Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 02:02 PM EDT

PDB ID	:	1Q4G
Title	:	2.0 Angstrom Crystal Structure of Ovine Prostaglandin H2 Synthase-1, in complex with alpha-methyl-4-biphenylacetic acid
Authors	:	Gupta, K.; Selinksy, B.S.; Kaub, C.J.; Katz, A.K.; Loll, P.J.
Deposited on	:	2003-08-03
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

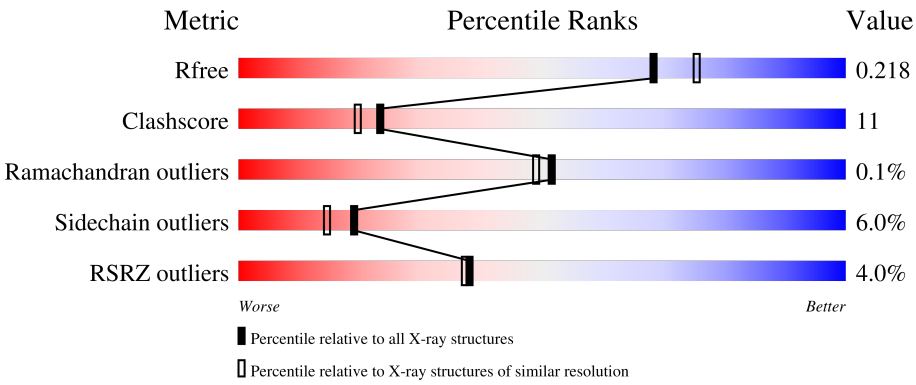
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% 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	553	5% 78% 19% •
1	B	553	3% 77% 20% •
2	C	2	50% 50%
2	F	2	50% 50%
3	D	4	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	4	25% 50% 25%
4	E	5	60% 40%
5	H	5	20% 20% 60%

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
2	NDG	C	2	-	-	-	X
3	BMA	D	3	-	-	-	X
3	BMA	D	4	-	-	-	X
3	BMA	G	4	-	-	-	X
4	MAN	E	4	-	-	-	X
4	MAN	E	5	-	-	-	X
5	BMA	H	4	-	-	-	X
5	BMA	H	5	-	-	-	X
6	BOG	A	752	-	-	-	X
6	BOG	A	754	-	-	-	X
6	BOG	B	1750	-	-	-	X
6	BOG	B	1752	-	-	-	X
6	BOG	B	1753	-	-	-	X
9	GOL	A	758	-	X	-	-
9	GOL	A	759	-	X	-	-
9	GOL	B	1758	-	X	-	-
9	GOL	B	1759	-	X	-	-
9	GOL	B	1760	-	X	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10336 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 Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4504	2918	762	795	29	0	2	0
1	B	553	4504	2918	762	795	29	0	2	0

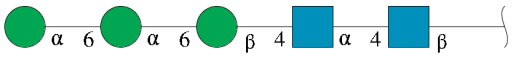
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 3 is an oligosaccharide called beta-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.

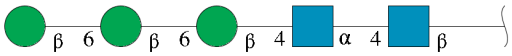
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	4	50	28	2	20	0	0	0
3	G	4	50	28	2	20	0	0	0

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



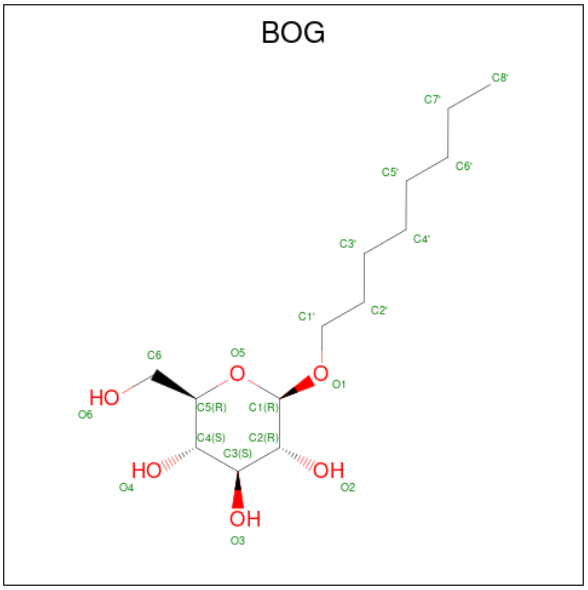
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	5	61	34	2	25	0	0	0

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



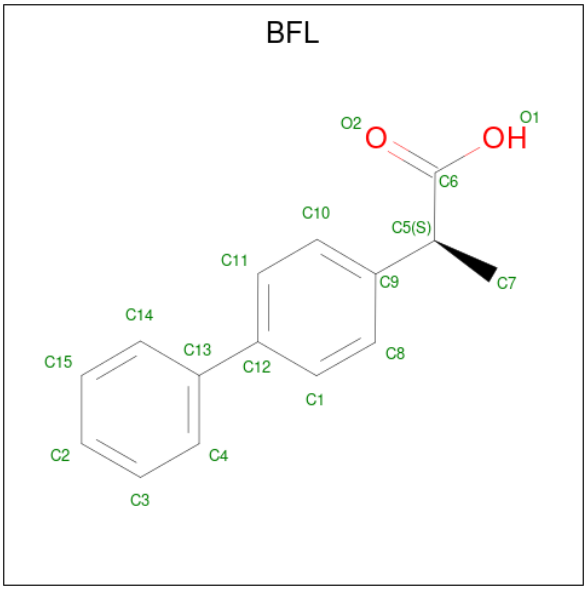
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	H	5	61	34	2	25	0	0	0

- Molecule 6 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



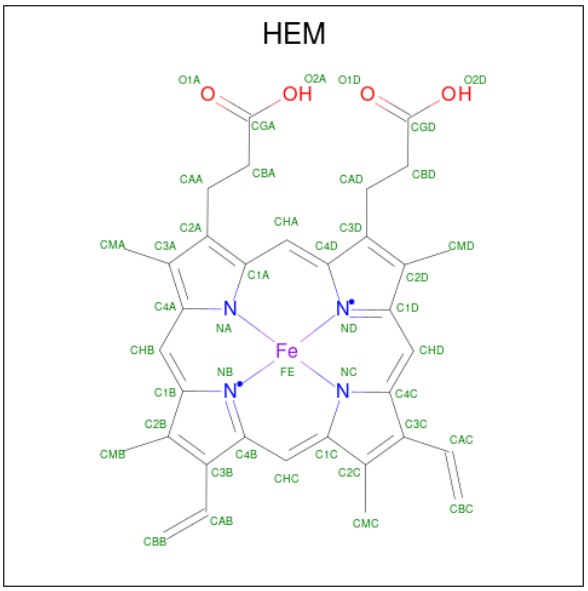
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	20	14	6	0	0
			Total	C	O		
6	A	1	20	14	6	0	0
			Total	C	O		
6	A	1	20	14	6	0	0
			Total	C	O		
6	A	1	20	14	6	0	0
			Total	C	O		
6	B	1	20	14	6	0	0
			Total	C	O		
6	B	1	20	14	6	0	0
			Total	C	O		
6	B	1	20	14	6	0	0
			Total	C	O		
6	B	1	20	14	6	0	0

- Molecule 7 is 2-(1,1'-BIPHENYL-4-YL)PROPANOIC ACID (three-letter code: BFL) (formula: $C_{15}H_{14}O_2$).



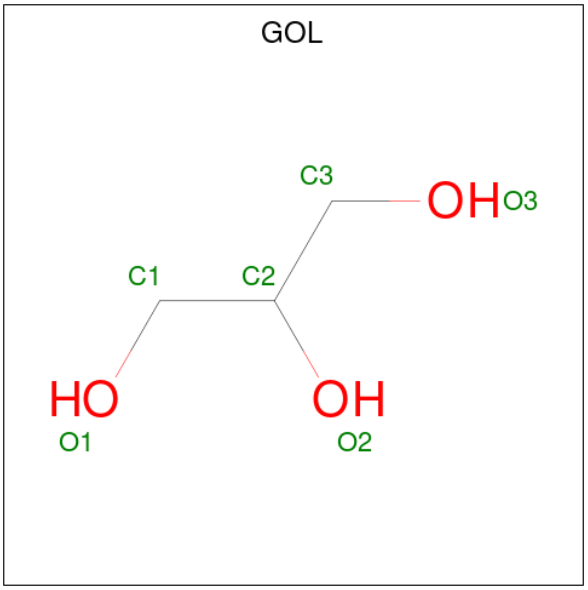
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	17	15	2	0	0
			Total	C	O		
7	B	1	17	15	2	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	86	68	2	8	8	0	1
			Total	C	Fe	N	O		
8	B	1	86	68	2	8	8	0	1

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	6	3	3	0	0
			Total	C	O		
9	A	1	6	3	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	6	3	3	0	0
			Total	C	O		
9	B	1	6	3	3	0	0
			Total	C	O		
9	B	1	6	3	3	0	0

- Molecule 10 is water.

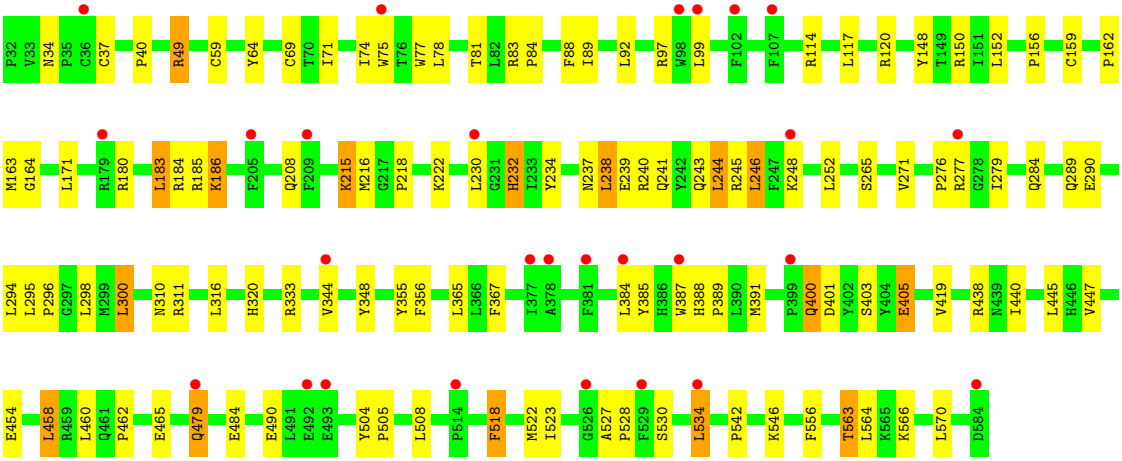
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	321	321	321	0	0
			Total	O		
10	B	333	333	333	0	0

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 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.

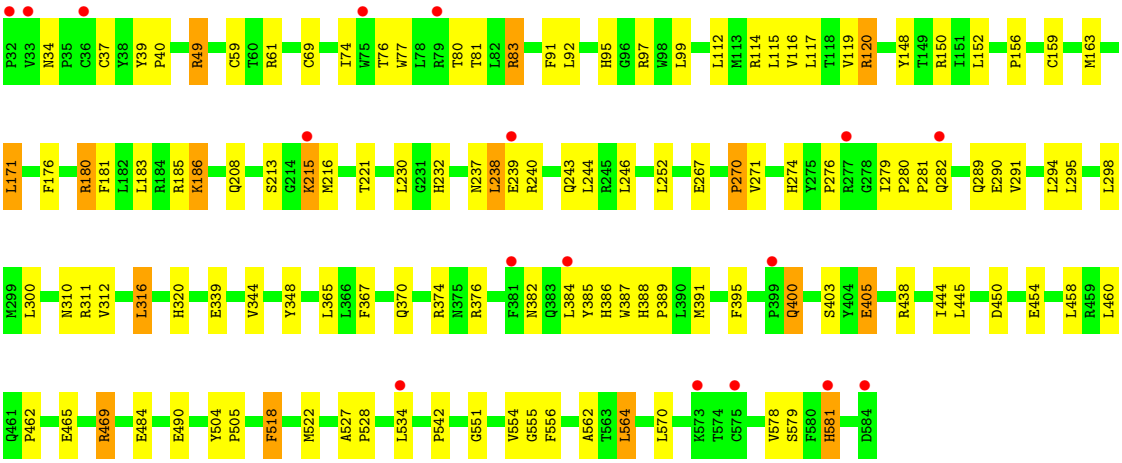
• Molecule 1: Prostaglandin G/H synthase 1

Chain A:



• Molecule 1: Prostaglandin G/H synthase 1

Chain B:



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

Chain C:

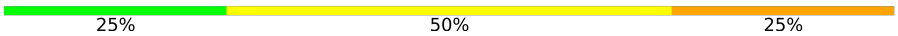
• Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

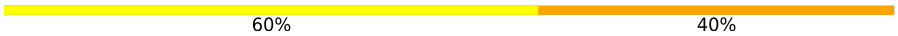
• Molecule 3: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 3: beta-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 G: 

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

Chain E: 

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.15Å 203.86Å 223.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 2.00 43.68 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.8 (43.68-2.00) 93.1 (43.68-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.231 0.203 , 0.218	Depositor DCC
R_{free} test set	10694 reflections (7.42%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10336	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, HEM, BOG, GOL, NDG, MAN, BFL, BMA

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	0.35	0/4643	0.59	1/6302 (0.0%)
1	B	0.37	0/4643	0.60	0/6302
All	All	0.36	0/9286	0.60	1/12604 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	TYR	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4504	0	4403	101	0
1	B	4504	0	4403	100	0
2	C	28	0	24	3	0
2	F	28	0	24	1	0
3	D	50	0	43	5	0
3	G	50	0	43	4	0
4	E	61	0	51	6	0
5	H	61	0	51	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	80	0	112	2	0
6	B	80	0	112	6	0
7	A	17	0	13	1	0
7	B	17	0	13	0	0
8	A	86	0	60	4	0
8	B	86	0	60	4	0
9	A	12	0	8	1	0
9	B	18	0	12	1	0
10	A	321	0	0	6	0
10	B	333	0	0	5	0
All	All	10336	0	9432	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (215) 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:185:ARG:HH21	1:A:438:ARG:NH1	1.56	1.02
1:A:59:CYS:SG	1:A:69[B]:CYS:HB2	2.01	1.01
1:A:59:CYS:SG	1:A:69[B]:CYS:CB	2.53	0.96
1:B:215:LYS:HE2	1:B:215:LYS:H	1.32	0.93
1:A:215:LYS:HE2	1:A:215:LYS:H	1.35	0.89
1:B:237:ASN:ND2	1:B:239:GLU:HG3	1.88	0.89
1:A:563:THR:HG22	1:A:566:LYS:H	1.35	0.88
2:C:1:NAG:H61	2:C:2:NDG:H8C1	1.57	0.86
1:B:215:LYS:H	1:B:215:LYS:CE	1.91	0.82
4:E:2:NDG:H4	4:E:3:BMA:O2	1.81	0.80
1:B:237:ASN:HD22	1:B:239:GLU:HG3	1.43	0.80
1:A:215:LYS:H	1:A:215:LYS:CE	1.98	0.76
1:B:216:MET:HG2	5:H:2:NDG:H8C1	1.71	0.73
5:H:4:BMA:O2	5:H:4:BMA:H62	1.88	0.73
1:A:185:ARG:HH21	1:A:438:ARG:HH11	1.34	0.73
1:A:185:ARG:HH21	1:A:438:ARG:HH12	1.37	0.71
1:A:387:TRP:HB2	8:A:801[A]:HEM:HAC	1.71	0.71
1:A:391:MET:HG3	8:A:801[A]:HEM:HAB	1.72	0.71
1:B:276:PRO:HD2	1:B:279:ILE:HD12	1.73	0.71
1:B:294:LEU:HG	1:B:295:LEU:HG	1.72	0.70
1:B:208:GLN:NE2	1:B:230:LEU:H	1.90	0.70
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.57	0.69
1:A:391:MET:HG3	8:A:801[B]:HEM:HAB	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:NAG:H4	3:D:3:BMA:O2	1.93	0.69
1:B:387:TRP:HB2	8:B:1601[A]:HEM:HAC	1.77	0.67
1:A:208:GLN:NE2	1:A:230:LEU:H	1.93	0.66
5:H:4:BMA:H62	5:H:5:BMA:HO2	1.60	0.66
1:B:83:ARG:NH1	6:B:1751:BOG:H3	2.10	0.65
1:A:40:PRO:HB3	2:C:1:NAG:H62	1.78	0.65
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.79	0.65
1:A:114:ARG:HD3	1:A:365:LEU:O	1.96	0.65
1:B:387:TRP:HB2	8:B:1601[B]:HEM:HAC	1.78	0.64
1:A:49:ARG:O	1:B:320:HIS:HD2	1.80	0.64
1:A:387:TRP:HB2	8:A:801[B]:HEM:HAC	1.79	0.64
5:H:4:BMA:H62	5:H:5:BMA:O2	1.98	0.64
1:B:208:GLN:HE21	1:B:230:LEU:H	1.44	0.63
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.37	0.63
1:B:180:ARG:O	1:B:438:ARG:NH1	2.31	0.63
1:A:150:ARG:HD3	1:A:152:LEU:O	1.99	0.62
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.39	0.62
1:B:150:ARG:HD3	1:B:152:LEU:O	1.99	0.61
1:B:243:GLN:OE1	1:B:270:PRO:HD2	1.99	0.61
1:A:216:MET:HE1	10:A:1062:HOH:O	2.00	0.61
1:A:99:LEU:HD23	6:A:754:BOG:H3'1	1.81	0.60
1:A:563:THR:HG21	10:A:1065:HOH:O	2.01	0.60
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.60
1:A:215:LYS:HG2	1:A:216:MET:H	1.66	0.60
1:B:554:VAL:HG13	1:B:555:GLY:N	2.16	0.60
1:B:518:PHE:CD1	1:B:522:MET:HG2	2.37	0.60
1:B:450:ASP:O	1:B:454:GLU:HG3	2.01	0.60
1:A:215:LYS:HD2	1:A:222:LYS:NZ	2.16	0.60
1:A:185:ARG:NH2	1:A:438:ARG:NH1	2.40	0.59
1:B:267:GLU:OE1	1:B:282:GLN:HG2	2.03	0.59
1:A:215:LYS:HD2	1:A:222:LYS:HZ3	1.67	0.59
1:B:115:LEU:HD21	6:B:1752:BOG:H2	1.84	0.59
1:A:294:LEU:HG	1:A:295:LEU:HG	1.84	0.58
4:E:2:NDG:H3	4:E:2:NDG:O7	2.02	0.58
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.02	0.58
1:B:183:LEU:HD13	1:B:445:LEU:HD22	1.85	0.58
1:A:454:GLU:HG3	1:A:458:LEU:HD22	1.86	0.58
1:A:320:HIS:HD2	1:B:49:ARG:O	1.86	0.57
1:A:64:TYR:HB2	1:A:69[B]:CYS:SG	2.44	0.56
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.86	0.56
5:H:2:NDG:H3	5:H:2:NDG:O7	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:SER:OG	1:A:405:GLU:HG2	2.06	0.56
1:B:311:ARG:NH2	1:B:570:LEU:HD23	2.20	0.56
1:B:391:MET:HE1	1:B:395:PHE:HE2	1.70	0.56
1:B:208:GLN:HE22	1:B:230:LEU:HD12	1.71	0.56
1:A:518:PHE:HE2	1:A:523:ILE:HD11	1.71	0.55
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.87	0.55
1:B:163:MET:CE	1:B:171:LEU:HD21	2.37	0.55
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.87	0.55
1:A:530[B]:SER:O	1:A:534:LEU:HD22	2.07	0.55
1:B:185:ARG:NH2	1:B:438:ARG:NH1	2.55	0.54
1:A:479:GLN:HE21	1:A:479:GLN:C	2.11	0.54
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.90	0.54
1:A:186:LYS:HB2	1:A:186:LYS:NZ	2.23	0.54
1:B:237:ASN:ND2	1:B:240:ARG:H	2.06	0.54
1:B:339:GLU:HG2	1:B:562:ALA:HB2	1.90	0.54
1:A:97:ARG:HG2	1:A:356:PHE:CE2	2.43	0.54
1:B:99:LEU:HD23	6:B:1753:BOG:H3'1	1.90	0.54
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.54	0.53
1:A:563:THR:HG23	10:A:832:HOH:O	2.07	0.53
1:A:215:LYS:HG2	1:A:216:MET:N	2.23	0.53
1:B:554:VAL:HG13	1:B:555:GLY:H	1.71	0.53
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.91	0.53
1:B:40:PRO:HB3	2:F:1:NAG:H62	1.90	0.53
1:A:180:ARG:O	1:A:438:ARG:NH1	2.42	0.53
1:B:186:LYS:HB2	1:B:186:LYS:NZ	2.24	0.52
1:B:237:ASN:ND2	1:B:239:GLU:CG	2.67	0.52
1:B:403:SER:OG	1:B:405:GLU:HG2	2.09	0.52
1:A:238:LEU:HD13	5:H:2:NDG:H6C2	1.91	0.52
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.92	0.52
1:B:215:LYS:HE2	1:B:215:LYS:N	2.14	0.52
1:B:367:PHE:CD2	1:B:542:PRO:HG3	2.45	0.52
1:A:530[A]:SER:O	1:A:534:LEU:HD22	2.08	0.52
10:A:1117:HOH:O	2:C:2:NDG:H3	2.09	0.52
1:A:185:ARG:HG2	1:A:185:ARG:NH1	2.24	0.52
1:A:344:VAL:O	1:A:348:TYR:HB3	2.10	0.51
1:A:208:GLN:HE22	1:A:230:LEU:HD12	1.76	0.51
1:A:218:PRO:HB3	1:A:454:GLU:OE2	2.10	0.51
4:E:2:NDG:C4	4:E:3:BMA:O2	2.55	0.51
1:B:150:ARG:CD	1:B:152:LEU:O	2.58	0.50
1:A:208:GLN:HE21	1:A:230:LEU:H	1.60	0.50
1:A:310:ASN:HB3	9:A:758:GOL:O1	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:HH22	6:B:1751:BOG:H5	1.75	0.50
1:A:185:ARG:NH2	1:A:438:ARG:HH11	2.06	0.50
1:B:405:GLU:CD	1:B:405:GLU:H	2.15	0.50
1:B:74:ILE:HG12	10:B:1877:HOH:O	2.12	0.50
1:B:176:PHE:CZ	1:B:180:ARG:HG3	2.47	0.50
1:A:244:LEU:HD13	1:A:271:VAL:HG11	1.93	0.50
3:D:2:NAG:C4	3:D:3:BMA:O2	2.60	0.49
1:B:391:MET:HG3	8:B:1601[B]:HEM:CBB	2.42	0.49
1:A:241:GLN:NE2	1:A:245:ARG:HH11	2.10	0.49
1:A:150:ARG:CD	1:A:152:LEU:O	2.61	0.49
1:A:388:HIS:N	1:A:389:PRO:CD	2.76	0.49
1:A:400:GLN:OE1	3:D:3:BMA:H62	2.11	0.49
4:E:2:NDG:O7	4:E:2:NDG:C3	2.61	0.48
1:B:163:MET:HE3	1:B:171:LEU:HD21	1.94	0.48
1:A:77:TRP:O	1:A:81:THR:HG23	2.14	0.48
1:B:49:ARG:HG3	10:B:1763:HOH:O	2.14	0.48
3:G:2:NAG:H4	3:G:3:BMA:O2	2.14	0.48
1:A:239:GLU:CD	1:A:239:GLU:H	2.17	0.47
1:B:83:ARG:NH1	1:B:83:ARG:HG3	2.29	0.47
1:A:246:LEU:HD13	1:A:248:LYS:HB3	1.96	0.47
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.96	0.47
1:B:444:ILE:HG21	8:B:1601[B]:HEM:HBB2	1.96	0.47
1:B:579:SER:OG	1:B:581:HIS:HD2	1.98	0.47
1:A:290:GLU:CD	1:A:290:GLU:H	2.18	0.47
1:B:311:ARG:NH2	10:B:1907:HOH:O	2.47	0.47
1:B:374:ARG:HD2	10:B:1942:HOH:O	2.14	0.47
1:B:240:ARG:NH1	1:B:271:VAL:HG13	2.30	0.46
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.79	0.46
1:B:290:GLU:H	1:B:290:GLU:CD	2.17	0.46
1:A:546:LYS:HE3	10:B:1818:HOH:O	2.15	0.46
1:B:388:HIS:N	1:B:389:PRO:CD	2.79	0.46
1:A:311:ARG:NH2	10:A:975:HOH:O	2.48	0.46
1:B:59:CYS:SG	1:B:69[B]:CYS:SG	3.13	0.46
1:A:163:MET:HE1	1:A:171:LEU:HD21	1.97	0.45
1:B:91:PHE:O	1:B:95:HIS:HD2	1.99	0.45
1:A:237:ASN:ND2	1:A:240:ARG:H	2.14	0.45
1:B:310:ASN:HB3	9:B:1759:GOL:O2	2.16	0.45
1:B:213:SER:OG	1:B:215:LYS:HE3	2.16	0.45
1:A:71:ILE:HD13	6:A:753:BOG:H3	1.97	0.45
1:B:77:TRP:O	1:B:81:THR:HG23	2.17	0.45
1:A:265:SER:HA	1:A:284:GLN:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2:NDG:O3	4:E:3:BMA:C1	2.65	0.44
1:A:183:LEU:HD22	1:A:184:ARG:O	2.18	0.44
1:B:181:PHE:HZ	1:B:490:GLU:HG2	1.82	0.44
1:A:74:ILE:HG23	1:A:75:TRP:N	2.33	0.44
1:A:215:LYS:HE2	1:A:215:LYS:N	2.17	0.44
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.53	0.44
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.00	0.44
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.57	0.44
1:A:218:PRO:HB3	1:A:454:GLU:CD	2.38	0.44
1:B:274:HIS:HD2	1:B:291:VAL:HG12	1.82	0.44
1:B:469:ARG:O	1:B:469:ARG:NE	2.46	0.44
5:H:2:NDG:O7	5:H:2:NDG:C3	2.65	0.44
1:A:159:CYS:HB3	1:A:164:GLY:O	2.18	0.43
1:A:163:MET:CE	1:A:171:LEU:HD21	2.48	0.43
1:A:400:GLN:CA	1:A:400:GLN:HE21	2.29	0.43
1:B:400:GLN:OE1	3:G:3:BMA:H62	2.18	0.43
1:A:542:PRO:O	1:B:61:ARG:NH1	2.50	0.43
1:B:579:SER:OG	1:B:581:HIS:CD2	2.72	0.43
1:B:344:VAL:O	1:B:348:TYR:HB3	2.19	0.43
1:A:162:PRO:HB2	1:A:171:LEU:HD13	1.99	0.43
1:B:384:LEU:HG	1:B:522:MET:SD	2.58	0.43
1:A:400:GLN:HE21	1:A:401:ASP:H	1.65	0.43
1:B:119:VAL:HG12	6:B:1751:BOG:H62	2.00	0.43
1:B:215:LYS:HG2	1:B:216:MET:H	1.84	0.43
1:B:237:ASN:HD21	1:B:239:GLU:CD	2.22	0.43
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.87	0.43
1:B:400:GLN:OE1	3:G:3:BMA:C6	2.66	0.43
1:A:311:ARG:NH2	1:A:570:LEU:HD23	2.34	0.43
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.54	0.43
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.53	0.42
3:D:3:BMA:O6	3:D:4:BMA:H62	2.18	0.42
1:A:518:PHE:HE2	1:A:523:ILE:CD1	2.32	0.42
1:B:83:ARG:HH12	6:B:1751:BOG:H3	1.81	0.42
1:B:382:ASN:OD1	1:B:386:HIS:HE1	2.02	0.42
1:A:355:TYR:CE1	7:A:701:BFL:H5	2.54	0.42
1:A:384:LEU:C	1:A:384:LEU:HD23	2.40	0.42
1:A:277:ARG:HD2	1:A:277:ARG:HA	1.84	0.42
1:B:215:LYS:HG2	1:B:216:MET:N	2.33	0.42
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.55	0.42
1:A:300:LEU:HD21	1:A:419:VAL:HG13	2.02	0.42
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:TYR:CZ	1:B:221:THR:HB	2.55	0.42
1:B:391:MET:HE1	1:B:395:PHE:CE2	2.53	0.42
1:A:88:PHE:O	1:A:92:LEU:HD13	2.20	0.42
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.55	0.42
1:B:564:LEU:HD13	1:B:578:VAL:HG22	2.02	0.42
1:B:114:ARG:HD3	1:B:365:LEU:O	2.20	0.41
1:B:238:LEU:HD12	4:E:1:NAG:H4	2.02	0.41
1:B:581:HIS:CD2	1:B:581:HIS:O	2.73	0.41
3:G:2:NAG:C4	3:G:3:BMA:O2	2.68	0.41
1:B:116:VAL:O	1:B:120:ARG:HB2	2.21	0.41
1:B:320:HIS:CE1	1:B:551:GLY:O	2.73	0.41
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.61	0.41
1:A:183:LEU:HG	1:A:445:LEU:HD22	2.01	0.41
1:A:295:LEU:HA	1:A:296:PRO:HD3	1.96	0.41
1:A:367:PHE:O	1:B:370:GLN:NE2	2.43	0.41
1:A:389:PRO:HG3	1:A:440:ILE:HG12	2.03	0.41
1:A:243:GLN:CD	5:H:5:BMA:H62	2.41	0.41
1:B:83:ARG:HH11	1:B:83:ARG:CG	2.33	0.41
1:B:112:LEU:O	1:B:116:VAL:HG23	2.20	0.41
1:A:83:ARG:HD3	10:A:944:HOH:O	2.21	0.41
1:B:39:TYR:N	1:B:40:PRO:CD	2.83	0.41
1:B:312:VAL:HG12	1:B:316:LEU:HD22	2.03	0.41
1:B:554:VAL:CG1	1:B:555:GLY:N	2.84	0.41
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.57	0.40
1:B:59:CYS:HB3	1:B:69[B]:CYS:SG	2.61	0.40
1:B:320:HIS:HE1	1:B:551:GLY:O	2.04	0.40
3:D:2:NAG:O3	3:D:3:BMA:C1	2.69	0.40
1:B:76:THR:O	1:B:80:THR:HG23	2.22	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	553/553 (100%)	537 (97%)	16 (3%)	0	100	100
1	B	553/553 (100%)	535 (97%)	17 (3%)	1 (0%)	47	44
All	All	1106/1106 (100%)	1072 (97%)	33 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	PRO

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	490/488 (100%)	462 (94%)	28 (6%)	20	16
1	B	490/488 (100%)	459 (94%)	31 (6%)	18	13
All	All	980/976 (100%)	921 (94%)	59 (6%)	19	14

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	78	LEU
1	A	117	LEU
1	A	120	ARG
1	A	183	LEU
1	A	186	LYS
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	289	GLN
1	A	298	LEU
1	A	300	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	316	LEU
1	A	385	TYR
1	A	400	GLN
1	A	405	GLU
1	A	458	LEU
1	A	460	LEU
1	A	479	GLN
1	A	484	GLU
1	A	518	PHE
1	A	534	LEU
1	A	556	PHE
1	A	563	THR
1	A	564	LEU
1	B	49	ARG
1	B	83	ARG
1	B	92	LEU
1	B	117	LEU
1	B	120	ARG
1	B	171	LEU
1	B	180	ARG
1	B	186	LYS
1	B	215	LYS
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	289	GLN
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	376	ARG
1	B	385	TYR
1	B	400	GLN
1	B	405	GLU
1	B	458	LEU
1	B	460	LEU
1	B	469	ARG
1	B	484	GLU
1	B	518	PHE
1	B	534	LEU
1	B	556	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	564	LEU
1	B	581	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	134	HIS
1	A	203	GLN
1	A	204	HIS
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	274	HIS
1	A	320	HIS
1	A	375	ASN
1	A	386	HIS
1	A	400	GLN
1	A	443	HIS
1	B	42	GLN
1	B	56	GLN
1	B	95	HIS
1	B	134	HIS
1	B	203	GLN
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	274	HIS
1	B	320	HIS
1	B	386	HIS
1	B	443	HIS
1	B	581	HIS

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)

22 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	1,2	14,14,15	0.67	0	17,19,21	0.65	0
2	NDG	C	2	2	14,14,15	0.59	0	17,19,21	0.90	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.49	0	17,19,21	0.68	1 (5%)
3	NAG	D	2	3	14,14,15	0.66	0	17,19,21	0.72	0
3	BMA	D	3	3	11,11,12	0.74	0	15,15,17	1.06	1 (6%)
3	BMA	D	4	3	11,11,12	0.60	0	15,15,17	0.90	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.74	0	17,19,21	1.02	0
4	NDG	E	2	4	14,14,15	0.89	1 (7%)	17,19,21	1.66	3 (17%)
4	BMA	E	3	4	11,11,12	0.85	0	15,15,17	1.68	3 (20%)
4	MAN	E	4	4	11,11,12	0.66	0	15,15,17	0.78	1 (6%)
4	MAN	E	5	4	11,11,12	0.54	0	15,15,17	0.70	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.64	0	17,19,21	0.89	1 (5%)
2	NDG	F	2	2	14,14,15	0.62	0	17,19,21	0.77	0
3	NAG	G	1	1,3	14,14,15	0.54	0	17,19,21	0.62	0
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	0.76	0
3	BMA	G	3	3	11,11,12	0.68	0	15,15,17	1.06	1 (6%)
3	BMA	G	4	3	11,11,12	0.60	0	15,15,17	0.89	1 (6%)
5	NAG	H	1	1,5	14,14,15	0.70	0	17,19,21	0.88	1 (5%)
5	NDG	H	2	5	14,14,15	0.73	1 (7%)	17,19,21	1.37	2 (11%)
5	BMA	H	3	5	11,11,12	0.53	0	15,15,17	0.65	0
5	BMA	H	4	5	11,11,12	0.65	0	15,15,17	1.05	1 (6%)
5	BMA	H	5	5	11,11,12	0.66	0	15,15,17	0.83	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NDG	C	2	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	1/1/1/1
3	BMA	D	4	3	-	2/2/19/22	1/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NDG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NDG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	1/1/1/1
3	BMA	G	4	3	-	2/2/19/22	1/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NDG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	BMA	H	4	5	-	2/2/19/22	0/1/1/1
5	BMA	H	5	5	-	1/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NDG	C1-C2	2.21	1.55	1.52
5	H	2	NDG	C1-C2	2.12	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	3	BMA	C1-O5-C5	4.73	118.61	112.19
4	E	2	NDG	C1-O5-C5	4.41	118.16	112.19
5	H	2	NDG	C1-O5-C5	3.83	117.38	112.19
4	E	2	NDG	C4-C3-C2	-3.43	106.00	111.02
4	E	3	BMA	C1-C2-C3	3.36	113.80	109.67
3	G	3	BMA	C1-O5-C5	3.31	116.67	112.19
5	H	4	BMA	C1-O5-C5	3.29	116.65	112.19
3	D	3	BMA	C1-O5-C5	3.25	116.59	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	BMA	C1-O5-C5	3.03	116.30	112.19
3	G	4	BMA	C1-O5-C5	3.02	116.28	112.19
5	H	2	NDG	C4-C3-C2	-2.83	106.87	111.02
5	H	5	BMA	C1-O5-C5	2.66	115.80	112.19
4	E	5	MAN	C1-O5-C5	2.58	115.69	112.19
4	E	2	NDG	C3-C4-C5	-2.54	105.71	110.24
4	E	4	MAN	C1-O5-C5	2.45	115.52	112.19
2	F	1	NAG	C2-N2-C7	-2.30	119.63	122.90
4	E	3	BMA	O5-C1-C2	2.25	114.25	110.77
2	C	2	NDG	C2-N2-C7	-2.19	119.78	122.90
5	H	1	NAG	C2-N2-C7	-2.06	119.97	122.90
3	D	1	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NDG	C8-C7-N2-C2
2	C	2	NDG	O7-C7-N2-C2
4	E	2	NDG	C3-C2-N2-C7
3	D	2	NAG	O5-C5-C6-O6
3	G	4	BMA	C4-C5-C6-O6
3	G	4	BMA	O5-C5-C6-O6
3	D	4	BMA	C4-C5-C6-O6
2	F	2	NDG	C4-C5-C6-O6
2	C	2	NDG	O5-C5-C6-O6
5	H	4	BMA	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	F	2	NDG	O5-C5-C6-O6
3	D	4	BMA	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
4	E	5	MAN	C4-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
5	H	5	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	3	BMA	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	2	NDG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
5	H	2	NDG	C3-C2-N2-C7
5	H	4	BMA	C4-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2

All (6) ring outliers are listed below:

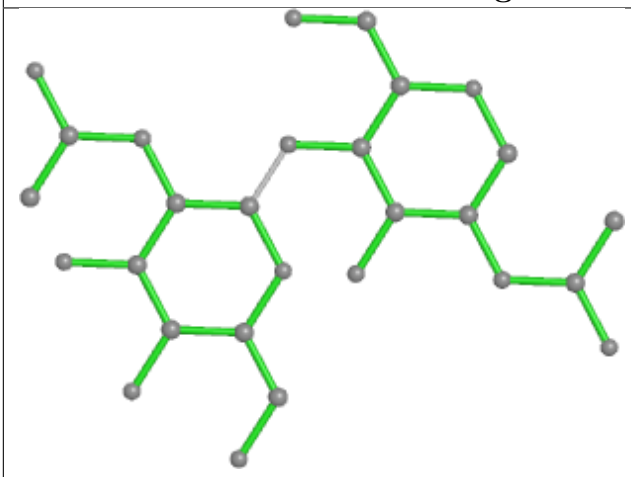
Mol	Chain	Res	Type	Atoms
5	H	5	BMA	C1-C2-C3-C4-C5-O5
4	E	5	MAN	C1-C2-C3-C4-C5-O5
3	D	4	BMA	C1-C2-C3-C4-C5-O5
3	G	4	BMA	C1-C2-C3-C4-C5-O5
3	D	3	BMA	C1-C2-C3-C4-C5-O5
3	G	3	BMA	C1-C2-C3-C4-C5-O5

14 monomers are involved in 27 short contacts:

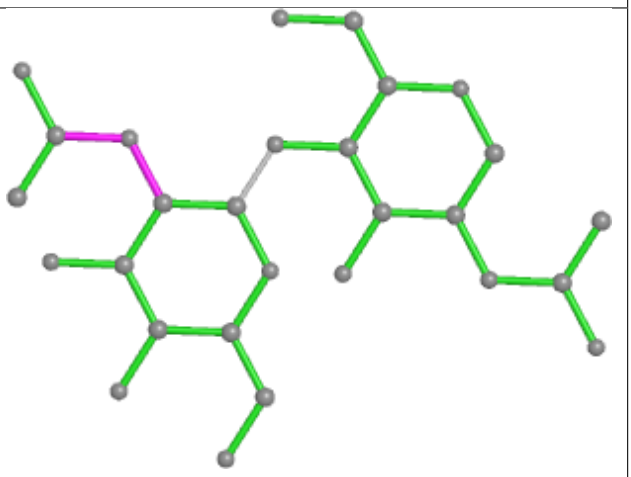
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3	BMA	3	0
2	C	1	NAG	2	0
5	H	5	BMA	3	0
4	E	1	NAG	1	0
3	D	3	BMA	5	0
2	C	2	NDG	2	0
4	E	2	NDG	5	0
5	H	4	BMA	3	0
3	D	2	NAG	3	0
3	G	2	NAG	2	0
3	G	3	BMA	4	0
5	H	2	NDG	4	0
3	D	4	BMA	1	0
2	F	1	NAG	1	0

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

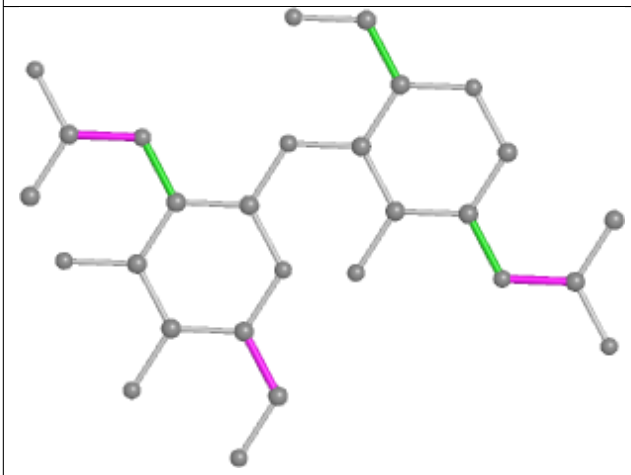
Oligosaccharide Chain C



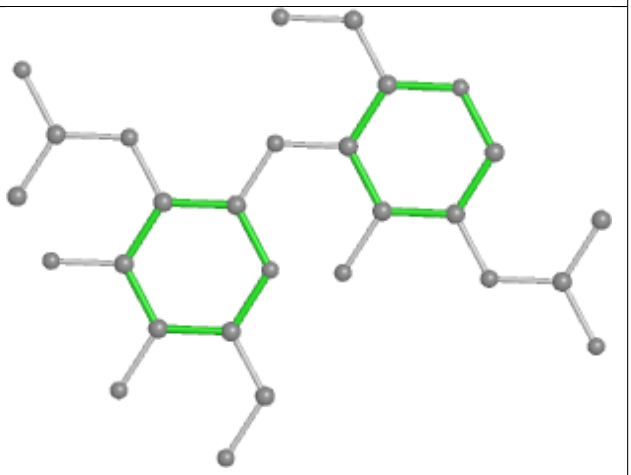
Bond lengths



Bond angles

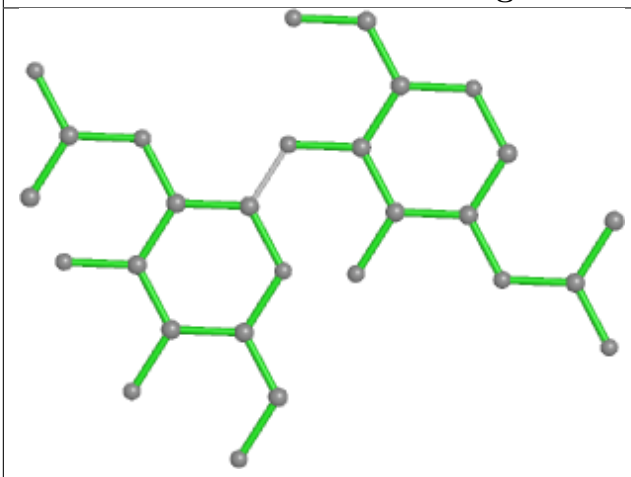


Torsions

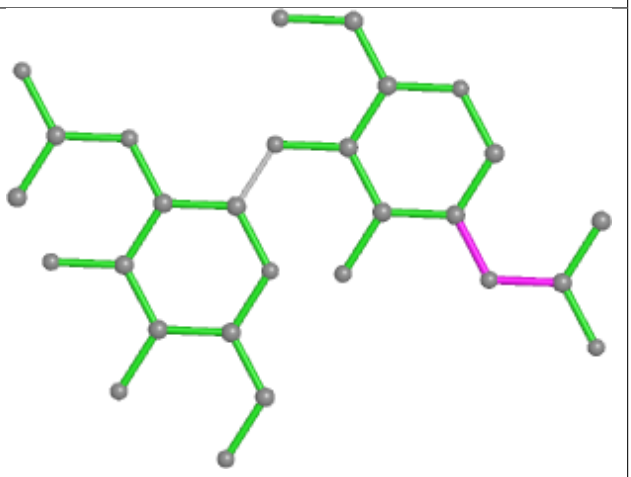


Rings

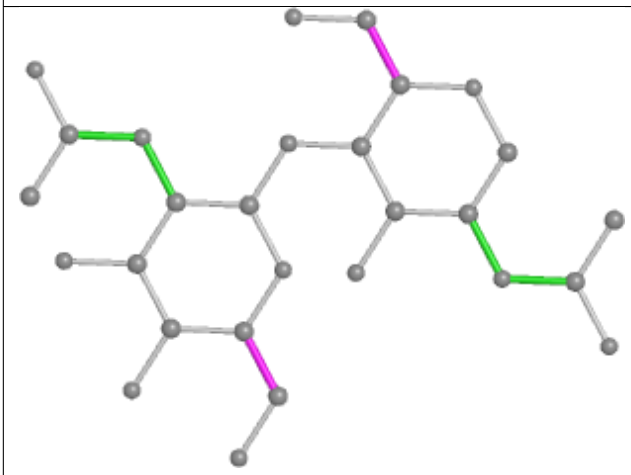
Oligosaccharide Chain F



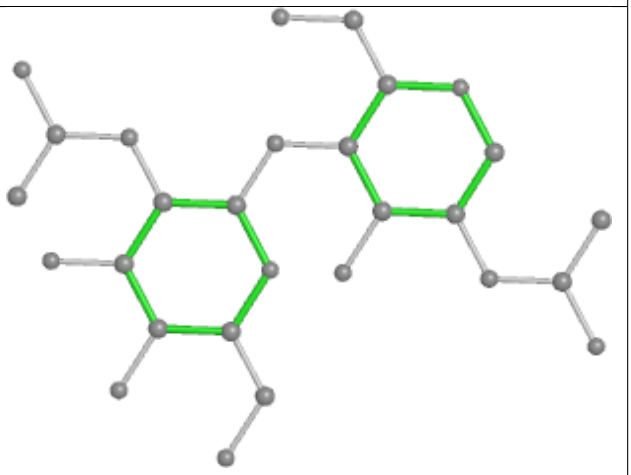
Bond lengths



Bond angles

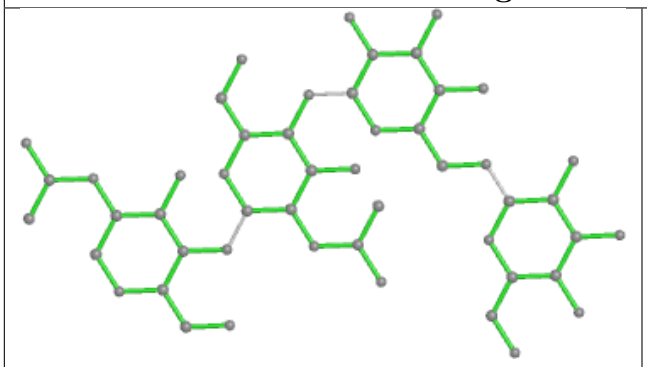


Torsions

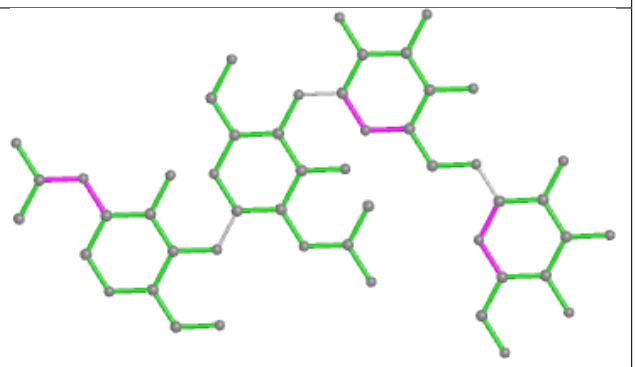


Rings

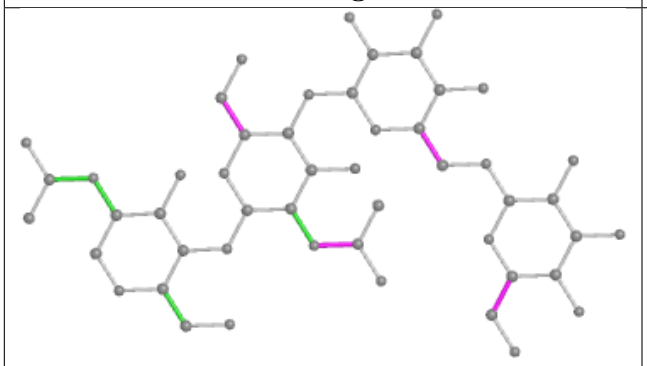
Oligosaccharide Chain D



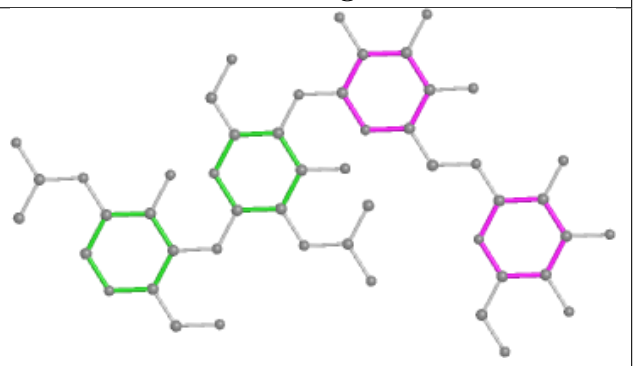
Bond lengths



Bond angles

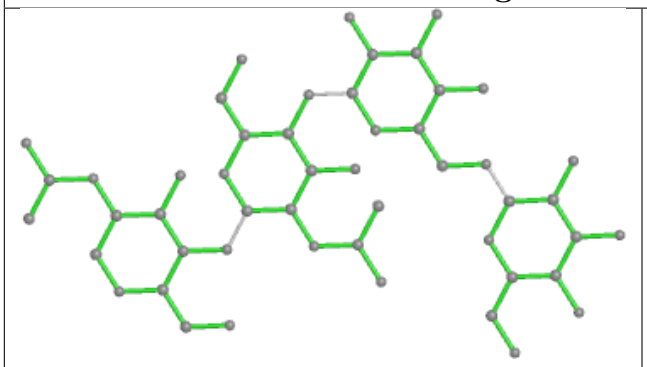


Torsions

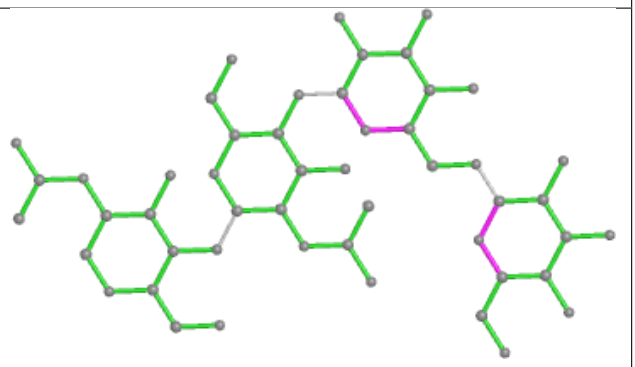


Rings

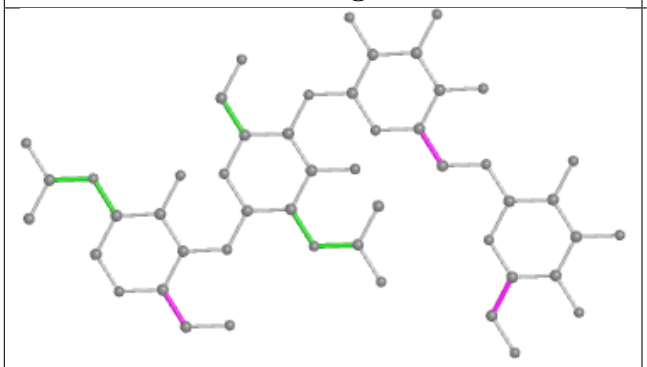
Oligosaccharide Chain G



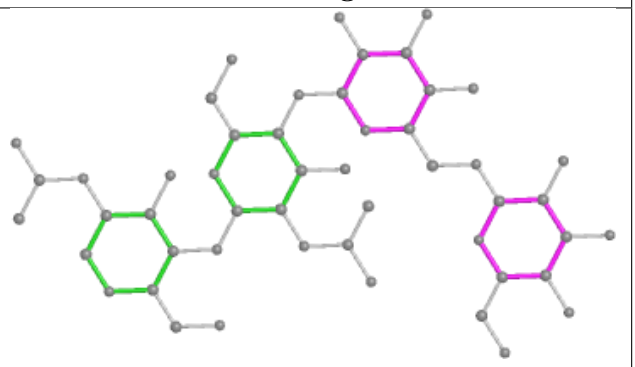
Bond lengths



Bond angles

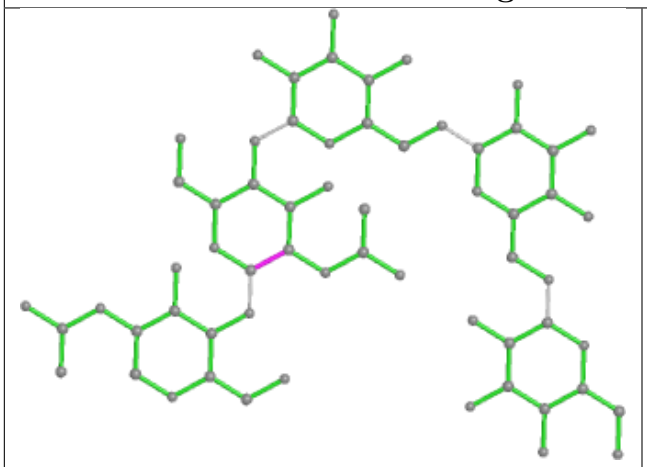


Torsions

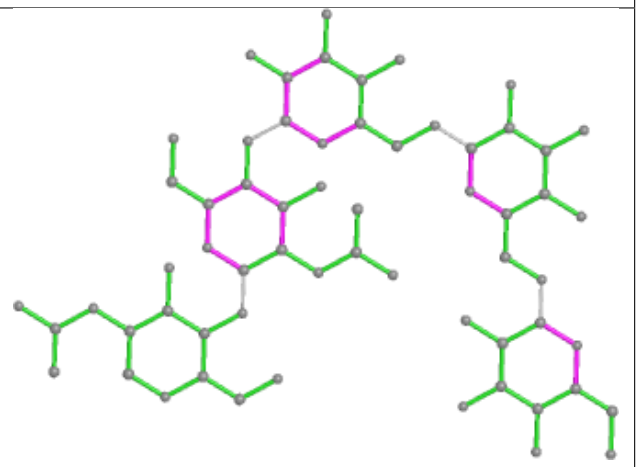


Rings

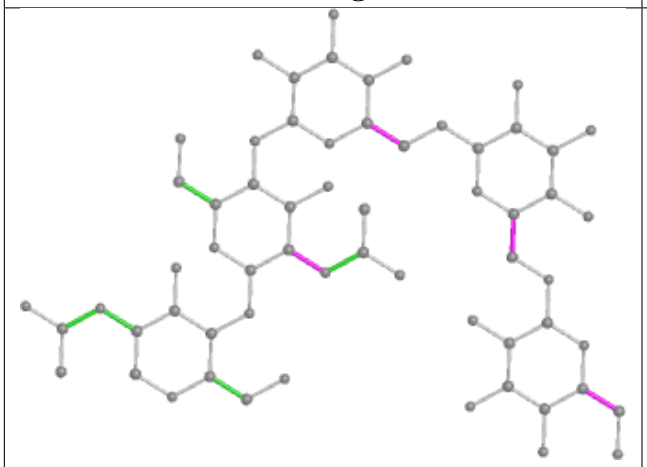
Oligosaccharide Chain E



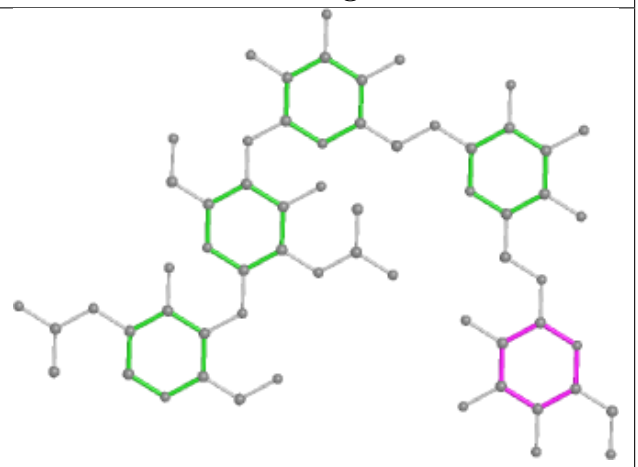
Bond lengths



Bond angles

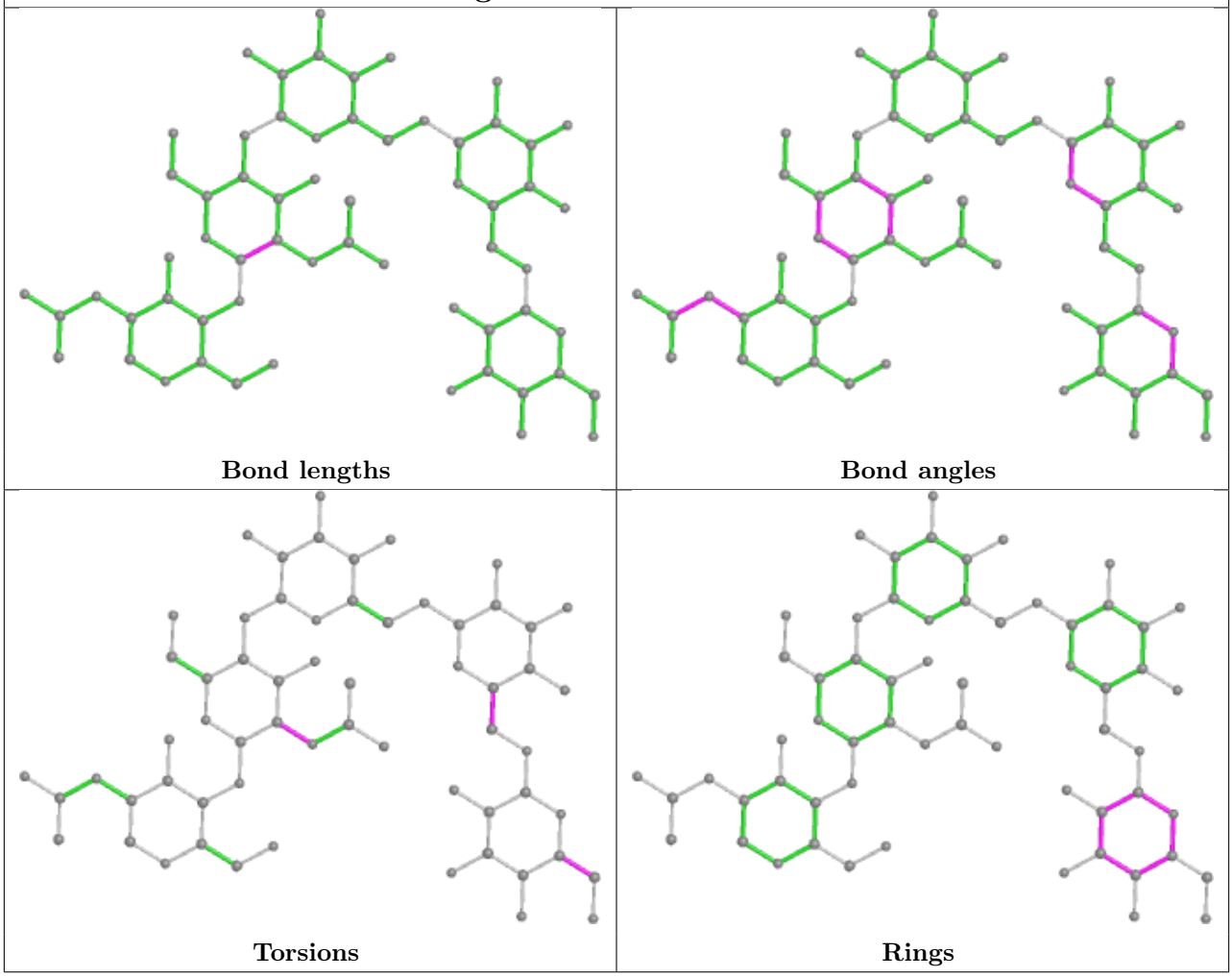


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

19 ligands 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	$\#\|Z\| > 2$
6	BOG	A	754	-	20,20,20	1.70	5 (25%)	25,25,25	0.92	2 (8%)
7	BFL	B	1701	-	17,18,18	2.08	6 (35%)	20,24,24	1.29	2 (10%)
8	HEM	A	801[B]	1	41,50,50	1.65	7 (17%)	45,82,82	7.41	30 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	GOL	B	1760	-	5,5,5	4.51	5 (100%)	5,5,5	5.82	3 (60%)
8	HEM	B	1601[B]	1	41,50,50	1.69	8 (19%)	45,82,82	6.56	25 (55%)
6	BOG	B	1752	-	20,20,20	1.71	5 (25%)	25,25,25	0.91	2 (8%)
6	BOG	B	1751	-	20,20,20	1.66	6 (30%)	25,25,25	0.76	1 (4%)
6	BOG	A	752	-	20,20,20	1.79	5 (25%)	25,25,25	0.88	2 (8%)
6	BOG	B	1750	-	20,20,20	1.72	5 (25%)	25,25,25	0.92	2 (8%)
6	BOG	B	1753	-	20,20,20	1.70	5 (25%)	25,25,25	0.90	2 (8%)
6	BOG	A	753	-	20,20,20	1.68	5 (25%)	25,25,25	0.87	1 (4%)
6	BOG	A	751	-	20,20,20	1.68	6 (30%)	25,25,25	0.82	1 (4%)
9	GOL	A	758	-	5,5,5	4.53	5 (100%)	5,5,5	5.70	3 (60%)
8	HEM	A	801[A]	1	41,50,50	1.67	6 (14%)	45,82,82	7.10	29 (64%)
9	GOL	B	1758	-	5,5,5	4.60	5 (100%)	5,5,5	5.71	3 (60%)
8	HEM	B	1601[A]	1	41,50,50	1.70	8 (19%)	45,82,82	6.88	25 (55%)
7	BFL	A	701	-	17,18,18	2.05	6 (35%)	20,24,24	1.30	3 (15%)
9	GOL	B	1759	-	5,5,5	4.57	5 (100%)	5,5,5	5.74	3 (60%)
9	GOL	A	759	-	5,5,5	4.50	5 (100%)	5,5,5	5.78	3 (60%)

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
6	BOG	A	754	-	-	6/11/31/31	0/1/1/1
7	BFL	B	1701	-	-	0/8/12/12	0/2/2/2
8	HEM	A	801[B]	1	-	2/12/54/54	-
9	GOL	B	1760	-	-	3/4/4/4	-
8	HEM	B	1601[B]	1	-	2/12/54/54	-
6	BOG	B	1752	-	-	4/11/31/31	0/1/1/1
6	BOG	B	1751	-	-	6/11/31/31	0/1/1/1
6	BOG	A	752	-	-	4/11/31/31	0/1/1/1
6	BOG	B	1750	-	-	3/11/31/31	0/1/1/1
6	BOG	B	1753	-	-	8/11/31/31	0/1/1/1
6	BOG	A	753	-	-	2/11/31/31	0/1/1/1
6	BOG	A	751	-	-	4/11/31/31	0/1/1/1
9	GOL	A	758	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	A	801[A]	1	-	1/12/54/54	-
9	GOL	B	1758	-	-	2/4/4/4	-
8	HEM	B	1601[A]	1	-	2/12/54/54	-
7	BFL	A	701	-	-	0/8/12/12	0/2/2/2
9	GOL	B	1759	-	-	2/4/4/4	-
9	GOL	A	759	-	-	2/4/4/4	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1758	GOL	C3-C2	-7.72	1.19	1.51
9	B	1759	GOL	C3-C2	-7.56	1.20	1.51
9	A	758	GOL	C3-C2	-7.39	1.21	1.51
9	B	1760	GOL	C3-C2	-7.32	1.21	1.51
9	A	759	GOL	C3-C2	-7.31	1.21	1.51
8	A	801[B]	HEM	C3C-C2C	-4.68	1.33	1.40
8	A	801[A]	HEM	CBB-CAB	4.67	1.53	1.30
8	A	801[A]	HEM	C3C-C2C	-4.66	1.33	1.40
8	A	801[B]	HEM	CBB-CAB	4.66	1.53	1.30
9	B	1760	GOL	O1-C1	4.66	1.62	1.42
8	B	1601[B]	HEM	CBB-CAB	4.61	1.53	1.30
8	B	1601[A]	HEM	CBB-CAB	4.58	1.53	1.30
9	A	759	GOL	O1-C1	4.58	1.61	1.42
9	B	1758	GOL	O1-C1	4.48	1.61	1.42
8	B	1601[A]	HEM	C3C-C2C	-4.45	1.34	1.40
9	B	1759	GOL	O1-C1	4.41	1.61	1.42
8	B	1601[B]	HEM	C3C-C2C	-4.36	1.34	1.40
9	A	758	GOL	O1-C1	4.33	1.60	1.42
6	A	752	BOG	O5-C1	3.93	1.51	1.41
8	B	1601[A]	HEM	FE-ND	3.90	2.16	1.96
6	A	753	BOG	O5-C1	3.77	1.51	1.41
6	B	1750	BOG	O5-C1	3.76	1.51	1.41
6	A	752	BOG	O5-C5	3.75	1.53	1.44
6	B	1751	BOG	O5-C1	3.72	1.51	1.41
6	B	1752	BOG	O5-C1	3.71	1.51	1.41
6	A	754	BOG	O5-C1	3.70	1.51	1.41
6	B	1753	BOG	O5-C1	3.66	1.51	1.41
6	A	751	BOG	O5-C1	3.63	1.51	1.41
6	A	754	BOG	O5-C5	3.55	1.53	1.44
6	A	753	BOG	O5-C5	3.53	1.52	1.44
6	B	1750	BOG	O5-C5	3.50	1.52	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1753	BOG	O5-C5	3.49	1.52	1.44
8	B	1601[B]	HEM	FE-ND	3.42	2.13	1.96
9	A	759	GOL	O3-C3	3.42	1.56	1.42
8	A	801[A]	HEM	FE-ND	3.39	2.13	1.96
9	B	1760	GOL	O3-C3	3.39	1.56	1.42
6	B	1752	BOG	O5-C5	3.39	1.52	1.44
8	B	1601[A]	HEM	CBC-CAC	3.38	1.51	1.29
8	B	1601[B]	HEM	CBC-CAC	3.36	1.51	1.29
6	B	1751	BOG	O5-C5	3.36	1.52	1.44
7	A	701	BFL	C10-C9	3.35	1.44	1.39
8	A	801[B]	HEM	CBC-CAC	3.32	1.51	1.29
8	A	801[A]	HEM	CBC-CAC	3.32	1.51	1.29
9	A	758	GOL	O3-C3	3.29	1.56	1.42
6	A	751	BOG	O5-C5	3.28	1.52	1.44
9	B	1759	GOL	O3-C3	3.26	1.56	1.42
7	B	1701	BFL	C10-C9	3.20	1.44	1.39
9	A	758	GOL	C1-C2	-3.19	1.38	1.51
7	B	1701	BFL	C11-C10	3.15	1.43	1.36
9	B	1758	GOL	O3-C3	3.13	1.55	1.42
7	A	701	BFL	C11-C10	3.08	1.43	1.36
9	B	1759	GOL	O2-C2	-3.07	1.34	1.43
7	B	1701	BFL	O1-C6	-3.05	1.20	1.30
8	B	1601[B]	HEM	FE-NB	3.01	2.11	1.96
7	B	1701	BFL	C3-C4	2.99	1.43	1.36
7	A	701	BFL	C15-C14	2.96	1.43	1.36
7	B	1701	BFL	C15-C14	2.93	1.43	1.36
7	A	701	BFL	C3-C4	2.93	1.43	1.36
9	B	1758	GOL	O2-C2	-2.91	1.34	1.43
7	A	701	BFL	O1-C6	-2.87	1.21	1.30
9	A	758	GOL	O2-C2	-2.84	1.34	1.43
8	A	801[B]	HEM	FE-ND	2.82	2.10	1.96
9	B	1758	GOL	C1-C2	-2.78	1.40	1.51
8	B	1601[A]	HEM	FE-NB	2.78	2.10	1.96
9	B	1760	GOL	O2-C2	-2.78	1.35	1.43
9	B	1759	GOL	C1-C2	-2.77	1.40	1.51
9	A	759	GOL	C1-C2	-2.76	1.40	1.51
9	A	759	GOL	O2-C2	-2.74	1.35	1.43
9	B	1760	GOL	C1-C2	-2.68	1.40	1.51
6	A	752	BOG	C4-C3	2.56	1.58	1.52
6	B	1752	BOG	C4-C3	2.56	1.58	1.52
6	B	1750	BOG	C4-C3	2.55	1.58	1.52
7	B	1701	BFL	O2-C6	2.54	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	751	BOG	C4-C3	2.51	1.58	1.52
6	A	752	BOG	C3'-C2'	-2.49	1.37	1.51
6	A	754	BOG	C3'-C2'	-2.48	1.37	1.51
6	B	1753	BOG	C3'-C2'	-2.48	1.37	1.51
6	B	1753	BOG	C4-C3	2.47	1.58	1.52
6	B	1750	BOG	C3'-C2'	-2.45	1.37	1.51
6	A	753	BOG	C3'-C2'	-2.44	1.37	1.51
6	A	754	BOG	C4-C3	2.43	1.58	1.52
6	A	753	BOG	C4-C3	2.42	1.58	1.52
7	A	701	BFL	O2-C6	2.41	1.29	1.22
6	B	1751	BOG	C3'-C2'	-2.41	1.38	1.51
6	B	1752	BOG	C3'-C2'	-2.39	1.38	1.51
6	B	1751	BOG	C4-C3	2.39	1.58	1.52
6	A	751	BOG	C3'-C2'	-2.38	1.38	1.51
6	A	752	BOG	C1-C2	2.38	1.59	1.52
6	B	1752	BOG	C1-C2	2.37	1.59	1.52
8	A	801[B]	HEM	CAB-C3B	2.30	1.53	1.47
8	A	801[A]	HEM	CAB-C3B	2.30	1.53	1.47
6	A	751	BOG	C1-C2	2.26	1.59	1.52
8	B	1601[A]	HEM	C3C-CAC	2.25	1.52	1.47
6	B	1750	BOG	C1-C2	2.22	1.58	1.52
8	B	1601[B]	HEM	C3C-CAC	2.22	1.52	1.47
6	A	754	BOG	C1-C2	2.21	1.58	1.52
6	B	1753	BOG	C1-C2	2.20	1.58	1.52
8	B	1601[B]	HEM	CAB-C3B	2.17	1.53	1.47
8	B	1601[A]	HEM	CAB-C3B	2.16	1.53	1.47
6	A	753	BOG	C1-C2	2.12	1.58	1.52
6	A	751	BOG	C4-C5	-2.12	1.48	1.53
8	A	801[A]	HEM	C3C-CAC	2.11	1.52	1.47
8	A	801[B]	HEM	C3C-CAC	2.11	1.52	1.47
6	B	1751	BOG	C1-C2	2.06	1.58	1.52
6	B	1751	BOG	C4-C5	-2.03	1.48	1.53
8	B	1601[A]	HEM	C4D-ND	-2.02	1.36	1.40
8	B	1601[B]	HEM	C4D-ND	-2.02	1.36	1.40
8	A	801[B]	HEM	FE-NB	2.02	2.06	1.96

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	801[A]	HEM	C4C-CHD-C1D	23.43	153.48	122.56
8	A	801[B]	HEM	C4C-CHD-C1D	23.36	153.39	122.56
8	A	801[B]	HEM	C4B-CHC-C1C	21.88	151.44	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1601[A]	HEM	C4C-CHD-C1D	21.81	151.35	122.56
8	B	1601[B]	HEM	C4C-CHD-C1D	21.42	150.82	122.56
8	B	1601[A]	HEM	C4B-CHC-C1C	21.39	150.79	122.56
8	B	1601[B]	HEM	C4B-CHC-C1C	21.35	150.74	122.56
8	A	801[A]	HEM	C4B-CHC-C1C	20.23	149.26	122.56
8	A	801[B]	HEM	CHA-C4D-ND	-15.55	105.17	124.38
8	A	801[B]	HEM	CHD-C1D-ND	-15.35	107.76	124.43
8	A	801[A]	HEM	CHD-C1D-ND	-13.57	109.69	124.43
8	B	1601[B]	HEM	CHC-C4B-NB	-13.33	109.95	124.43
8	B	1601[A]	HEM	CHC-C4B-NB	-13.10	110.20	124.43
8	A	801[A]	HEM	CHB-C1B-NB	-12.68	108.72	124.38
8	A	801[B]	HEM	CHC-C4B-NB	-12.65	110.69	124.43
8	A	801[B]	HEM	CHB-C1B-NB	-12.28	109.21	124.38
8	A	801[A]	HEM	CHC-C4B-NB	-12.03	111.36	124.43
8	B	1601[A]	HEM	CHC-C4B-C3B	11.55	142.25	124.57
8	B	1601[A]	HEM	CHB-C1B-NB	-11.47	110.21	124.38
8	A	801[A]	HEM	CHA-C4D-ND	-11.33	110.38	124.38
8	B	1601[A]	HEM	C3B-C2B-C1B	-11.31	98.10	106.49
8	B	1601[A]	HEM	CHD-C1D-ND	-11.29	112.17	124.43
8	B	1601[B]	HEM	CHD-C1D-ND	-11.24	112.22	124.43
8	A	801[A]	HEM	C3B-C2B-C1B	-11.11	98.25	106.49
8	B	1601[B]	HEM	CHC-C4B-C3B	10.72	140.97	124.57
8	B	1601[B]	HEM	CHB-C1B-NB	-10.70	111.16	124.38
8	A	801[B]	HEM	CHC-C4B-C3B	10.69	140.93	124.57
9	B	1760	GOL	O3-C3-C2	10.60	161.01	110.20
9	A	759	GOL	O3-C3-C2	10.52	160.65	110.20
9	B	1759	GOL	O3-C3-C2	10.43	160.20	110.20
9	B	1758	GOL	O3-C3-C2	10.39	160.03	110.20
8	A	801[A]	HEM	CHC-C4B-C3B	10.25	140.27	124.57
9	A	758	GOL	O3-C3-C2	10.19	159.07	110.20
8	A	801[B]	HEM	C3B-C2B-C1B	-8.48	100.19	106.49
8	B	1601[B]	HEM	C3B-C2B-C1B	-8.44	100.22	106.49
8	B	1601[B]	HEM	CHA-C4D-ND	-8.36	114.05	124.38
8	B	1601[A]	HEM	C4B-C3B-C2B	8.17	113.60	107.11
8	B	1601[A]	HEM	CHA-C4D-ND	-7.95	114.56	124.38
8	A	801[A]	HEM	C4B-C3B-C2B	7.46	113.03	107.11
8	B	1601[A]	HEM	CHA-C4D-C3D	7.33	139.08	125.33
8	A	801[B]	HEM	C4D-ND-C1D	-7.14	97.70	105.07
8	B	1601[A]	HEM	C4A-C3A-C2A	-7.11	102.05	107.00
8	B	1601[B]	HEM	CHA-C4D-C3D	7.03	138.52	125.33
8	A	801[A]	HEM	C4A-C3A-C2A	-7.01	102.12	107.00
8	A	801[A]	HEM	C2B-C1B-NB	7.00	118.13	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	758	GOL	O2-C2-C3	6.96	139.79	109.12
8	A	801[A]	HEM	CHA-C4D-C3D	6.83	138.14	125.33
8	B	1601[A]	HEM	CHD-C1D-C2D	6.76	135.54	124.98
8	B	1601[A]	HEM	C2B-C1B-NB	6.74	117.83	109.84
9	A	759	GOL	O2-C2-C3	6.72	138.73	109.12
9	B	1760	GOL	O2-C2-C3	6.70	138.64	109.12
9	B	1759	GOL	O2-C2-C3	6.68	138.53	109.12
8	B	1601[B]	HEM	CHD-C1D-C2D	6.66	135.38	124.98
8	A	801[B]	HEM	CHA-C4D-C3D	6.65	137.81	125.33
8	A	801[B]	HEM	C2D-C1D-ND	6.64	117.83	109.88
9	B	1758	GOL	O2-C2-C3	6.57	138.05	109.12
8	A	801[A]	HEM	C1D-C2D-C3D	-6.48	100.15	106.96
8	B	1601[B]	HEM	C4A-C3A-C2A	-6.46	102.50	107.00
8	A	801[B]	HEM	C4B-C3B-C2B	5.96	111.85	107.11
8	A	801[A]	HEM	CMA-C3A-C2A	5.78	135.83	124.94
8	B	1601[B]	HEM	C2B-C1B-NB	5.69	116.58	109.84
8	A	801[B]	HEM	CMB-C2B-C3B	5.56	141.92	128.30
8	B	1601[A]	HEM	C1D-C2D-C3D	-5.47	101.21	106.96
8	B	1601[B]	HEM	C4B-C3B-C2B	5.35	111.36	107.11
8	A	801[B]	HEM	C3D-C4D-ND	5.24	116.00	110.17
8	A	801[A]	HEM	C2D-C1D-ND	5.22	116.13	109.88
8	A	801[A]	HEM	CHD-C1D-C2D	5.21	133.11	124.98
8	A	801[B]	HEM	C2B-C1B-NB	5.20	116.00	109.84
8	A	801[B]	HEM	C1D-C2D-C3D	-5.17	101.52	106.96
8	A	801[B]	HEM	CHD-C1D-C2D	5.16	133.04	124.98
8	A	801[B]	HEM	CMB-C2B-C1B	-5.12	117.24	125.04
8	A	801[A]	HEM	CMB-C2B-C3B	5.07	140.72	128.30
8	B	1601[B]	HEM	C1D-C2D-C3D	-4.98	101.72	106.96
8	B	1601[A]	HEM	CMB-C2B-C3B	4.48	139.26	128.30
8	B	1601[A]	HEM	CMA-C3A-C2A	4.39	133.23	124.94
8	A	801[B]	HEM	CBA-CAA-C2A	4.37	120.08	112.62
8	A	801[A]	HEM	CMA-C3A-C4A	-4.30	121.86	128.46
8	A	801[B]	HEM	C4A-C3A-C2A	-4.23	104.05	107.00
8	B	1601[B]	HEM	CAA-CBA-CGA	4.23	125.62	113.76
8	B	1601[A]	HEM	C4D-C3D-C2D	4.15	112.94	106.90
8	B	1601[A]	HEM	CMC-C2C-C3C	3.65	131.50	124.68
8	B	1601[B]	HEM	CMC-C2C-C3C	3.54	131.29	124.68
8	B	1601[B]	HEM	C4D-C3D-C2D	3.50	112.00	106.90
8	A	801[B]	HEM	CMA-C3A-C2A	3.50	131.54	124.94
8	B	1601[A]	HEM	C3D-C4D-ND	-3.46	106.31	110.17
8	B	1601[A]	HEM	CAD-C3D-C4D	-3.46	118.62	124.66
8	A	801[B]	HEM	O2A-CGA-O1A	-3.44	114.72	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1760	GOL	O1-C1-C2	3.38	126.43	110.20
8	A	801[B]	HEM	O1D-CGD-CBD	-3.38	112.22	123.08
9	B	1758	GOL	O1-C1-C2	3.34	126.24	110.20
9	A	759	GOL	O1-C1-C2	3.30	126.02	110.20
9	B	1759	GOL	O1-C1-C2	3.27	125.87	110.20
8	A	801[A]	HEM	C4D-ND-C1D	-3.19	101.78	105.07
8	B	1601[B]	HEM	CAD-C3D-C4D	-3.11	119.22	124.66
9	A	758	GOL	O1-C1-C2	3.09	124.99	110.20
8	A	801[B]	HEM	CBB-CAB-C3B	3.08	142.94	127.62
8	A	801[A]	HEM	CMB-C2B-C1B	-3.07	120.36	125.04
6	A	754	BOG	C1'-O1-C1	3.05	118.90	113.84
8	B	1601[B]	HEM	CMA-C3A-C2A	3.04	130.68	124.94
8	A	801[A]	HEM	CBB-CAB-C3B	2.97	142.39	127.62
8	A	801[B]	HEM	CHB-C1B-C2B	2.90	134.75	126.72
6	B	1750	BOG	C1'-O1-C1	2.90	118.65	113.84
6	A	753	BOG	C1'-O1-C1	2.87	118.59	113.84
8	A	801[A]	HEM	C1B-NB-C4B	-2.83	102.15	105.07
6	A	752	BOG	C1'-O1-C1	2.83	118.53	113.84
8	A	801[B]	HEM	O2D-CGD-CBD	2.79	122.99	114.03
8	B	1601[B]	HEM	CMB-C2B-C3B	2.76	135.07	128.30
8	A	801[A]	HEM	C4D-C3D-C2D	2.74	110.88	106.90
6	B	1752	BOG	C1'-O1-C1	2.73	118.36	113.84
6	B	1753	BOG	C1'-O1-C1	2.71	118.33	113.84
8	A	801[B]	HEM	CMA-C3A-C4A	-2.66	124.37	128.46
6	A	751	BOG	O1-C1-C2	2.62	112.39	108.30
7	A	701	BFL	O2-C6-C5	-2.59	112.98	122.85
6	B	1752	BOG	O1-C1-C2	2.57	112.32	108.30
8	B	1601[A]	HEM	CMA-C3A-C4A	-2.55	124.54	128.46
8	B	1601[B]	HEM	C3D-C4D-ND	-2.54	107.34	110.17
8	A	801[B]	HEM	CMD-C2D-C1D	2.51	128.87	125.04
8	B	1601[B]	HEM	C1B-NB-C4B	-2.49	102.51	105.07
8	B	1601[B]	HEM	O2A-CGA-O1A	-2.48	117.13	123.30
7	B	1701	BFL	O2-C6-C5	-2.45	113.51	122.85
6	B	1753	BOG	O1-C1-C2	2.45	112.13	108.30
8	A	801[A]	HEM	CMC-C2C-C3C	2.43	129.22	124.68
6	B	1750	BOG	O1-C1-C2	2.41	112.06	108.30
6	B	1751	BOG	O1-C1-C2	2.33	111.94	108.30
8	A	801[B]	HEM	CMC-C2C-C3C	2.33	129.04	124.68
8	A	801[A]	HEM	CMD-C2D-C1D	2.33	128.58	125.04
8	A	801[A]	HEM	CHB-C1B-C2B	2.31	133.10	126.72
8	A	801[B]	HEM	CAA-CBA-CGA	2.28	120.14	113.76
6	A	754	BOG	O1-C1-C2	2.27	111.85	108.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1601[A]	HEM	C1B-NB-C4B	-2.27	102.73	105.07
8	A	801[A]	HEM	O2A-CGA-O1A	-2.24	117.71	123.30
7	A	701	BFL	O1-C6-C5	2.22	124.27	114.30
7	B	1701	BFL	O1-C6-C5	2.17	124.03	114.30
8	B	1601[A]	HEM	C4D-ND-C1D	2.14	107.28	105.07
8	B	1601[A]	HEM	CAA-CBA-CGA	2.10	119.64	113.76
8	B	1601[B]	HEM	C2D-C1D-ND	2.10	112.39	109.88
6	A	752	BOG	O1-C1-C2	2.05	111.51	108.30
8	A	801[A]	HEM	CAA-CBA-CGA	2.05	119.51	113.76
8	A	801[A]	HEM	CAB-C3B-C2B	-2.03	121.90	128.60
8	B	1601[A]	HEM	CMD-C2D-C1D	2.03	128.13	125.04
8	B	1601[B]	HEM	CBB-CAB-C3B	-2.01	117.62	127.62
7	A	701	BFL	C8-C1-C12	2.00	123.93	120.82

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1601[A]	HEM	C2B-C3B-CAB-CBB
8	B	1601[B]	HEM	C2B-C3B-CAB-CBB
9	A	758	GOL	C1-C2-C3-O3
9	A	759	GOL	O1-C1-C2-O2
9	A	759	GOL	C1-C2-C3-O3
9	B	1758	GOL	C1-C2-C3-O3
9	B	1759	GOL	C1-C2-C3-O3
9	B	1760	GOL	C1-C2-C3-O3
6	A	754	BOG	O5-C5-C6-O6
6	B	1753	BOG	O5-C5-C6-O6
9	A	758	GOL	O1-C1-C2-O2
6	B	1753	BOG	C4-C5-C6-O6
6	A	754	BOG	C4-C5-C6-O6
6	B	1751	BOG	C2-C1-O1-C1'
6	B	1752	BOG	C2'-C3'-C4'-C5'
9	B	1758	GOL	O1-C1-C2-O2
9	B	1759	GOL	O1-C1-C2-O2
9	B	1760	GOL	O1-C1-C2-O2
6	A	751	BOG	C3'-C4'-C5'-C6'
6	A	752	BOG	C2'-C3'-C4'-C5'
6	A	753	BOG	C2'-C3'-C4'-C5'
6	B	1750	BOG	C3'-C4'-C5'-C6'
6	A	754	BOG	C3'-C4'-C5'-C6'
6	A	754	BOG	C1'-C2'-C3'-C4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	1752	BOG	C1'-C2'-C3'-C4'
6	B	1751	BOG	C3'-C4'-C5'-C6'
8	B	1601[B]	HEM	C4B-C3B-CAB-CBB
6	B	1752	BOG	O1-C1'-C2'-C3'
6	B	1751	BOG	O1-C1'-C2'-C3'
6	A	754	BOG	C2'-C3'-C4'-C5'
6	B	1753	BOG	C1'-C2'-C3'-C4'
6	B	1751	BOG	O5-C1-O1-C1'
6	B	1750	BOG	C1'-C2'-C3'-C4'
6	B	1753	BOG	C2-C1-O1-C1'
6	B	1752	BOG	C3'-C4'-C5'-C6'
6	B	1750	BOG	O1-C1'-C2'-C3'
6	A	751	BOG	C2'-C3'-C4'-C5'
6	A	751	BOG	C1'-C2'-C3'-C4'
6	A	752	BOG	C3'-C4'-C5'-C6'
6	B	1753	BOG	C3'-C4'-C5'-C6'
6	B	1753	BOG	C2'-C3'-C4'-C5'
8	A	801[A]	HEM	C2B-C3B-CAB-CBB
8	B	1601[A]	HEM	C4B-C3B-CAB-CBB
6	B	1751	BOG	C1'-C2'-C3'-C4'
6	A	752	BOG	C2-C1-O1-C1'
6	A	753	BOG	O1-C1'-C2'-C3'
6	B	1753	BOG	O1-C1'-C2'-C3'
6	B	1753	BOG	O5-C1-O1-C1'
9	B	1760	GOL	O1-C1-C2-C3
6	A	752	BOG	O5-C1-O1-C1'
6	B	1751	BOG	C2'-C3'-C4'-C5'
6	A	754	BOG	O1-C1'-C2'-C3'
6	A	751	BOG	O1-C1'-C2'-C3'
8	A	801[B]	HEM	CAD-CBD-CGD-O1D
8	A	801[B]	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	754	BOG	1	0
8	A	801[B]	HEM	2	0
8	B	1601[B]	HEM	3	0
6	B	1752	BOG	1	0
6	B	1751	BOG	4	0
6	B	1753	BOG	1	0

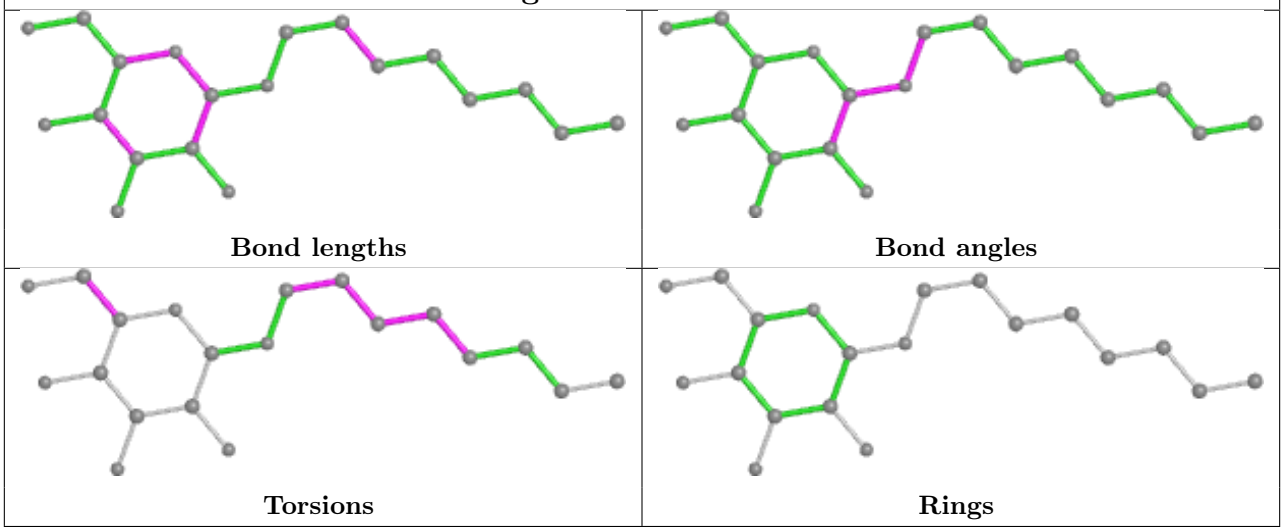
Continued on next page...

Continued from previous page...

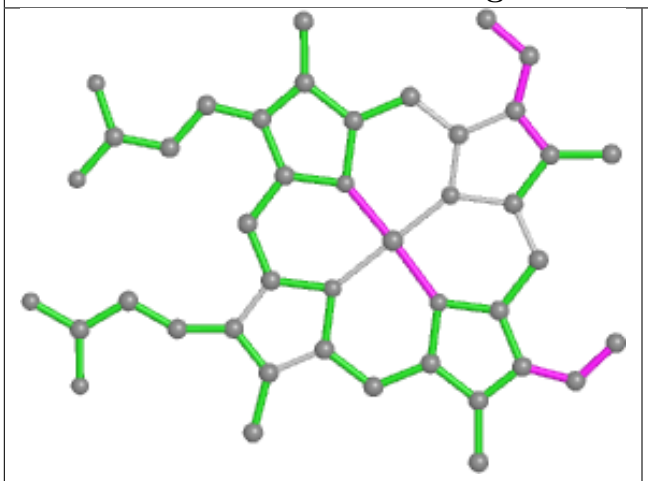
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	753	BOG	1	0
9	A	758	GOL	1	0
8	A	801[A]	HEM	2	0
8	B	1601[A]	HEM	1	0
7	A	701	BFL	1	0
9	B	1759	GOL	1	0

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

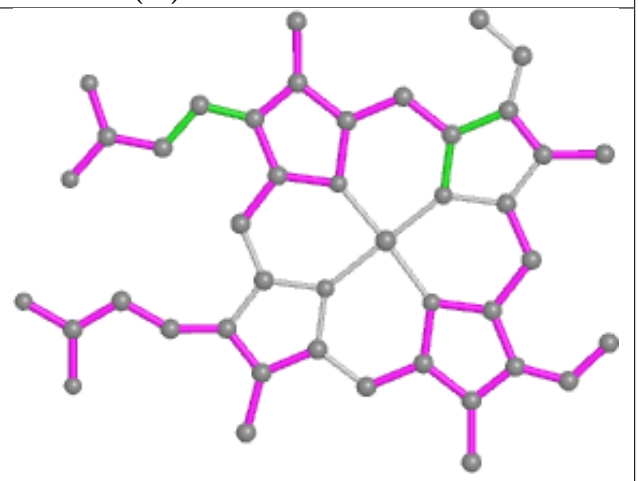
Ligand BOG A 754



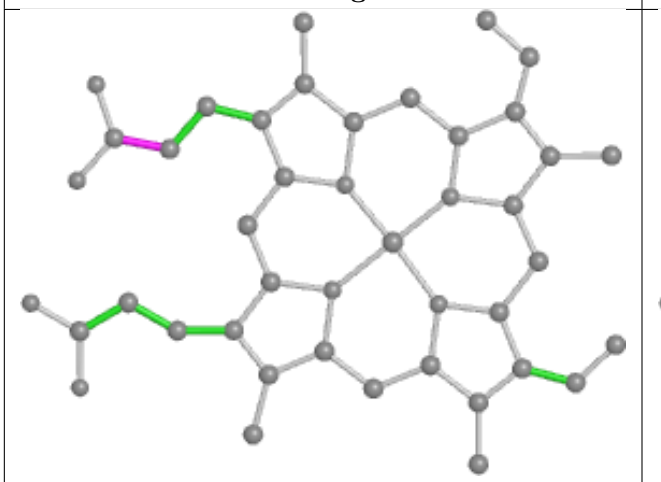
Ligand HEM A 801 (B)



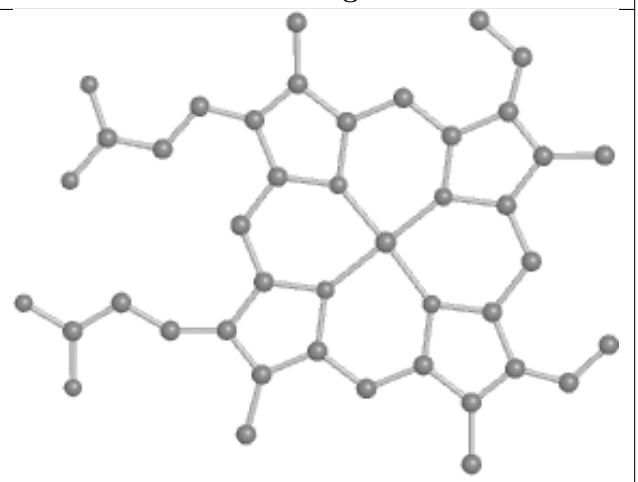
Bond lengths



Bond angles

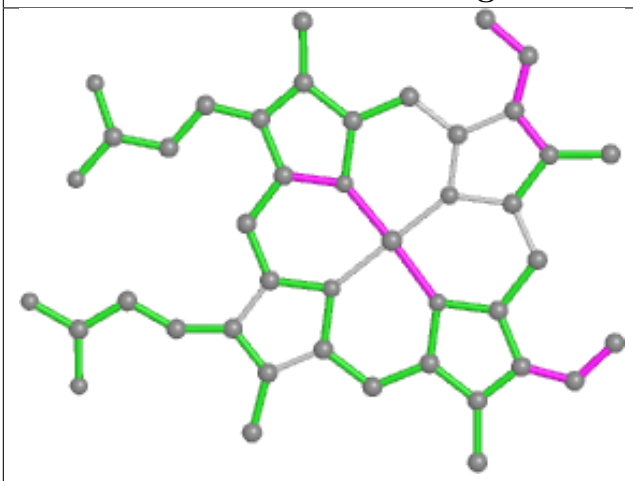


Torsions

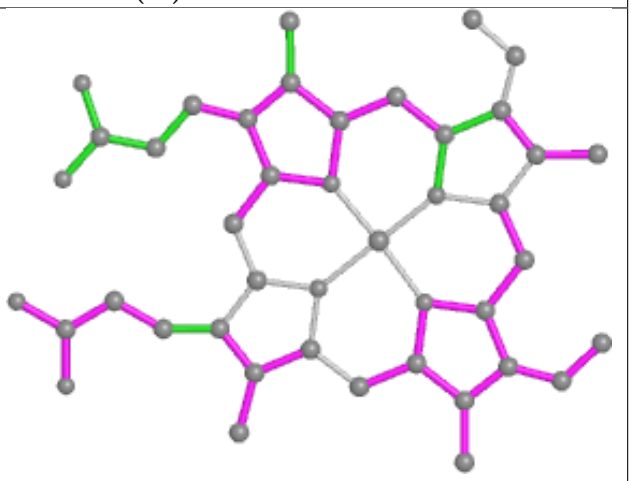


Rings

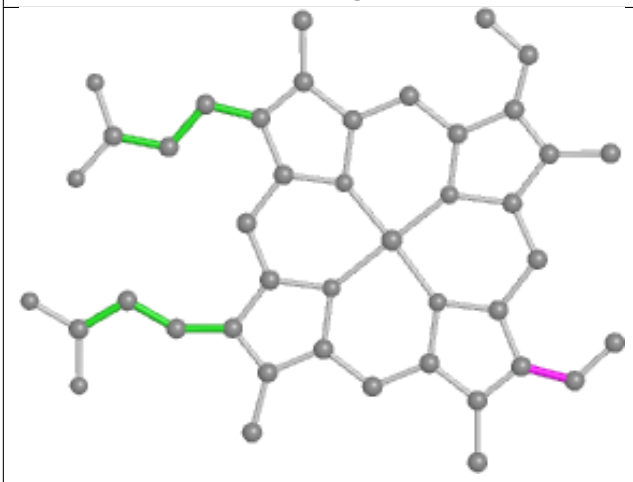
Ligand HEM B 1601 (B)



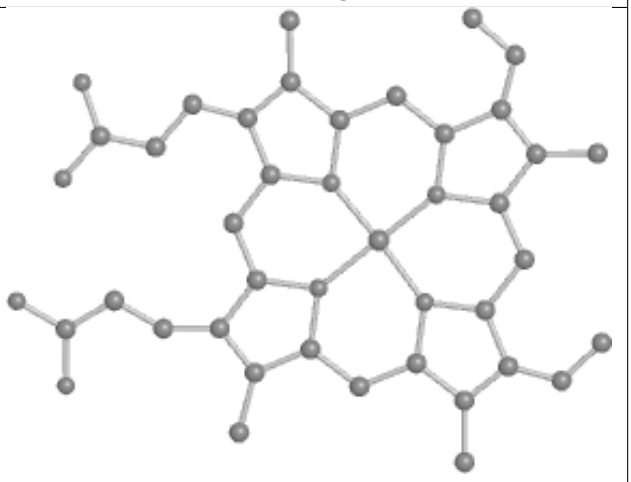
Bond lengths



Bond angles

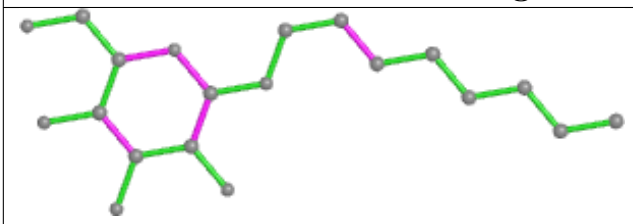


Torsions

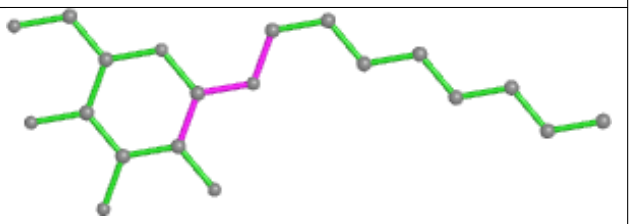


Rings

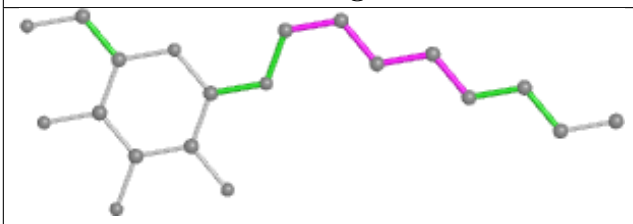
Ligand BOG B 1752



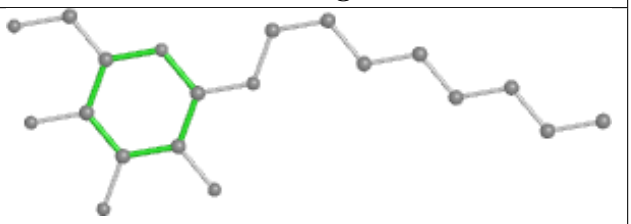
Bond lengths



Bond angles

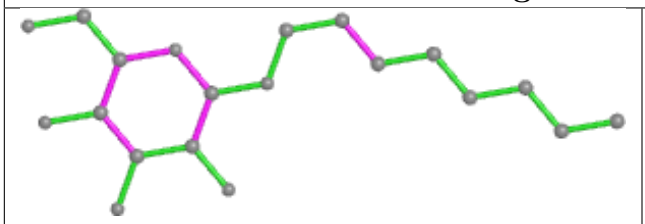


Torsions

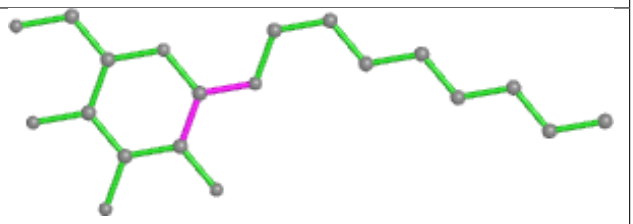


Rings

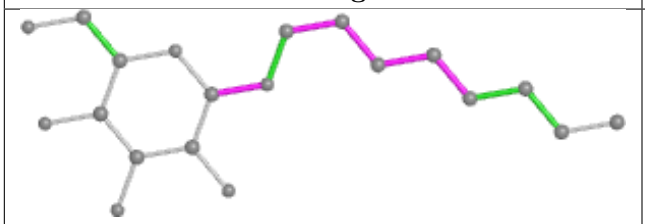
Ligand BOG B 1751



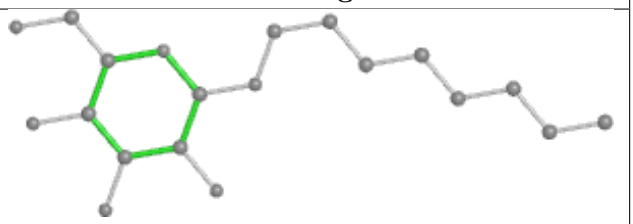
Bond lengths



Bond angles

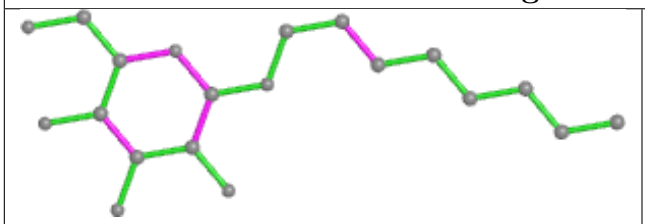


Torsions

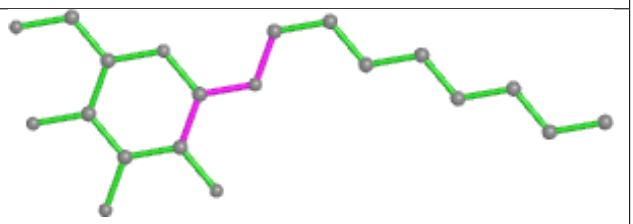


Rings

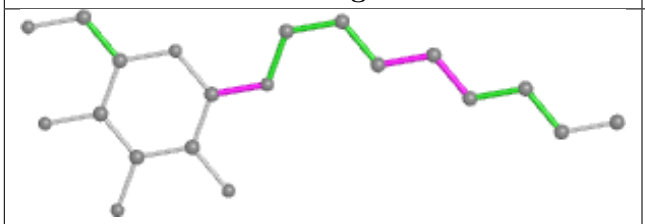
Ligand BOG A 752



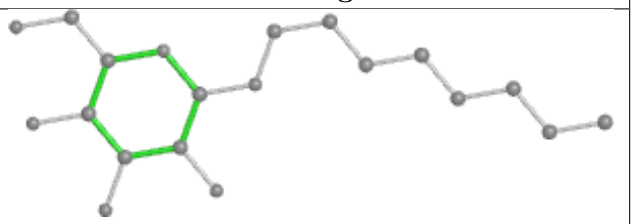
Bond lengths



Bond angles

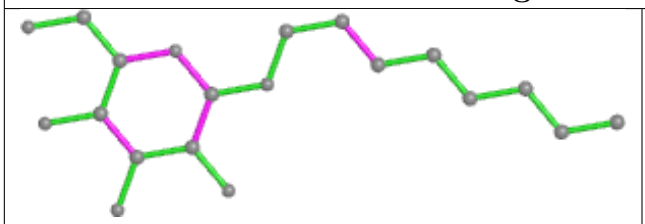


Torsions

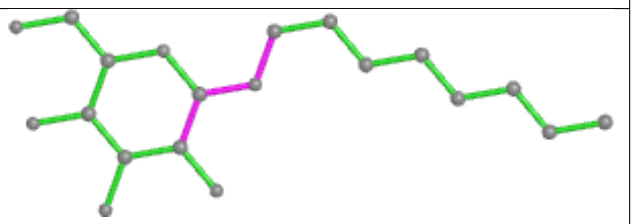


Rings

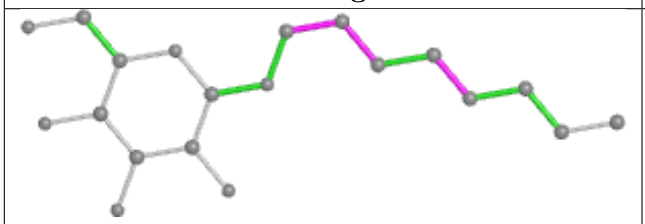
Ligand BOG B 1750



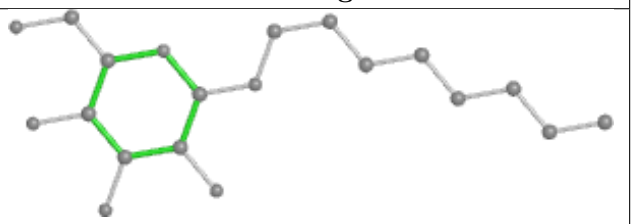
Bond lengths



Bond angles

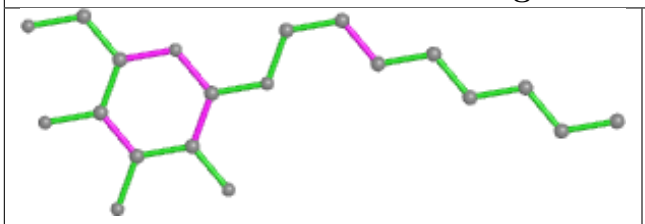


Torsions

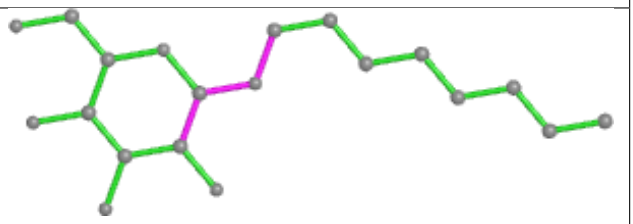


Rings

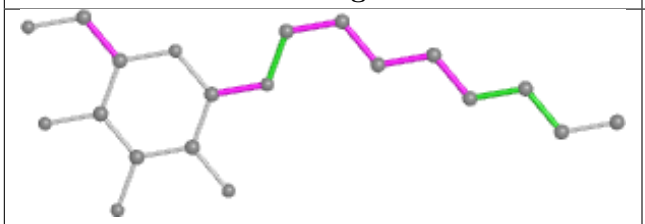
Ligand BOG B 1753



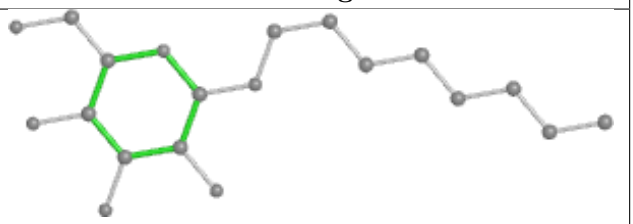
Bond lengths



Bond angles

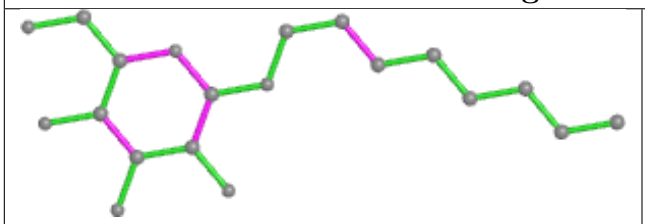


Torsions

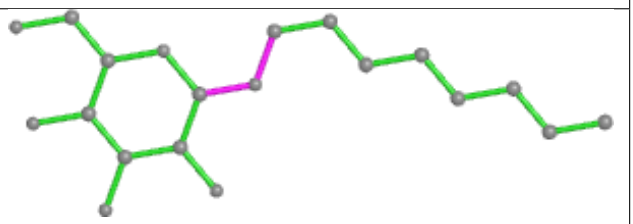


Rings

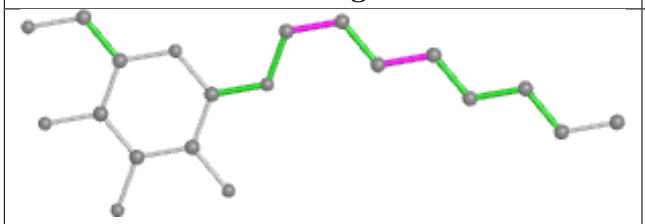
Ligand BOG A 753



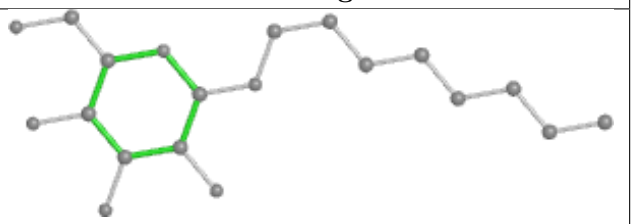
Bond lengths



Bond angles

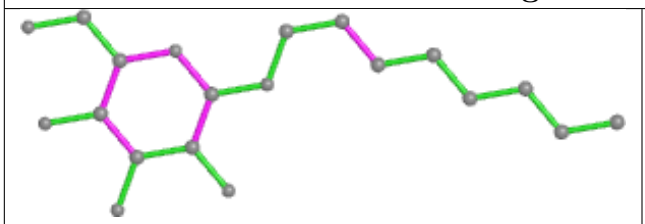


Torsions

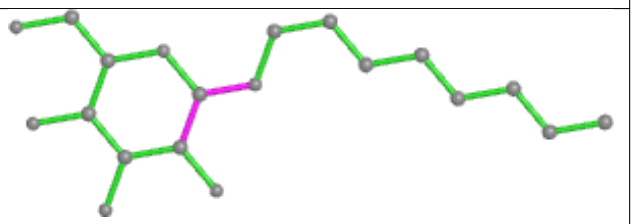


Rings

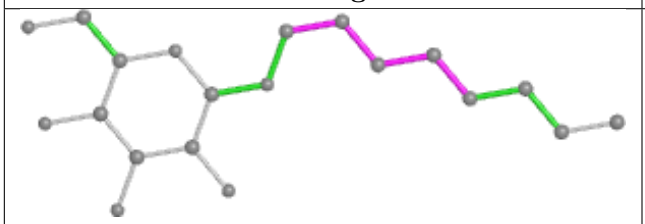
Ligand BOG A 751



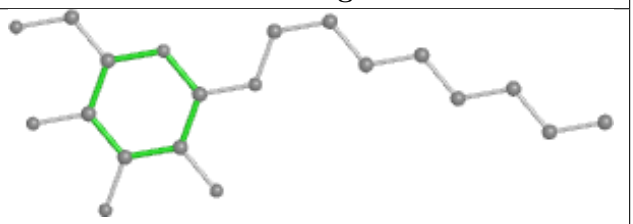
Bond lengths



Bond angles

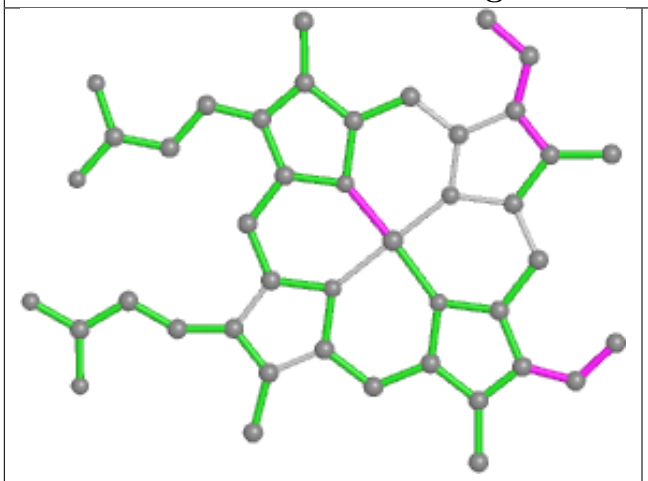


Torsions

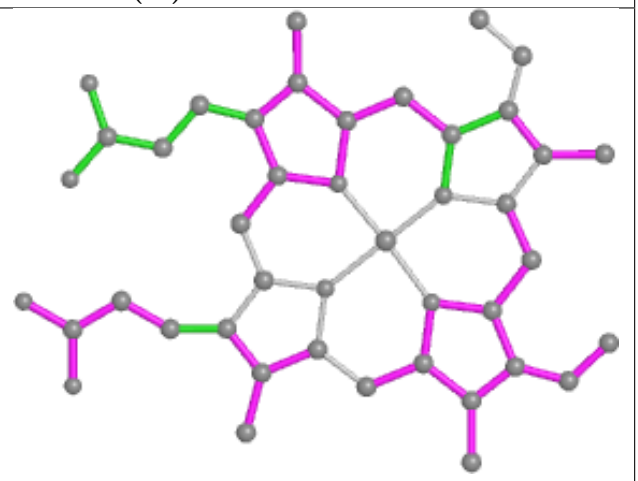


Rings

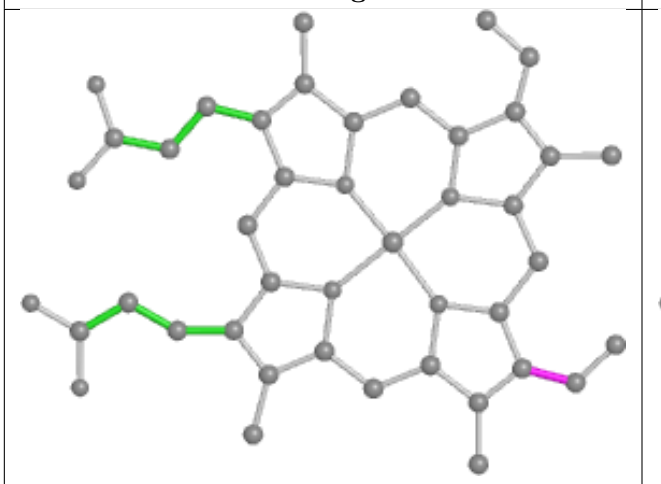
Ligand HEM A 801 (A)



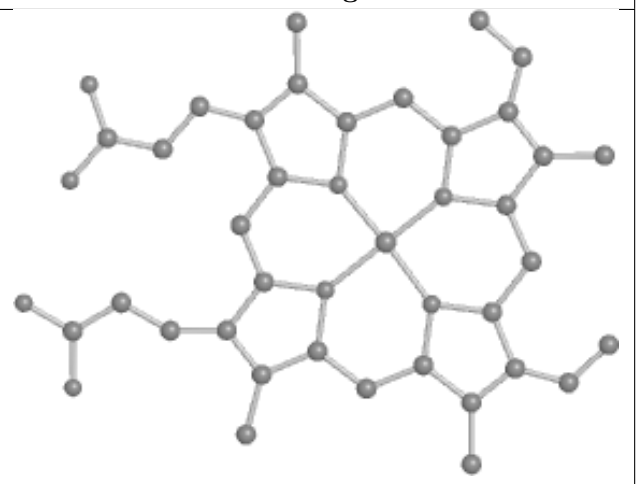
Bond lengths



Bond angles

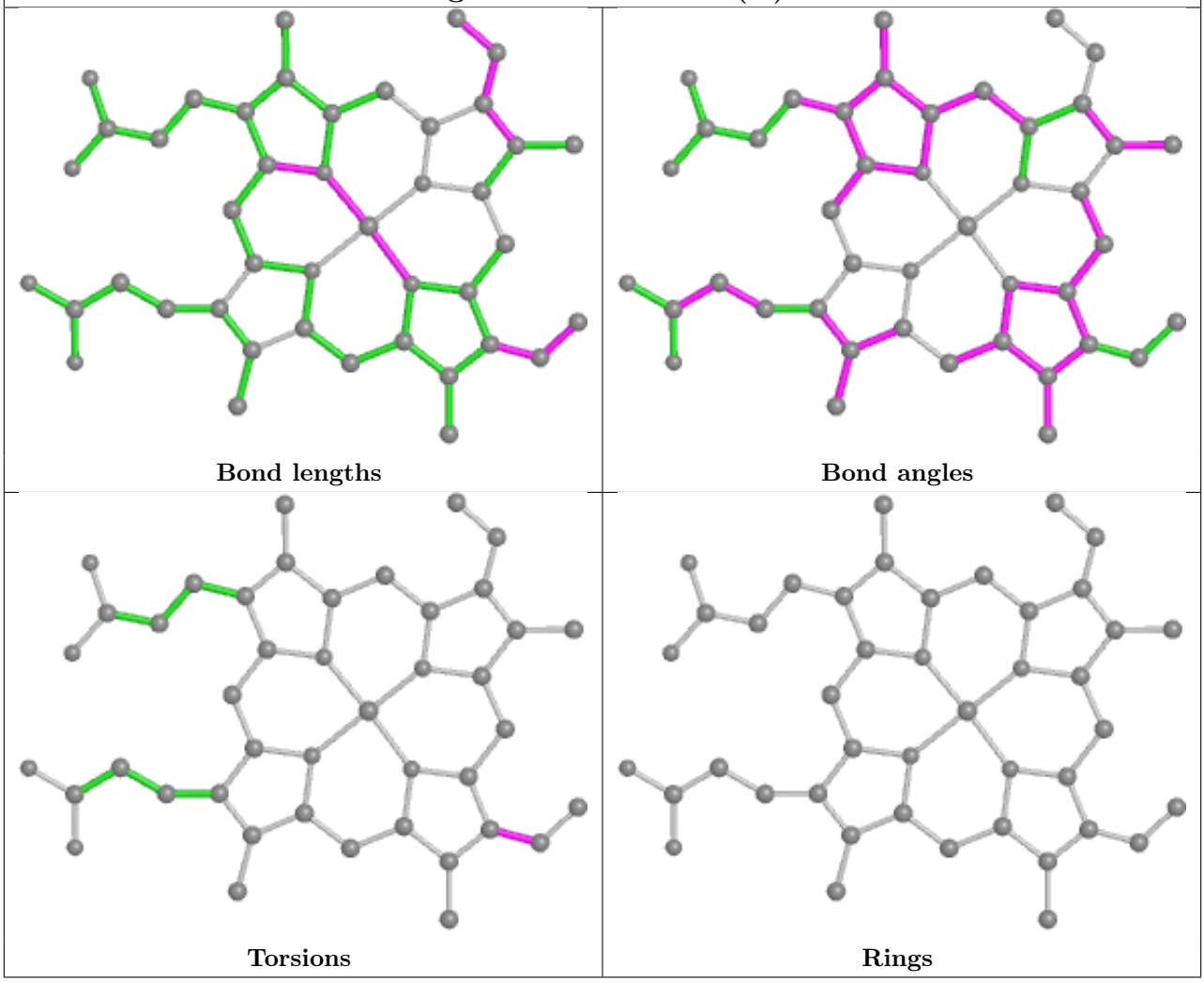


Torsions



Rings

Ligand HEM B 1601 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	553/553 (100%)	0.19	27 (4%)	29	28	30, 41, 55, 65	0
1	B	553/553 (100%)	0.12	17 (3%)	49	48	29, 41, 54, 66	0
All	All	1106/1106 (100%)	0.15	44 (3%)	38	37	29, 41, 55, 66	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	584	ASP	6.1
1	A	98	TRP	6.0
1	A	107	PHE	5.4
1	B	33	VAL	4.8
1	B	75	TRP	4.7
1	B	32	PRO	4.5
1	A	584	ASP	3.7
1	A	75	TRP	3.1
1	B	384	LEU	2.9
1	A	514	PRO	2.9
1	B	573	LYS	2.9
1	A	492	GLU	2.8
1	B	215	LYS	2.7
1	A	377	ILE	2.7
1	A	529	PHE	2.7
1	A	493	GLU	2.6
1	A	381	PHE	2.6
1	A	205	PHE	2.5
1	A	277	ARG	2.5
1	B	575	CYS	2.5
1	A	534	LEU	2.5
1	A	36	CYS	2.4
1	B	399	PRO	2.4
1	B	277	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	36	CYS	2.4
1	A	399	PRO	2.3
1	A	526	GLY	2.3
1	A	479	GLN	2.3
1	A	344	VAL	2.3
1	B	79	ARG	2.3
1	A	179	ARG	2.2
1	A	248	LYS	2.2
1	B	381	PHE	2.2
1	A	99	LEU	2.2
1	A	387	TRP	2.2
1	B	239	GLU	2.1
1	A	102	PHE	2.1
1	A	209	PHE	2.1
1	B	282	GLN	2.1
1	A	384	LEU	2.1
1	B	581	HIS	2.1
1	A	230	LEU	2.0
1	A	378	ALA	2.0
1	B	534	LEU	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	H	4	11/12	0.41	0.55	84,86,88,90	0
3	BMA	D	4	11/12	0.54	0.59	89,90,91,91	0
2	NDG	C	2	14/15	0.55	0.51	72,74,75,75	0
3	BMA	G	4	11/12	0.67	0.48	81,82,82,83	0
3	BMA	D	3	11/12	0.68	0.50	78,81,85,88	0
5	BMA	H	5	11/12	0.71	0.45	90,91,92,92	0
4	MAN	E	5	11/12	0.75	0.40	92,93,93,94	0
5	BMA	H	3	11/12	0.78	0.31	70,73,78,81	0

Continued on next page...

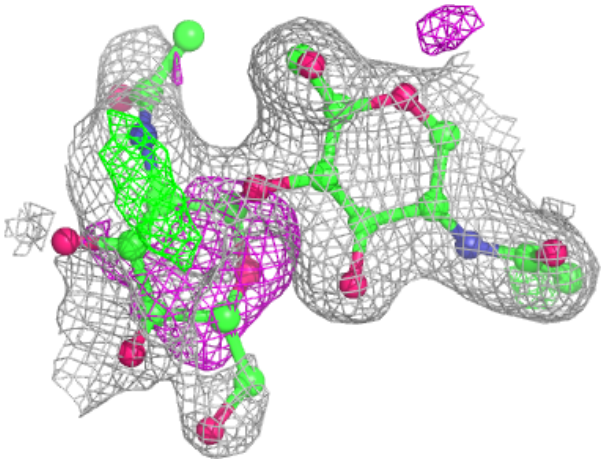
Continued from previous page...

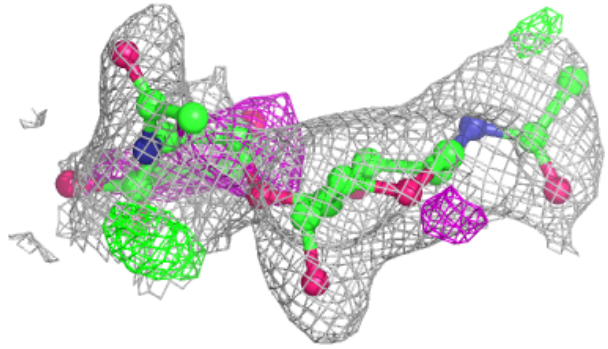
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	E	4	11/12	0.80	0.47	86,88,90,91	0
4	BMA	E	3	11/12	0.81	0.34	71,74,79,83	0
3	BMA	G	3	11/12	0.81	0.34	69,71,76,79	0
2	NDG	F	2	14/15	0.82	0.35	68,70,71,71	0
2	NAG	C	1	14/15	0.83	0.20	57,61,63,68	0
3	NAG	D	2	14/15	0.84	0.19	63,66,69,74	0
2	NAG	F	1	14/15	0.84	0.17	59,62,64,66	0
5	NDG	H	2	14/15	0.84	0.23	53,56,60,65	0
4	NDG	E	2	14/15	0.85	0.21	53,56,60,65	0
3	NAG	G	2	14/15	0.92	0.13	54,55,59,64	0
3	NAG	D	1	14/15	0.93	0.10	50,53,56,60	0
5	NAG	H	1	14/15	0.94	0.10	36,37,41,47	0
4	NAG	E	1	14/15	0.95	0.10	37,38,42,47	0
3	NAG	G	1	14/15	0.97	0.07	43,45,49,50	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:

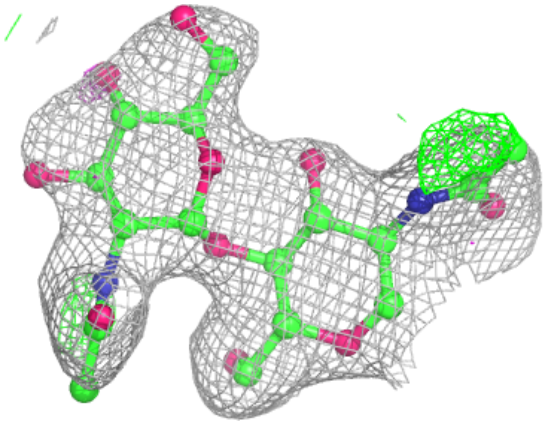
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

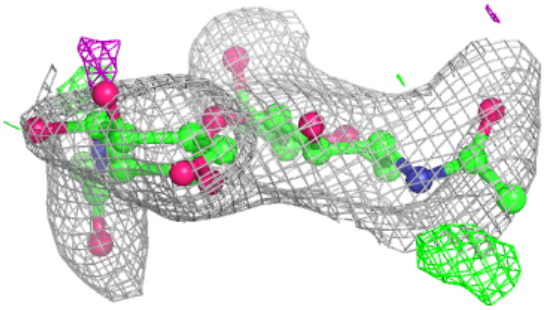


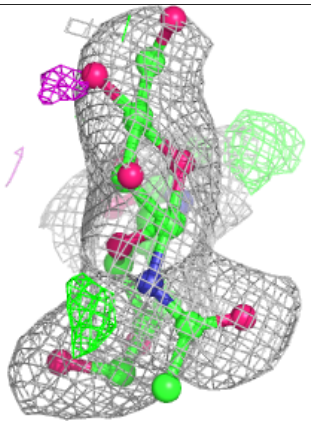


Electron density around Chain F:

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

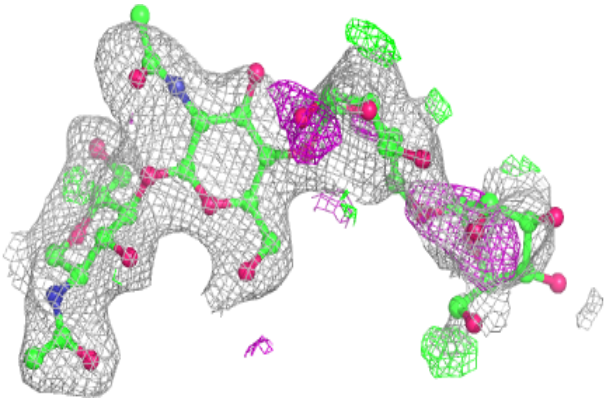


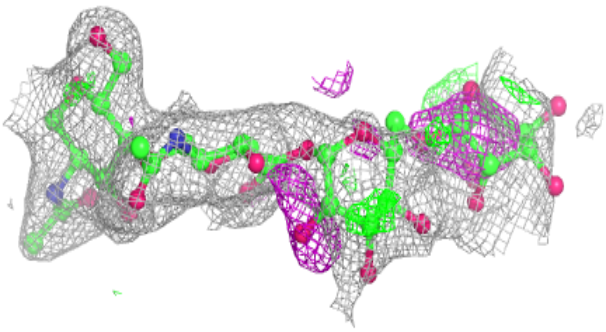


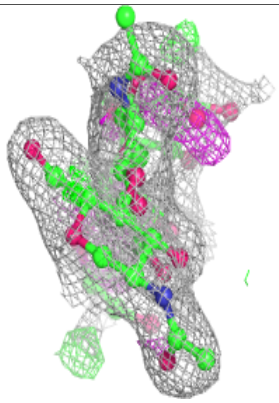


Electron density around Chain D:

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

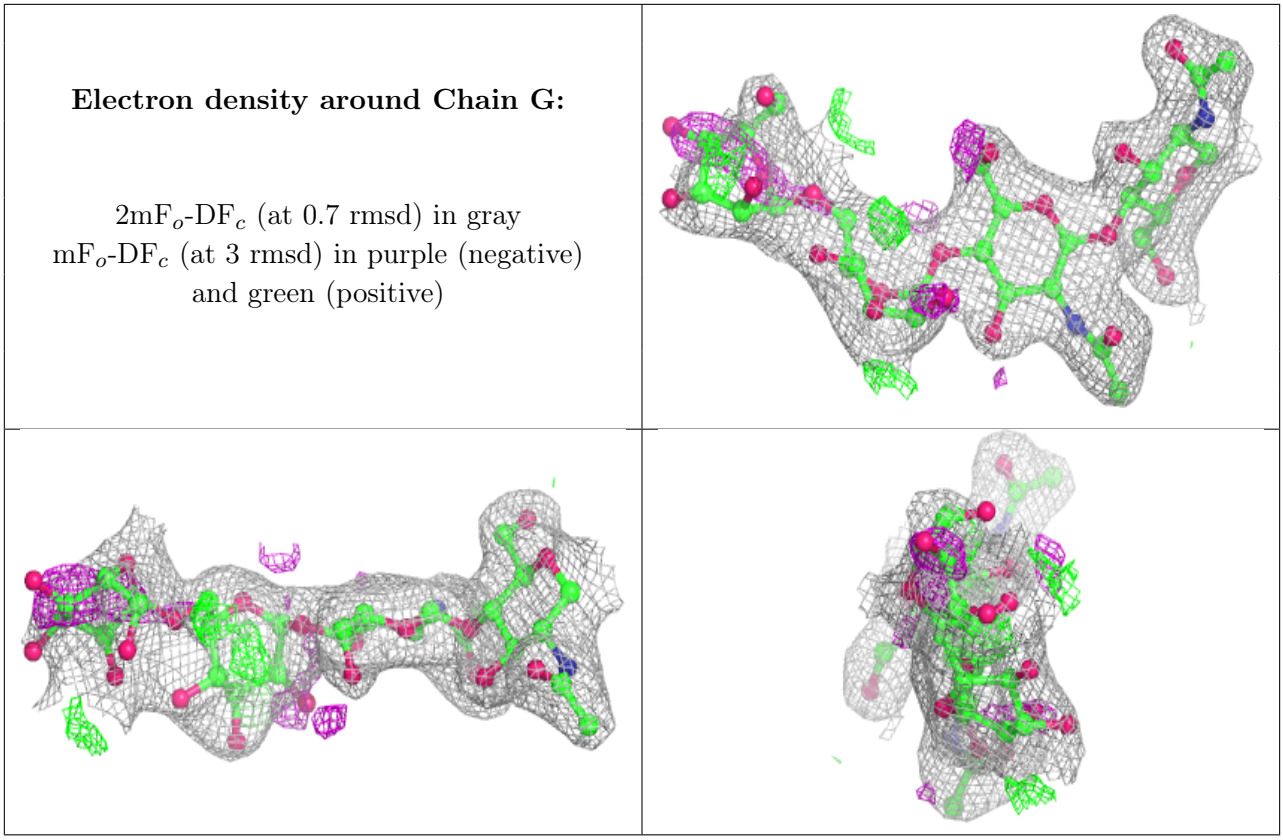






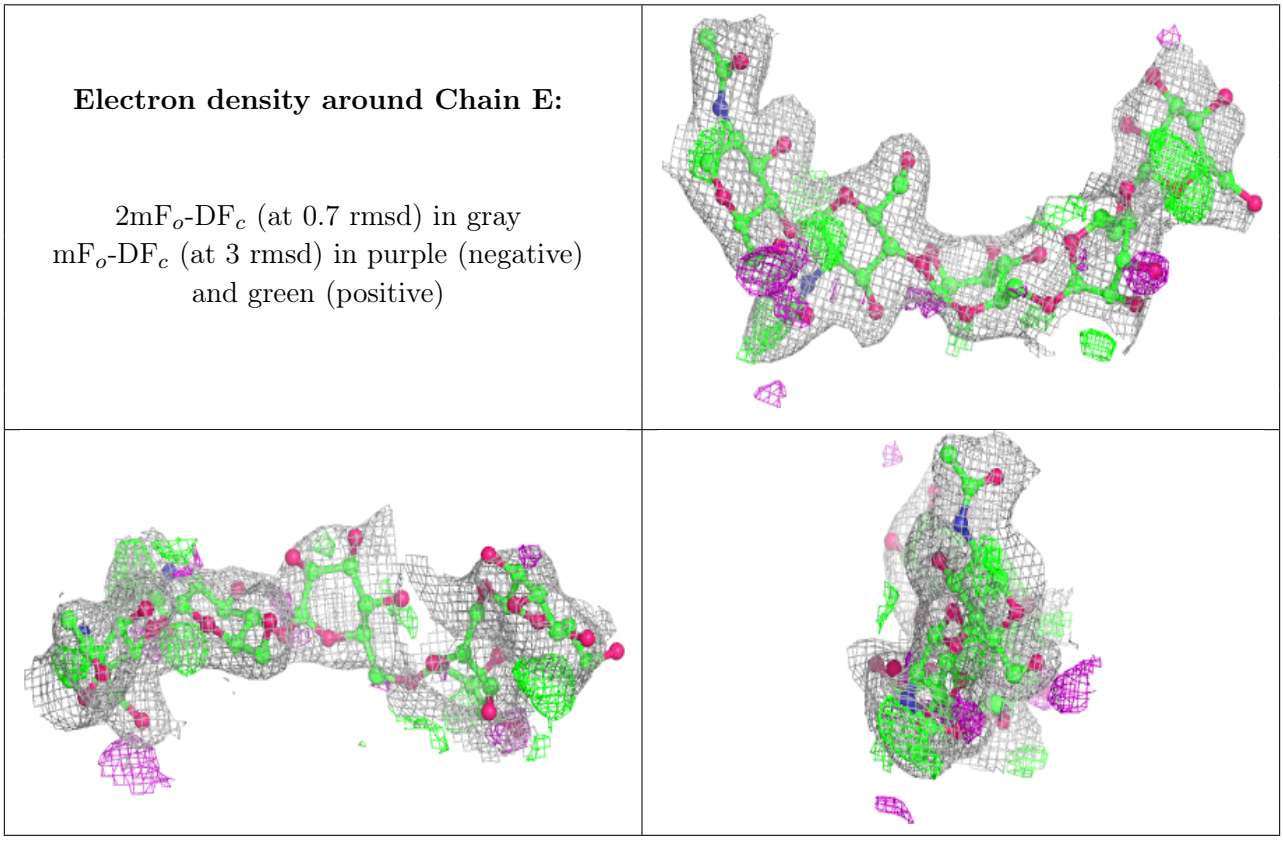
Electron density around Chain G:

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



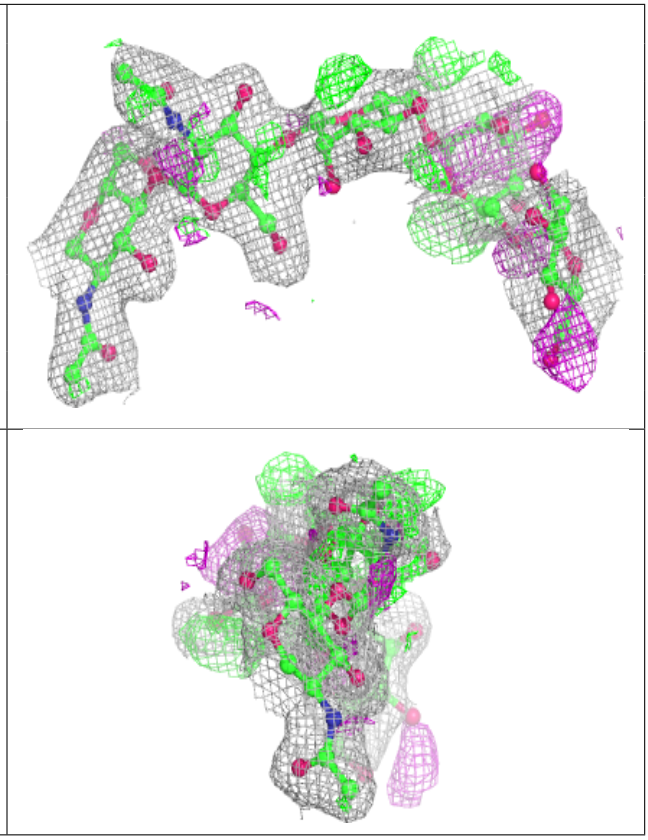
Electron density around Chain E:

$2mF_o$-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 H:

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



6.4 Ligands (i)

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
6	BOG	A	752	20/20	0.09	0.54	96,104,105,105	0
6	BOG	B	1752	20/20	0.30	0.47	112,113,113,113	0
6	BOG	B	1753	20/20	0.34	0.48	101,103,104,104	0
6	BOG	A	754	20/20	0.47	0.68	103,105,106,106	0
9	GOL	B	1760	6/6	0.51	0.40	78,79,79,79	0
9	GOL	B	1758	6/6	0.60	0.39	79,82,82,83	0
7	BFL	A	701	17/17	0.66	0.29	51,53,57,58	0
6	BOG	A	753	20/20	0.72	0.25	73,80,82,82	0
9	GOL	A	758	6/6	0.73	0.24	57,60,61,61	0
9	GOL	B	1759	6/6	0.77	0.17	50,53,56,59	0
6	BOG	B	1750	20/20	0.77	0.42	91,91,94,94	0
7	BFL	B	1701	17/17	0.79	0.26	52,53,57,57	0
9	GOL	A	759	6/6	0.83	0.32	77,77,77,77	0
6	BOG	B	1751	20/20	0.83	0.19	76,78,78,78	0

Continued on next page...

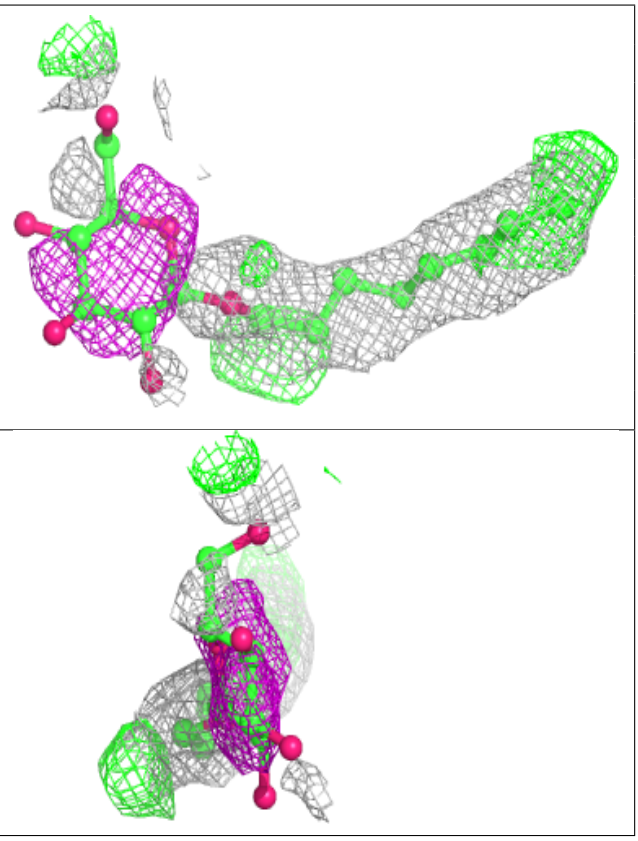
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BOG	A	751	20/20	0.90	0.18	70,71,73,73	0
8	HEM	A	801[B]	43/43	0.94	0.15	39,41,46,48	43
8	HEM	A	801[A]	43/43	0.94	0.15	41,42,48,50	43
8	HEM	B	1601[B]	43/43	0.95	0.15	40,42,47,49	43
8	HEM	B	1601[A]	43/43	0.95	0.15	40,41,47,49	43

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.

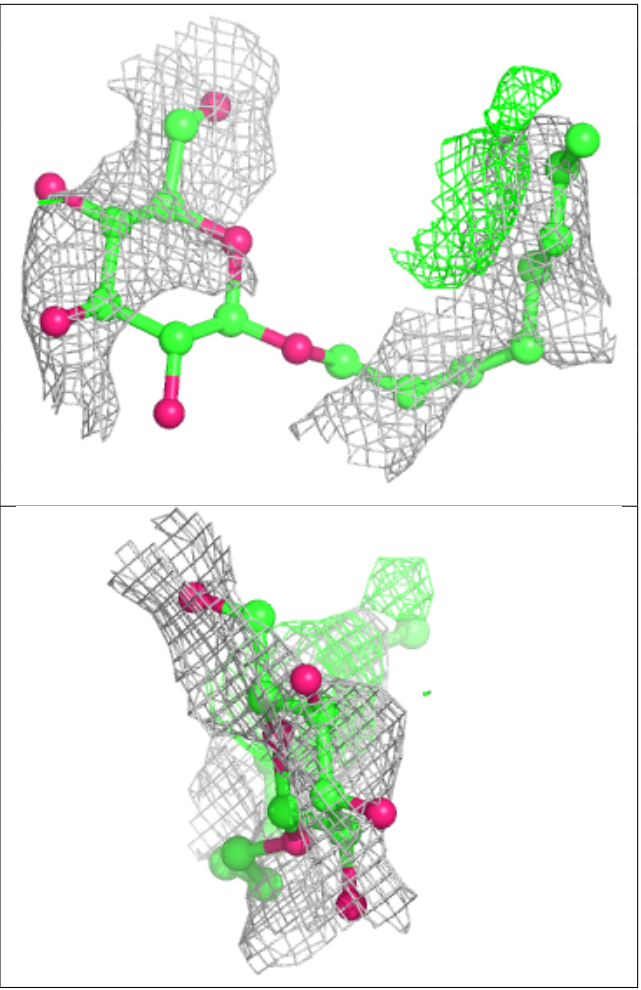
Electron density around BOG A 752:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



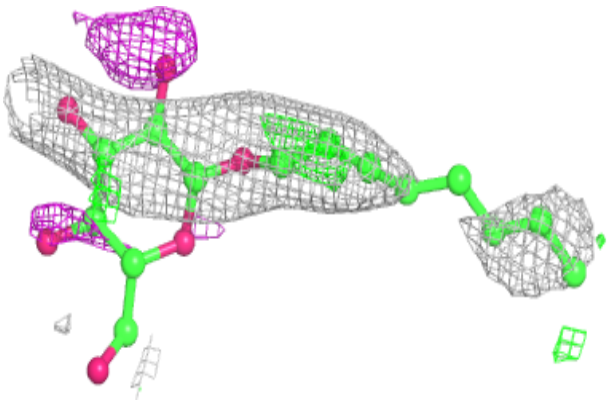
Electron density around BOG B 1752:

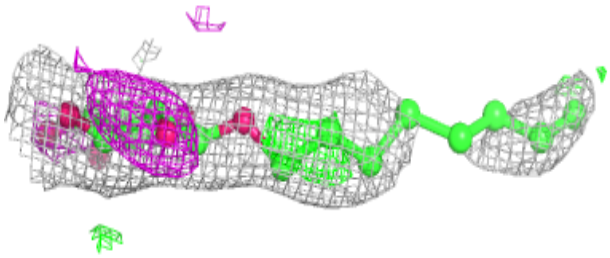
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

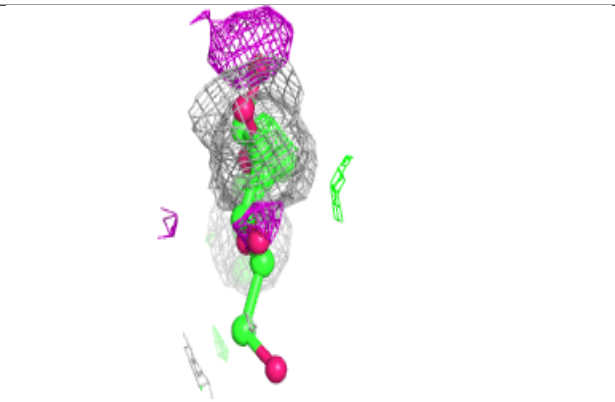


Electron density around BOG B 1753:

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

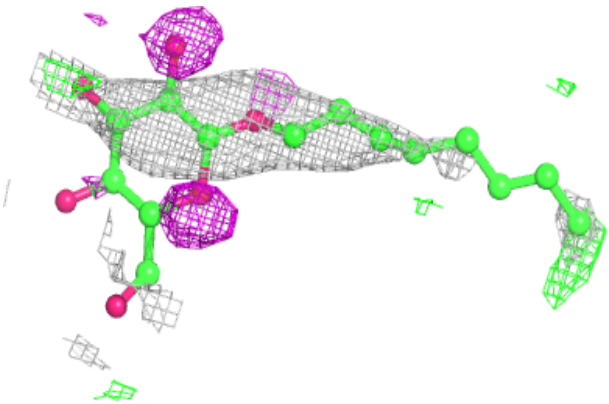


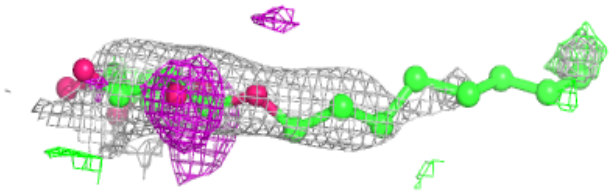


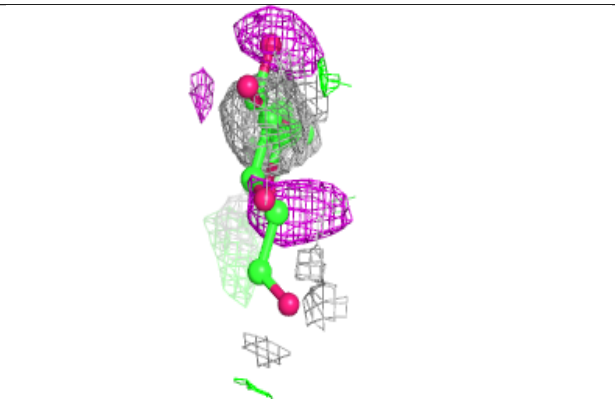


Electron density around BOG A 754:

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

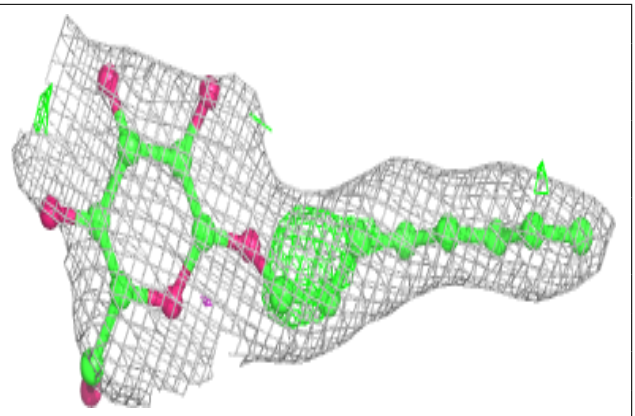


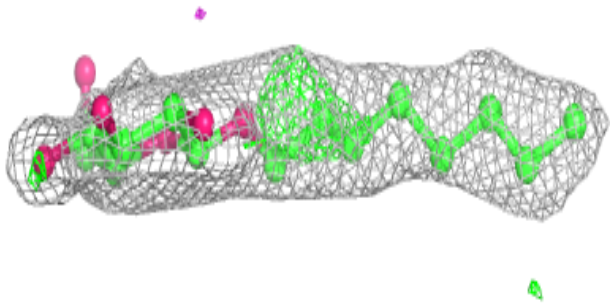


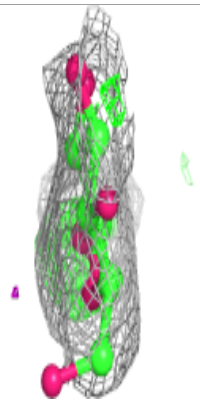


Electron density around BOG A 753:

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

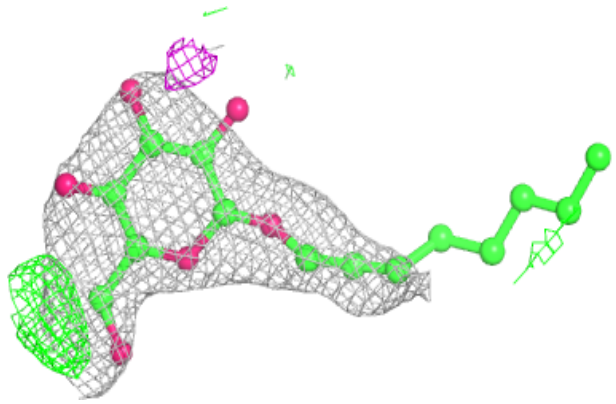


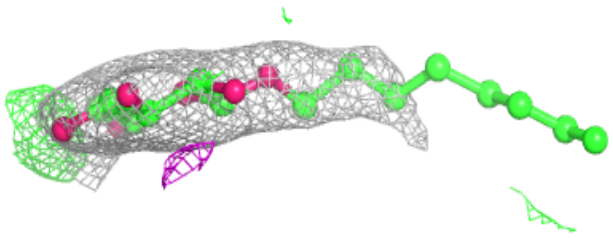


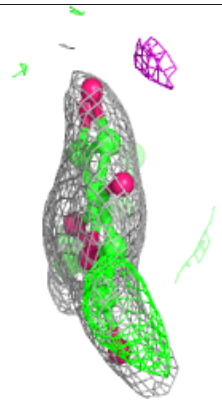


Electron density around BOG B 1750:

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

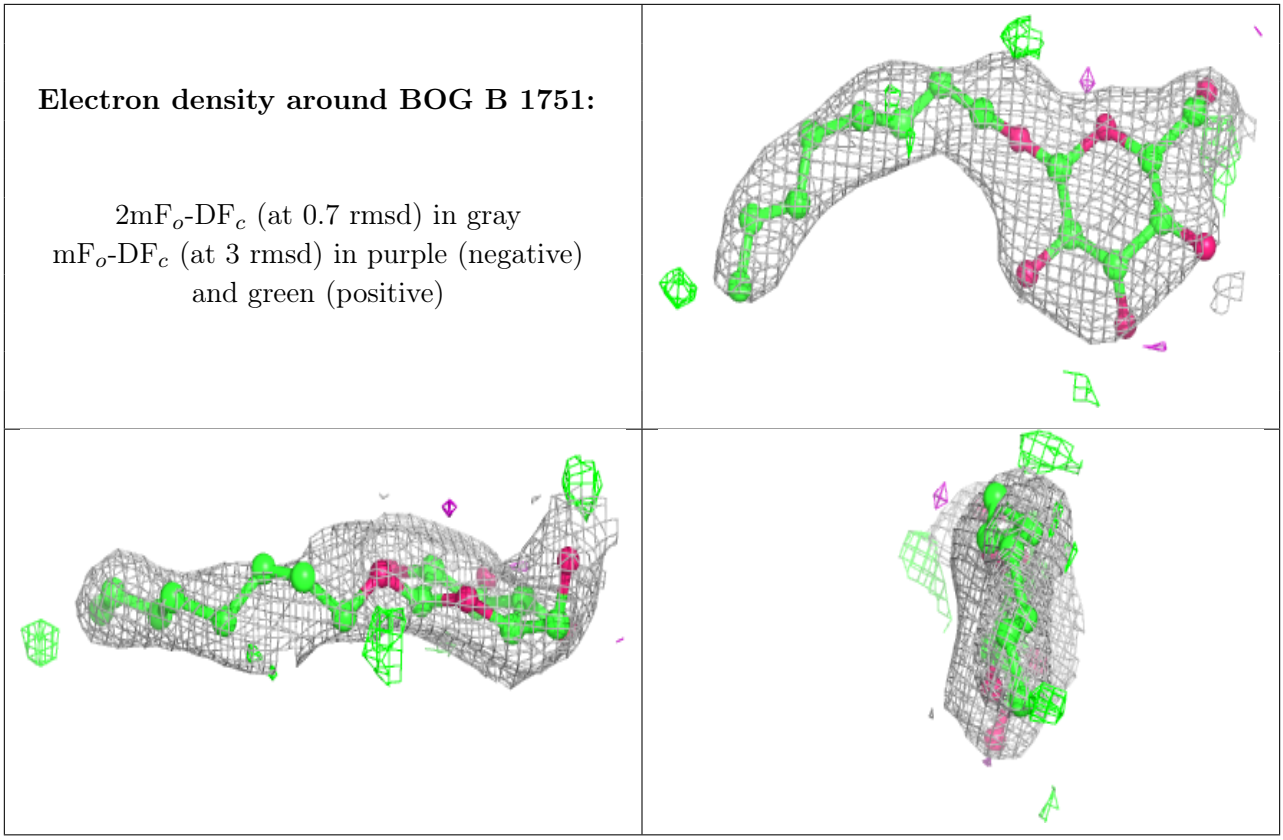






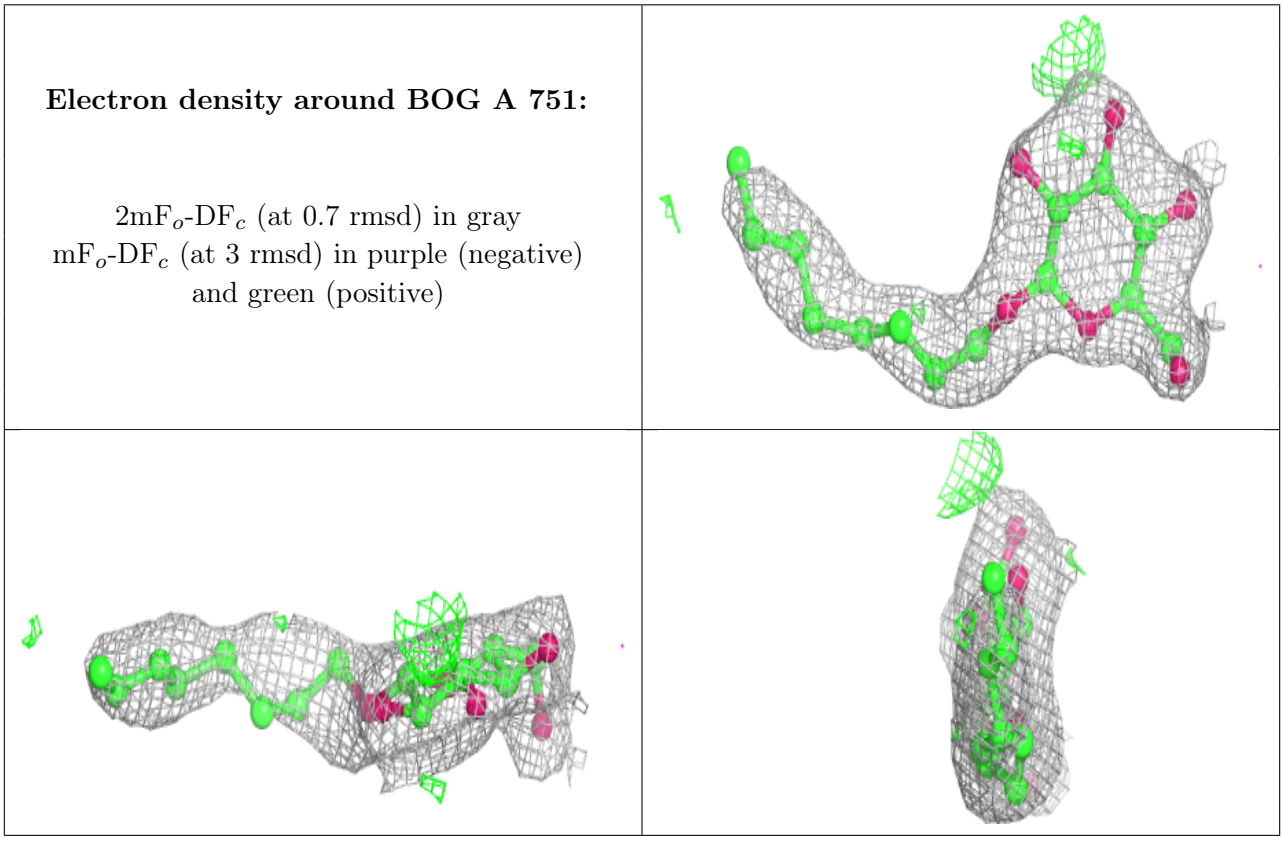
Electron density around BOG B 1751:

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



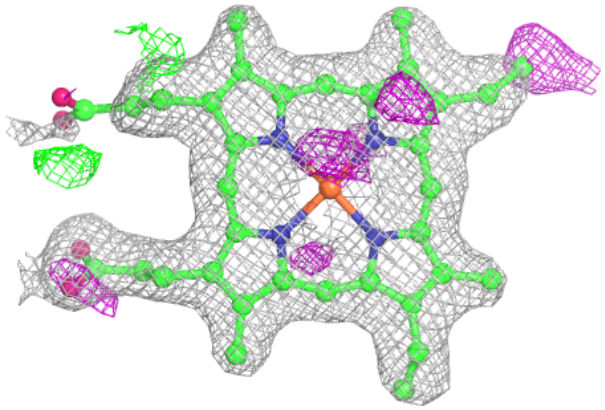
Electron density around BOG A 751:

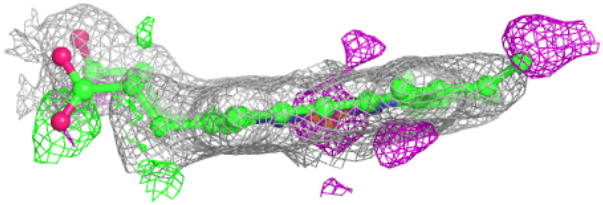
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

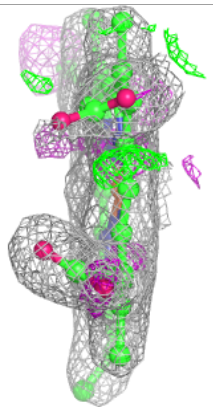


Electron density around HEM A 801 (B):

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

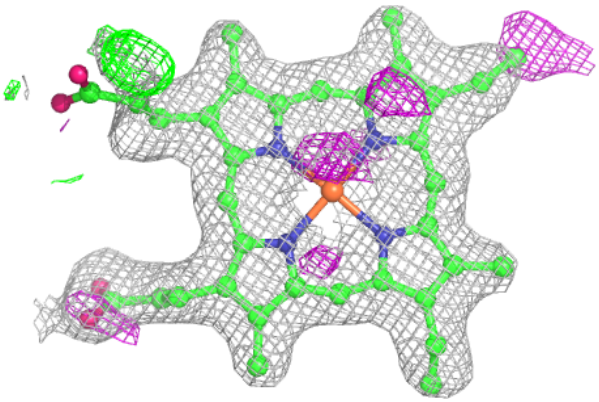


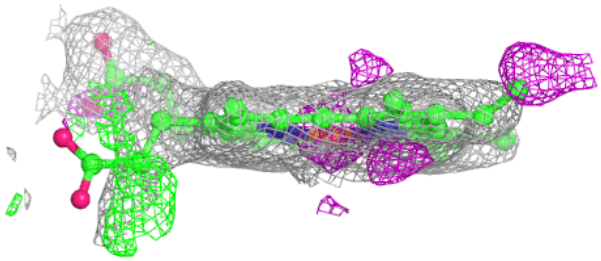


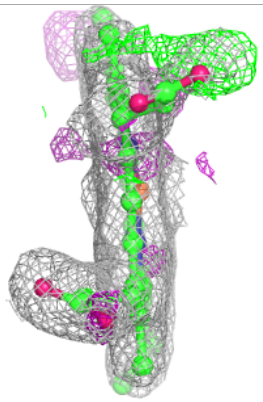


Electron density around HEM A 801 (A):

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

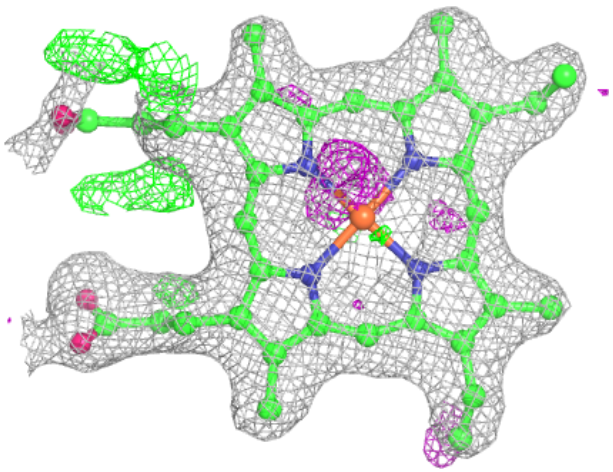


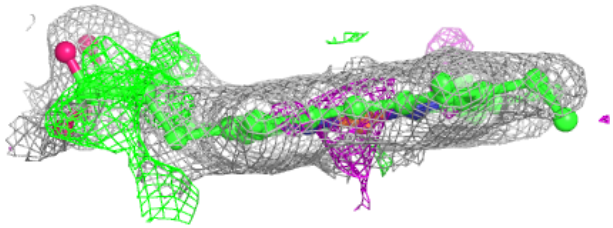




Electron density around HEM B 1601 (B):

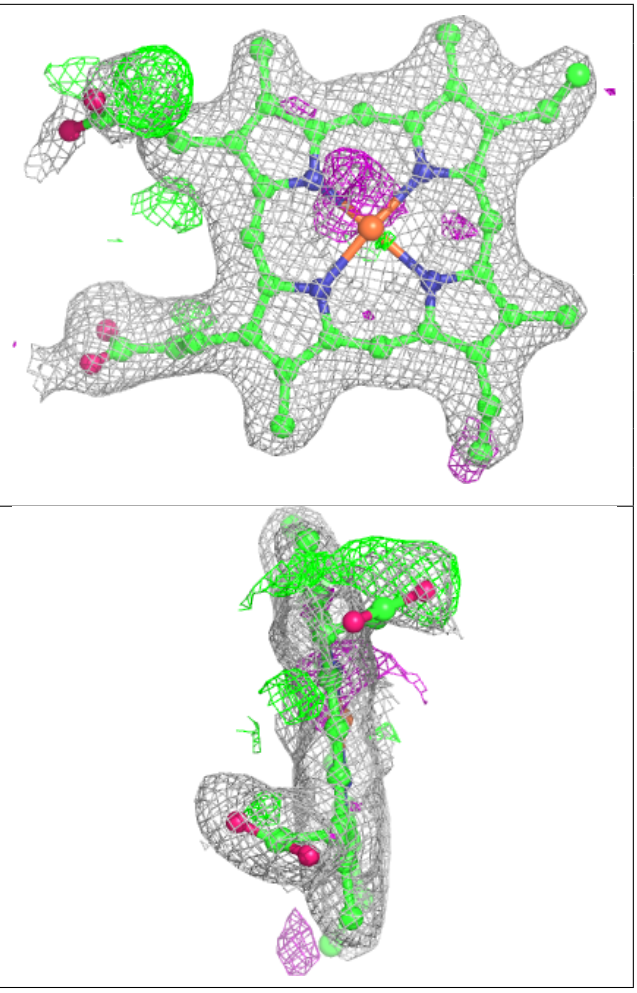
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEM B 1601 (A):

$2mF_o$-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.