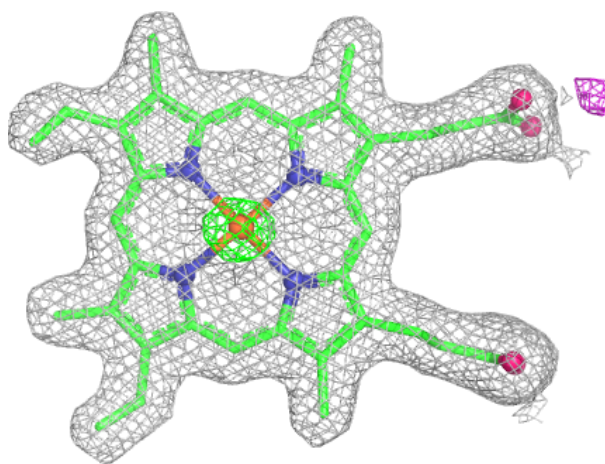
Electron density around HEM A 1307:

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 1306:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.