wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 12:40 PM EDT

PDB ID	:	1PXX
Title	:	CRYSTAL STRUCTURE OF DICLOFENAC BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2
Authors	:	Kiefer, J.R.; Rowlinson, S.W.; Prusakiewicz, J.J.; Pawlitz, J.L.; Kozak, K.R.; Kalgutkar, A.S.; Stallings, W.C.; Marnett, L.J.; Kurumbail, R.G.
Deposited on	:	2003-07-07
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

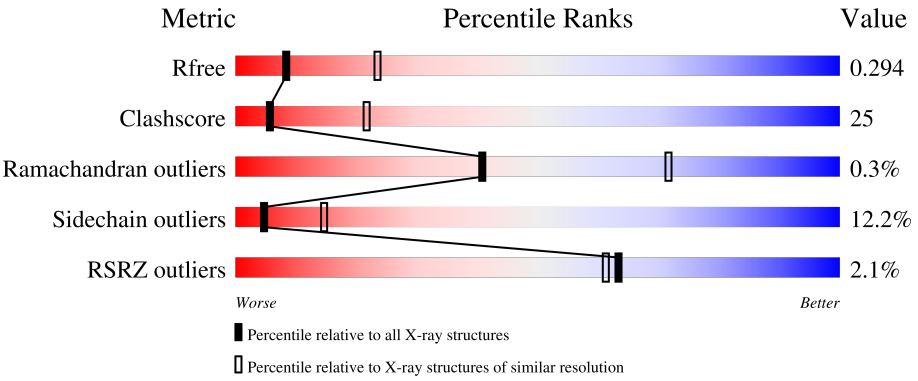
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	604	2% 50% 35% 6% 9%
1	B	604	2% 49% 36% 6% 9%
1	C	604	% 50% 36% 6% 9%
1	D	604	2% 50% 36% 6% 9%

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Mol	Chain	Length	Quality of chain
2	E	3	33% 67%
2	F	3	33% 67%
2	G	3	33% 67%
2	H	3	33% 67%

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	NAG	E	3	-	-	-	X
2	NAG	F	3	-	-	-	X
2	NAG	G	3	-	-	-	X
2	NAG	H	3	-	-	-	X
3	NAG	A	661	-	-	-	X
3	NAG	C	2661	-	-	X	-
3	NAG	D	3661	-	-	-	X
4	BOG	D	3703	-	-	X	-

2 Entry composition (i)

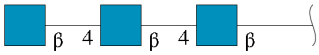
There are 7 unique types of molecules in this entry. The entry contains 18778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2.

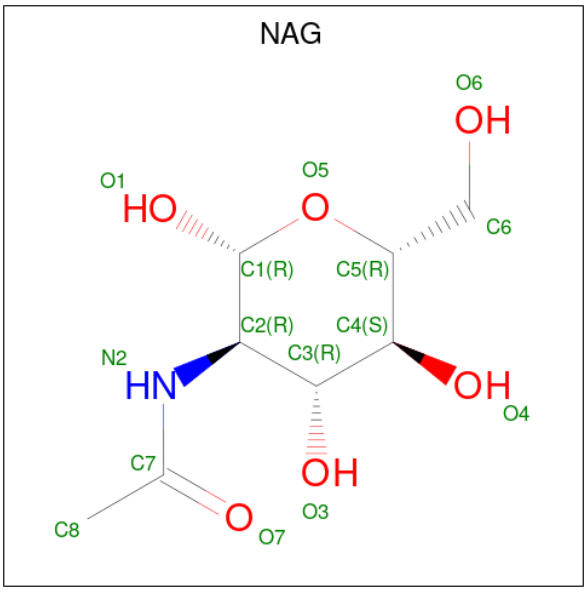
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4472	2885	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



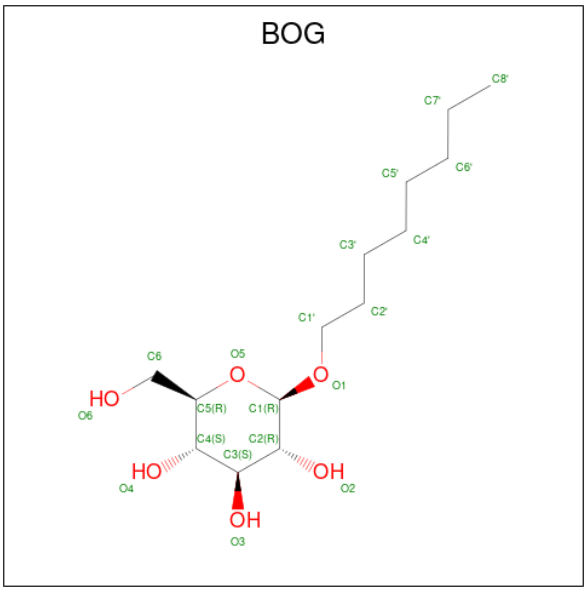
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	F	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	G	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	H	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



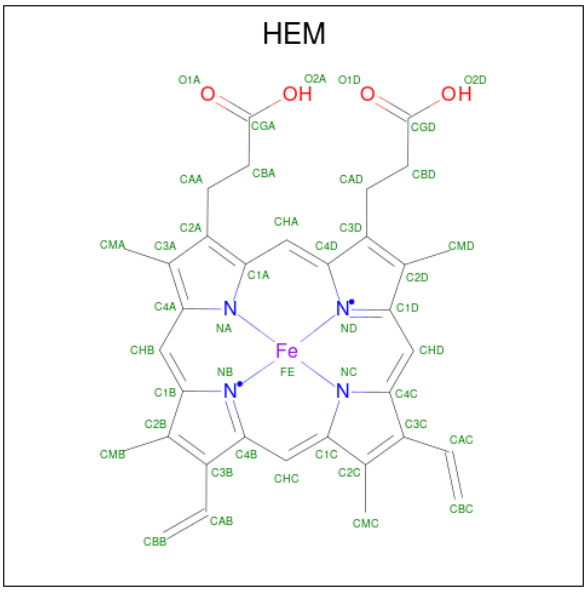
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	D	1	Total C O 19 13 6	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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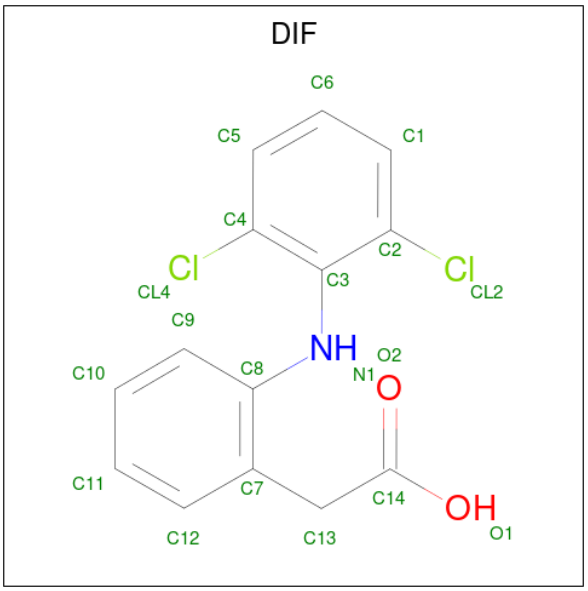
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is 2-[2,6-DICHLOROPHENYL)AMINO]BENZENEACETIC ACID (three-letter code: DIF) (formula: $C_{14}H_{11}Cl_2NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	B	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	C	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		
6	D	1	Total	C	Cl	N	O	0	0
			19	14	2	1	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		
7	B	93	Total	O	0	0
			93	93		

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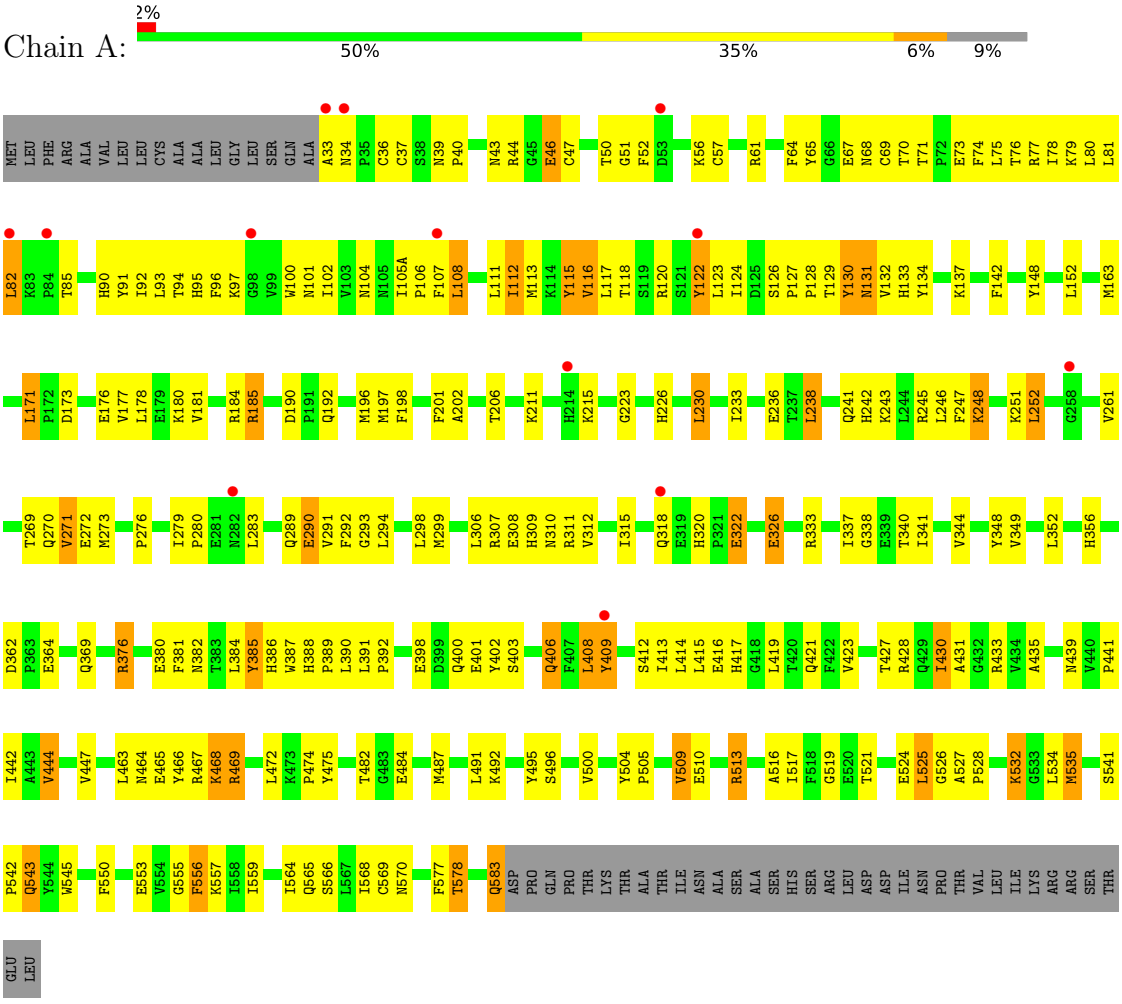
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	69	Total O 69 69	0	0
7	D	95	Total O 95 95	0	0

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.

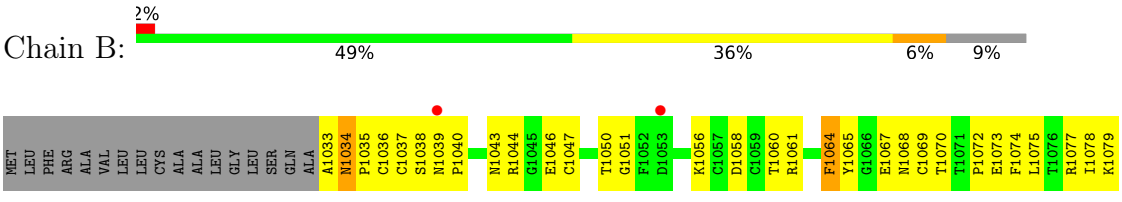
• Molecule 1: Prostaglandin G/H synthase 2

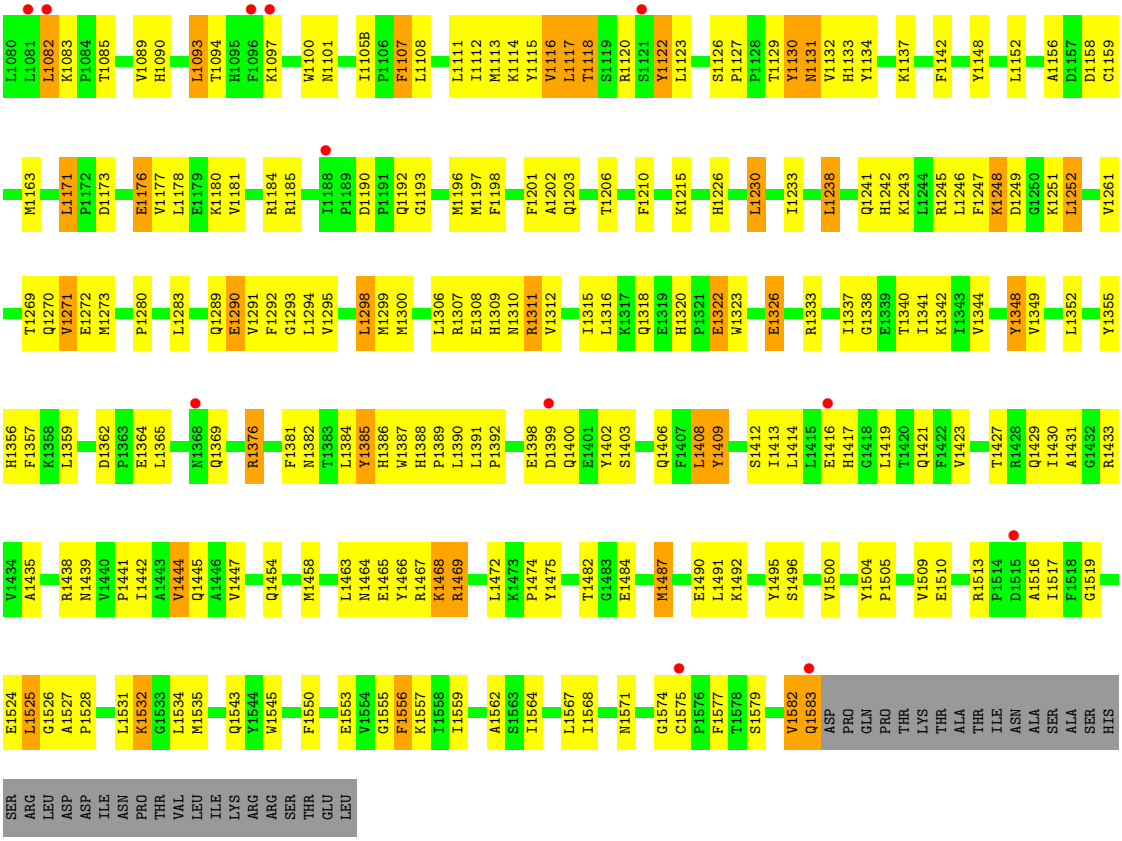
Chain A:



• Molecule 1: Prostaglandin G/H synthase 2

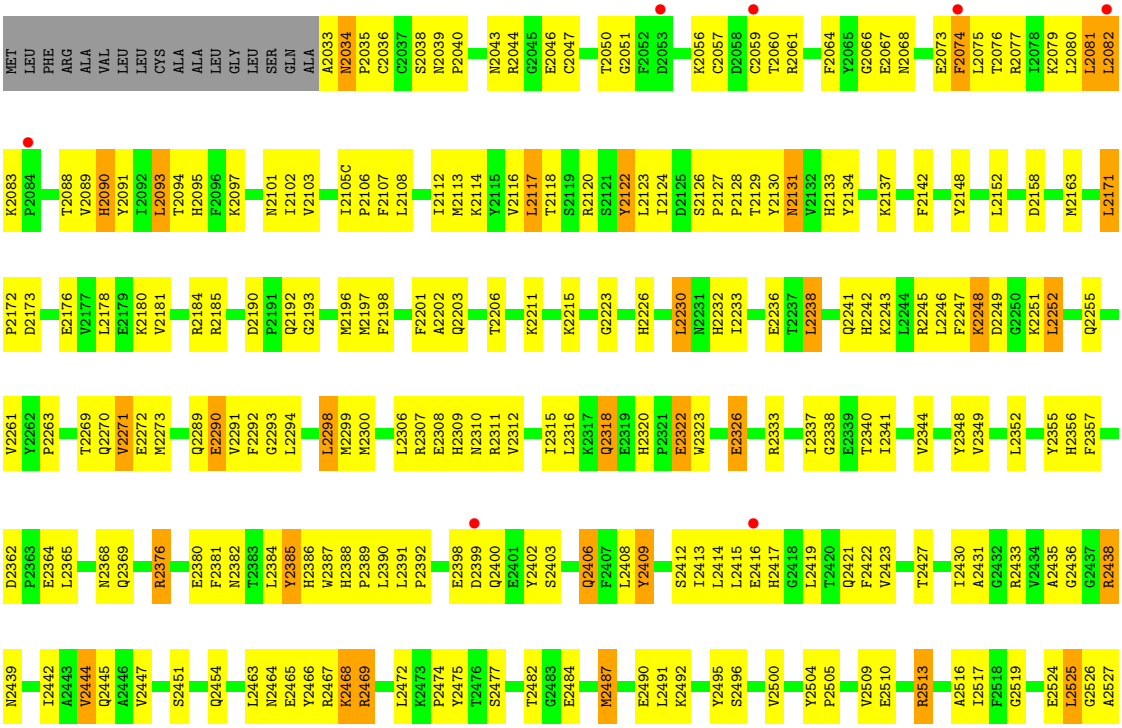
Chain B:

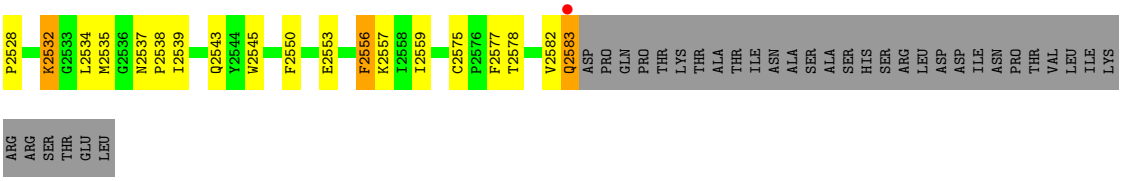




• Molecule 1: Prostaglandin G/H synthase 2

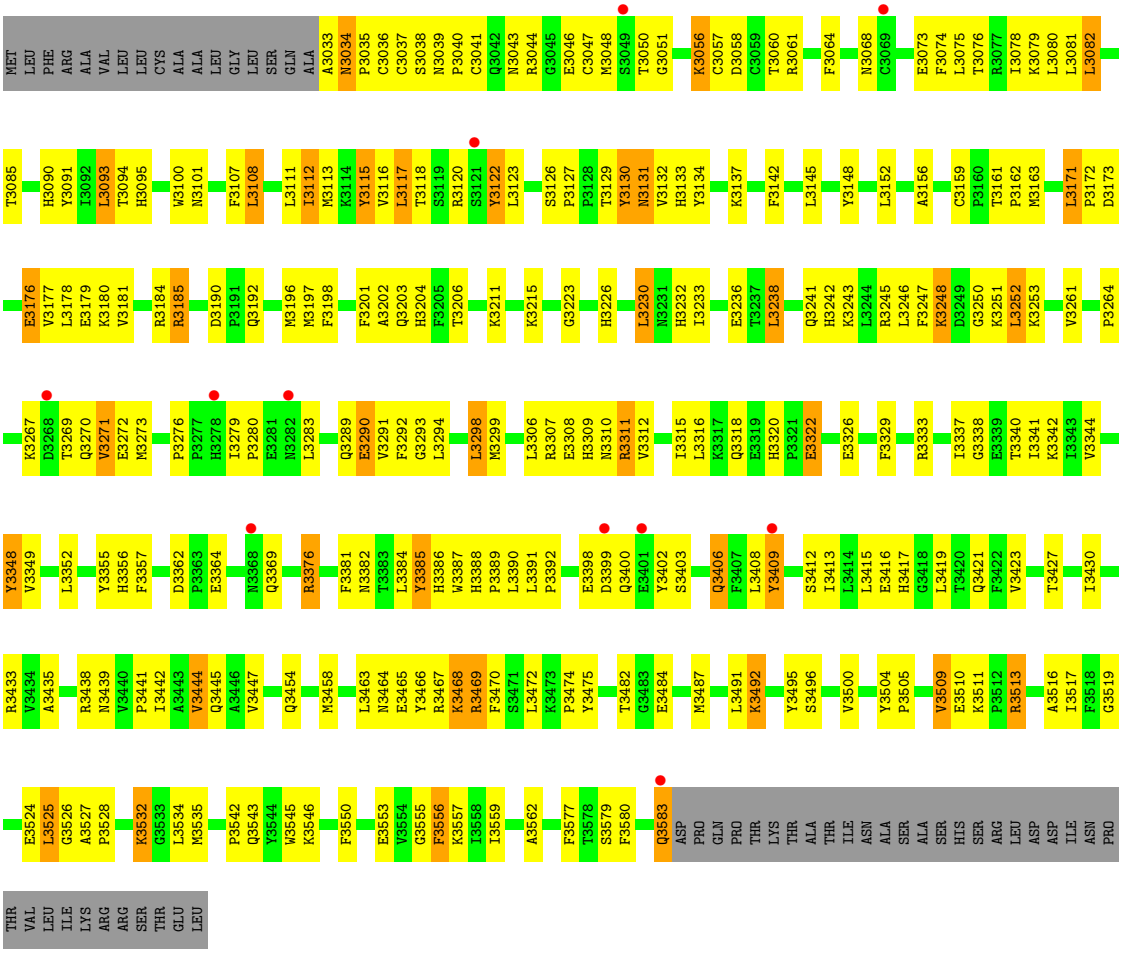
Chain C:





• Molecule 1: Prostaglandin G/H synthase 2

Chain D:



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

Chain E:

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

Chain F:

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

Chain G:

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	181.15Å 135.09Å 124.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.6 (20.00-2.90) 83.3 (19.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	6.15 (at 2.88Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.254 , 0.302 0.245 , 0.294	Depositor DCC
R_{free} test set	5475 reflections (9.63%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18778	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4672e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIF, NAG, HEM, BOG

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	0.47	0/4598	0.66	1/6232 (0.0%)
1	B	0.47	0/4601	0.66	1/6239 (0.0%)
1	C	0.47	0/4601	0.66	1/6239 (0.0%)
1	D	0.47	0/4601	0.66	1/6239 (0.0%)
All	All	0.47	0/18401	0.66	4/24949 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1148	TYR	N-CA-C	-5.71	95.57	111.00
1	D	3148	TYR	N-CA-C	-5.42	96.38	111.00
1	C	2148	TYR	N-CA-C	-5.38	96.47	111.00
1	A	148	TYR	N-CA-C	-5.31	96.67	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1348	TYR	Sidechain
1	D	3348	TYR	Sidechain

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	4472	0	4366	231	0
1	B	4474	0	4372	234	1
1	C	4474	0	4372	235	1
1	D	4474	0	4372	227	0
2	E	42	0	37	3	0
2	F	42	0	37	1	0
2	G	42	0	37	2	0
2	H	42	0	37	3	0
3	A	28	0	26	5	0
3	B	28	0	26	6	0
3	C	28	0	26	7	0
3	D	28	0	26	4	0
4	A	20	0	28	5	1
4	D	19	0	25	9	1
5	A	43	0	30	4	0
5	B	43	0	30	7	0
5	C	43	0	30	4	0
5	D	43	0	30	4	0
6	A	19	0	10	3	0
6	B	19	0	10	3	0
6	C	19	0	10	4	0
6	D	19	0	10	1	0
7	A	60	0	0	9	0
7	B	93	0	0	9	0
7	C	69	0	0	8	0
7	D	95	0	0	7	0
All	All	18778	0	17947	928	2

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 25.

The worst 5 of 928 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:D:3294:LEU:HD22	1:D:3409:TYR:HD2	1.03	1.15
1:A:294:LEU:HD22	1:A:409:TYR:CD2	1.80	1.14
1:D:3294:LEU:HD22	1:D:3409:TYR:CD2	1.84	1.12
1:A:294:LEU:HD22	1:A:409:TYR:HD2	1.00	1.11
1:D:3442:ILE:HD13	4:D:3703:BOG:H62	1.34	1.08

All (2) 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)
1:B:1490:GLU:OE1	4:A:703:BOG:O2[4_555]	2.18	0.02
1:C:2490:GLU:OE1	4:D:3703:BOG:O2[4_456]	2.18	0.02

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	549/604 (91%)	516 (94%)	31 (6%)	2 (0%)	34	66
1	B	550/604 (91%)	513 (93%)	36 (6%)	1 (0%)	47	78
1	C	550/604 (91%)	510 (93%)	37 (7%)	3 (0%)	29	61
1	D	550/604 (91%)	510 (93%)	40 (7%)	0	100	100
All	All	2199/2416 (91%)	2049 (93%)	144 (6%)	6 (0%)	41	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	C	2106	PRO
1	C	2074	PHE
1	C	2438	ARG
1	A	106	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	492/537 (92%)	432 (88%)	60 (12%)	5 15
1	B	493/537 (92%)	430 (87%)	63 (13%)	4 13
1	C	493/537 (92%)	439 (89%)	54 (11%)	6 19
1	D	493/537 (92%)	430 (87%)	63 (13%)	4 13
All	All	1971/2148 (92%)	1731 (88%)	240 (12%)	5 15

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1525	LEU
1	D	3409	TYR
1	C	2271	VAL
1	D	3406	GLN
1	D	3535	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2034	ASN
1	D	3464	ASN
1	C	2242	HIS
1	D	3454	GLN
1	D	3242	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)

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.47	0	17,19,21	0.65	0
2	NAG	E	2	2	14,14,15	0.81	0	17,19,21	0.77	1 (5%)
2	NAG	E	3	2	14,14,15	0.83	0	17,19,21	0.82	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
2	NAG	F	2	2	14,14,15	0.77	0	17,19,21	0.80	1 (5%)
2	NAG	F	3	2	14,14,15	0.96	1 (7%)	17,19,21	0.78	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.46	0	17,19,21	0.67	0
2	NAG	G	2	2	14,14,15	0.69	0	17,19,21	0.78	1 (5%)
2	NAG	G	3	2	14,14,15	0.91	1 (7%)	17,19,21	0.66	0
2	NAG	H	1	1,2	14,14,15	0.58	0	17,19,21	0.66	0
2	NAG	H	2	2	14,14,15	0.85	0	17,19,21	0.82	1 (5%)
2	NAG	H	3	2	14,14,15	0.93	1 (7%)	17,19,21	0.85	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	3	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	3	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	3	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	3	2	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	NAG	C1-C2	2.54	1.56	1.52
2	G	3	NAG	C1-C2	2.51	1.56	1.52
2	H	3	NAG	C1-C2	2.22	1.55	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	3	NAG	C1-O5-C5	2.60	115.72	112.19
2	G	2	NAG	C4-C3-C2	-2.25	107.72	111.02
2	F	2	NAG	C4-C3-C2	-2.21	107.78	111.02
2	H	3	NAG	C1-O5-C5	2.14	115.10	112.19
2	H	2	NAG	O5-C1-C2	-2.13	107.93	111.29

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C1-C2-N2-C7
2	E	3	NAG	C3-C2-N2-C7
2	G	3	NAG	C3-C2-N2-C7
2	H	3	NAG	C3-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	F	3	NAG	1	0
2	H	2	NAG	2	0
2	E	2	NAG	2	0
2	H	1	NAG	1	0
2	E	3	NAG	3	0
2	F	2	NAG	1	0
2	H	3	NAG	2	0

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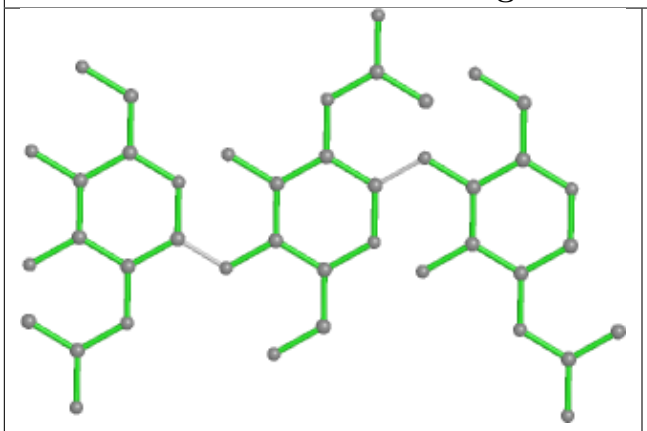
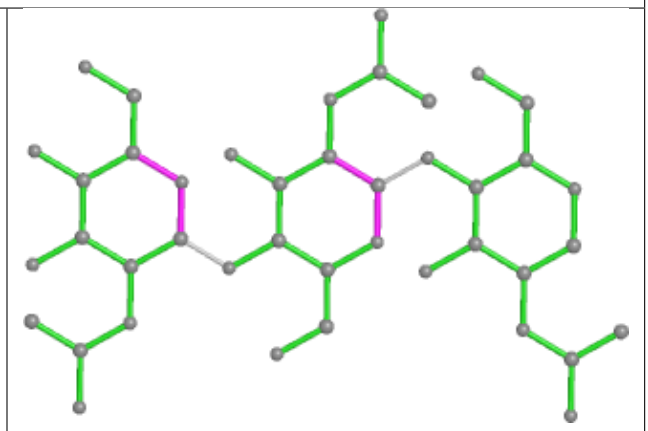
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	NAG	2	0

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

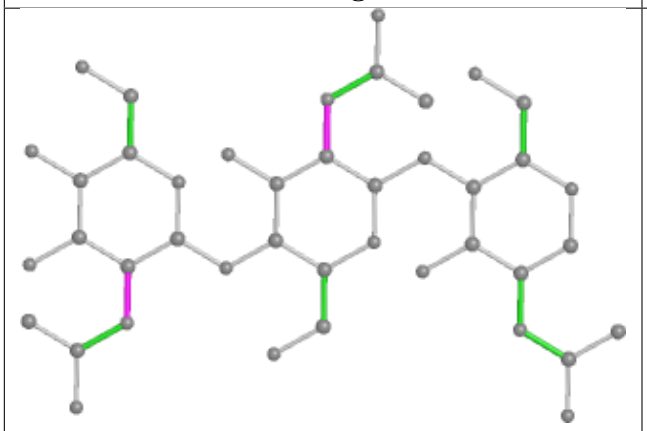
Oligosaccharide Chain E



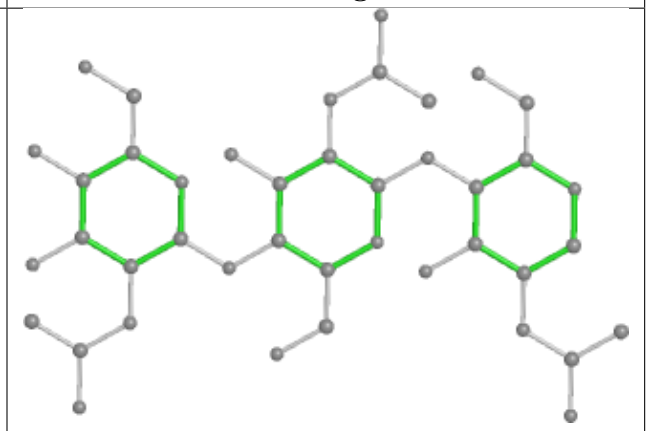
Bond lengths



Bond angles

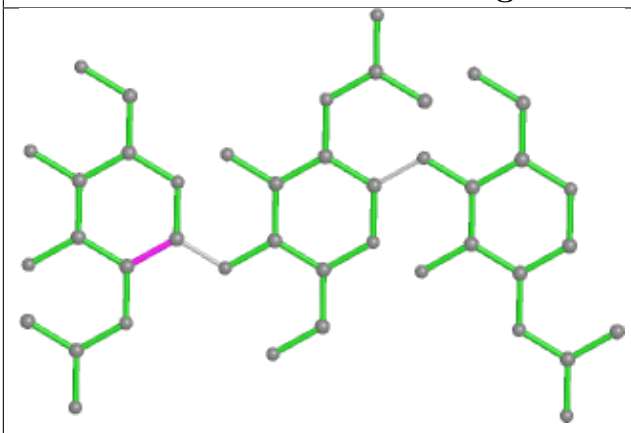


Torsions

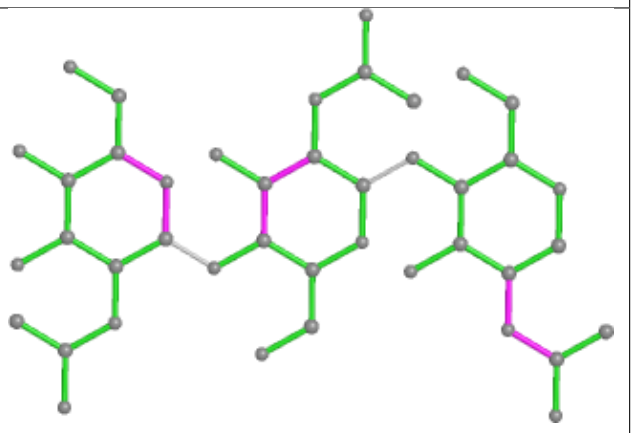


Rings

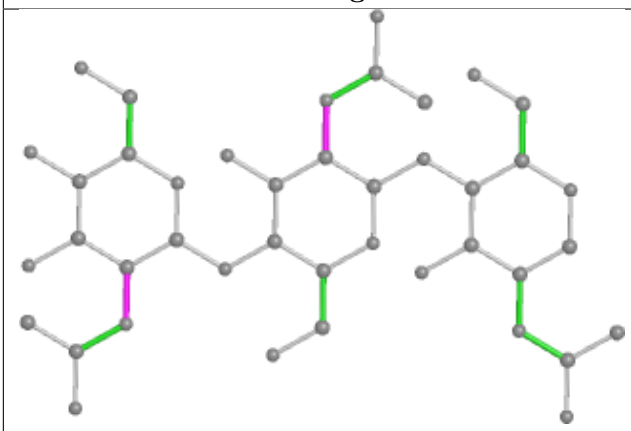
Oligosaccharide Chain F



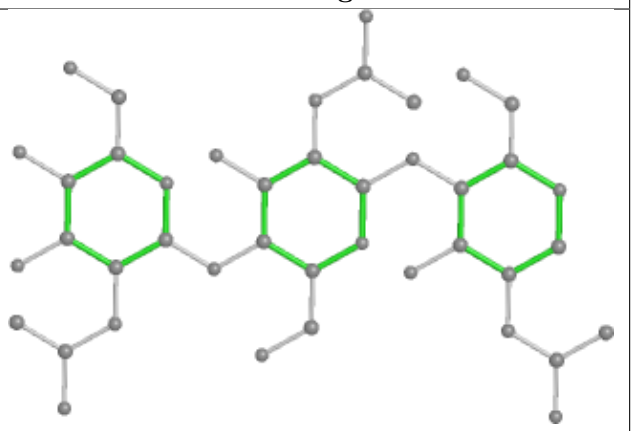
Bond lengths



Bond angles

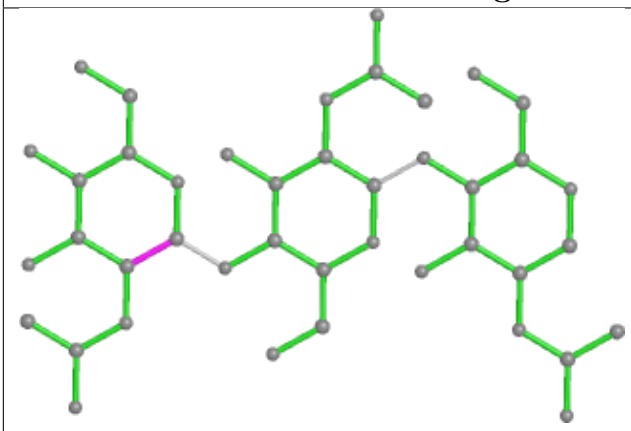


Torsions

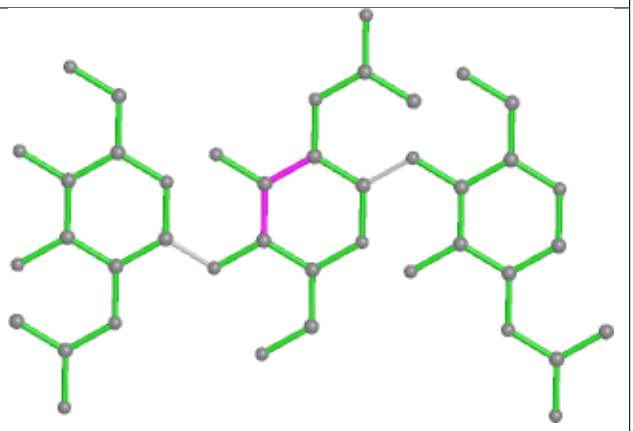


Rings

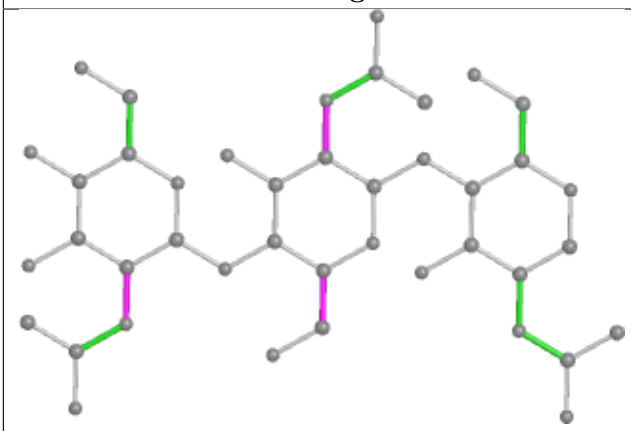
Oligosaccharide Chain G



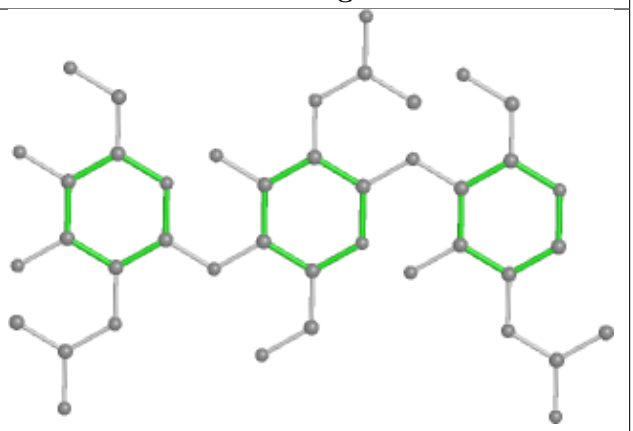
Bond lengths



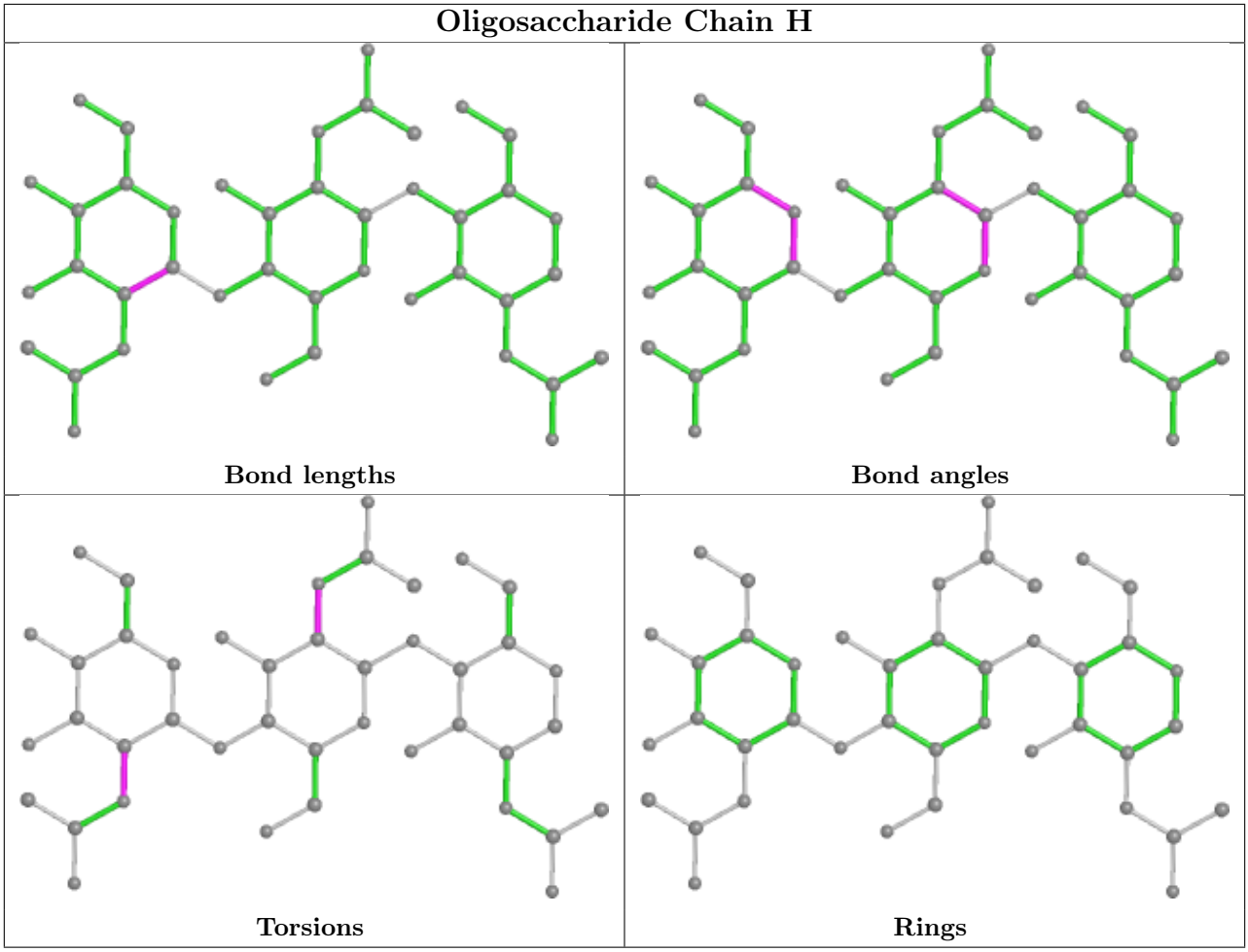
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
5	HEM	A	704	1	41,50,50	1.51	6 (14%)	45,82,82	1.10	1 (2%)
3	NAG	A	661	1	14,14,15	0.54	0	17,19,21	0.63	0
4	BOG	A	703	-	20,20,20	0.72	1 (5%)	25,25,25	0.64	0
3	NAG	C	2681	1	14,14,15	0.48	0	17,19,21	1.02	2 (11%)
5	HEM	D	3601	1	41,50,50	1.41	6 (14%)	45,82,82	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	HEM	B	1601	1	41,50,50	1.42	4 (9%)	45,82,82	1.10	1 (2%)
6	DIF	A	701	-	20,20,20	1.45	3 (15%)	27,27,27	2.30	7 (25%)
3	NAG	B	1681	1	14,14,15	0.46	0	17,19,21	0.80	0
6	DIF	B	1701	-	20,20,20	1.36	3 (15%)	27,27,27	1.96	6 (22%)
3	NAG	B	1661	1	14,14,15	0.48	0	17,19,21	0.68	0
6	DIF	C	2701	-	20,20,20	1.48	3 (15%)	27,27,27	1.77	7 (25%)
4	BOG	D	3703	-	17,17,20	0.37	0	18,18,25	0.84	1 (5%)
3	NAG	C	2661	1	14,14,15	0.59	0	17,19,21	0.62	0
3	NAG	D	3661	1	14,14,15	0.71	0	17,19,21	0.81	1 (5%)
3	NAG	A	681	1	14,14,15	0.58	0	17,19,21	0.75	0
6	DIF	D	3701	-	20,20,20	1.43	3 (15%)	27,27,27	2.05	7 (25%)
3	NAG	D	3681	1	14,14,15	0.47	0	17,19,21	0.86	0
5	HEM	C	2601	1	41,50,50	1.57	5 (12%)	45,82,82	1.06	2 (4%)

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
5	HEM	A	704	1	-	4/12/54/54	-
3	NAG	A	661	1	-	1/6/23/26	0/1/1/1
4	BOG	A	703	-	-	6/11/31/31	0/1/1/1
3	NAG	C	2681	1	-	1/6/23/26	0/1/1/1
5	HEM	D	3601	1	-	4/12/54/54	-
5	HEM	B	1601	1	-	6/12/54/54	-
6	DIF	A	701	-	-	0/8/8/8	0/2/2/2
3	NAG	B	1681	1	-	2/6/23/26	0/1/1/1
6	DIF	B	1701	-	-	0/8/8/8	0/2/2/2
3	NAG	B	1661	1	-	1/6/23/26	0/1/1/1
6	DIF	C	2701	-	-	0/8/8/8	0/2/2/2
4	BOG	D	3703	-	-	5/18/18/31	-
3	NAG	C	2661	1	-	1/6/23/26	0/1/1/1
3	NAG	D	3661	1	-	1/6/23/26	0/1/1/1
3	NAG	A	681	1	-	2/6/23/26	0/1/1/1
6	DIF	D	3701	-	-	0/8/8/8	0/2/2/2
3	NAG	D	3681	1	-	2/6/23/26	0/1/1/1
5	HEM	C	2601	1	-	4/12/54/54	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2601	HEM	C3C-CAC	-4.26	1.39	1.47
5	B	1601	HEM	C3C-CAC	-4.16	1.39	1.47
6	B	1701	DIF	O2-C14	4.15	1.35	1.22
5	D	3601	HEM	C3C-CAC	-4.09	1.39	1.47
5	C	2601	HEM	C3C-C2C	-4.08	1.34	1.40

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	701	DIF	C7-C8-N1	5.52	122.98	118.60
6	A	701	DIF	C4-C3-N1	-5.36	115.08	122.04
6	D	3701	DIF	C4-C3-N1	-5.17	115.33	122.04
6	A	701	DIF	C2-C3-N1	5.08	128.64	122.04
6	B	1701	DIF	C7-C8-N1	5.00	122.57	118.60

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1661	NAG	C3-C2-N2-C7
3	C	2661	NAG	C3-C2-N2-C7
3	D	3661	NAG	C3-C2-N2-C7
5	B	1601	HEM	C2B-C3B-CAB-CBB
5	B	1601	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

14 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	HEM	4	0
3	A	661	NAG	5	0
4	A	703	BOG	5	1
5	D	3601	HEM	4	0
5	B	1601	HEM	7	0
6	A	701	DIF	3	0
6	B	1701	DIF	3	0
3	B	1661	NAG	6	0
6	C	2701	DIF	4	0
4	D	3703	BOG	9	1
3	C	2661	NAG	7	0

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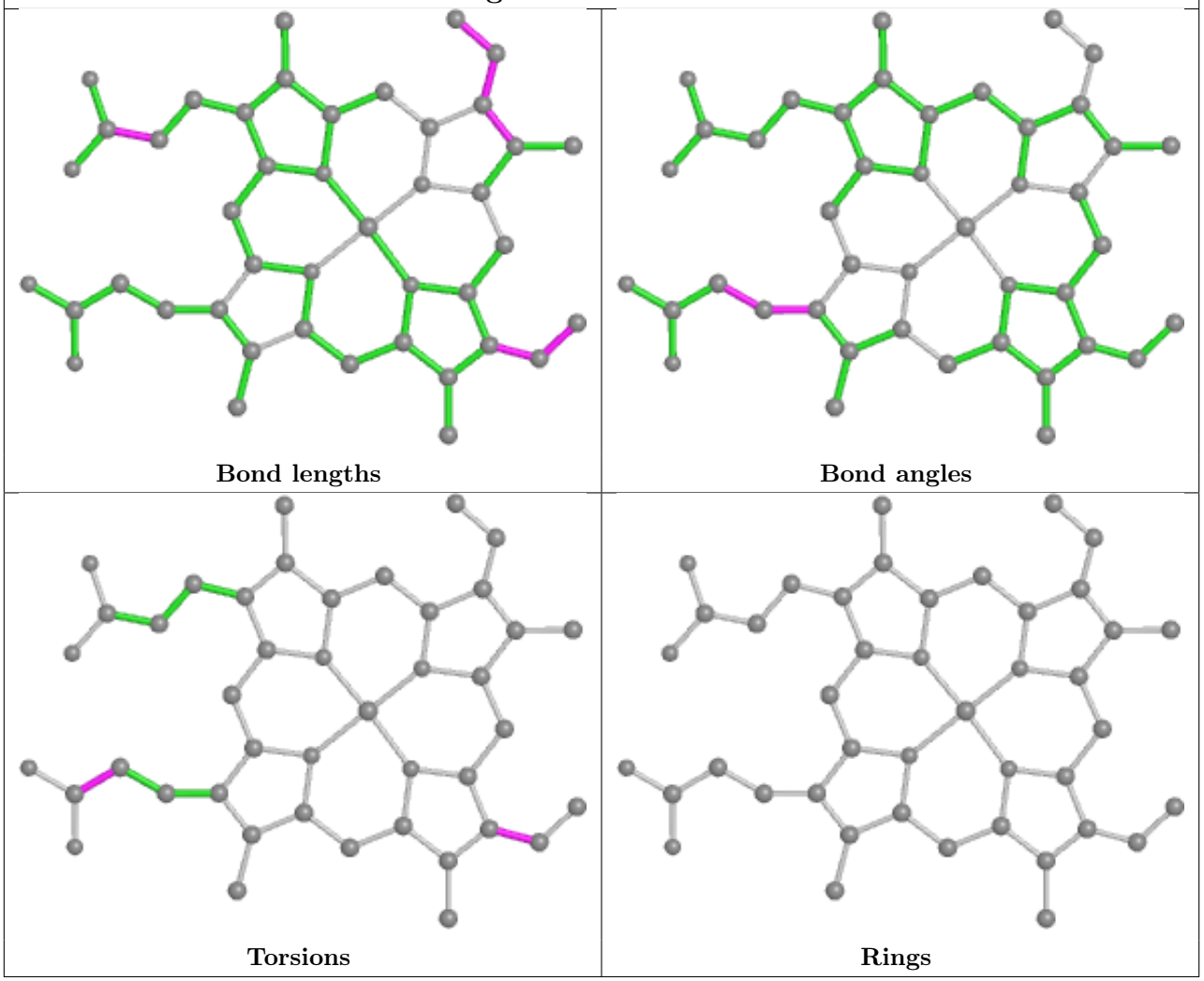
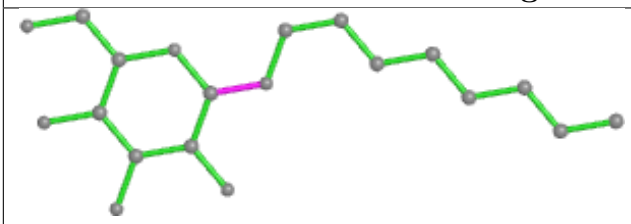
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3661	NAG	4	0
6	D	3701	DIF	1	0
5	C	2601	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

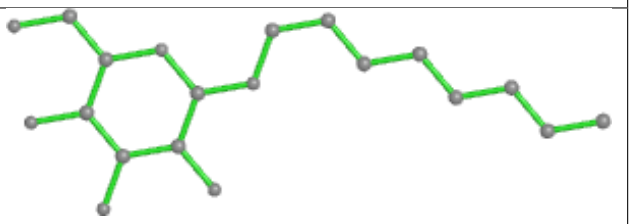
Ligand HEM A 704



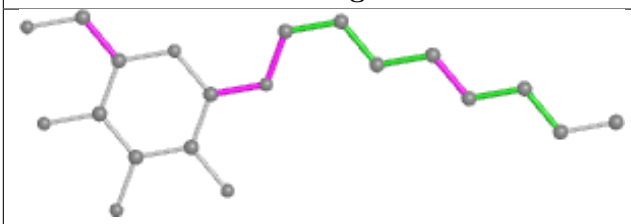
Ligand BOG A 703



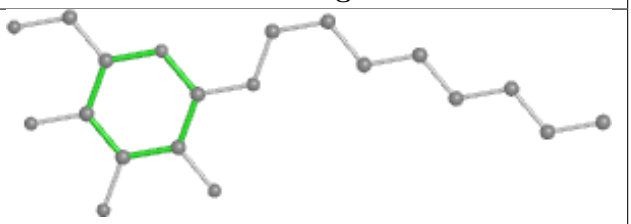
Bond lengths



Bond angles

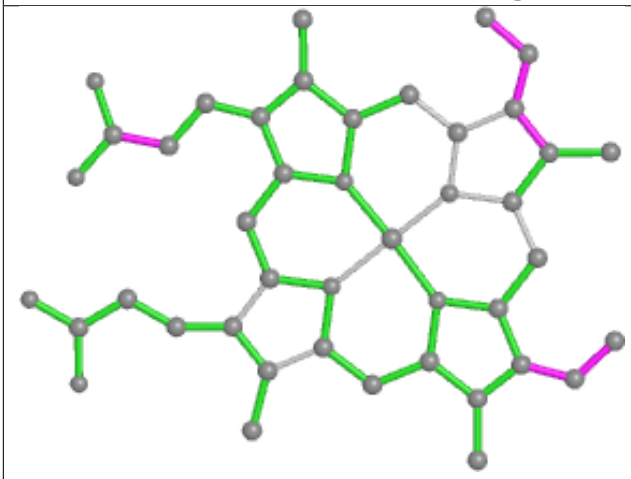


Torsions

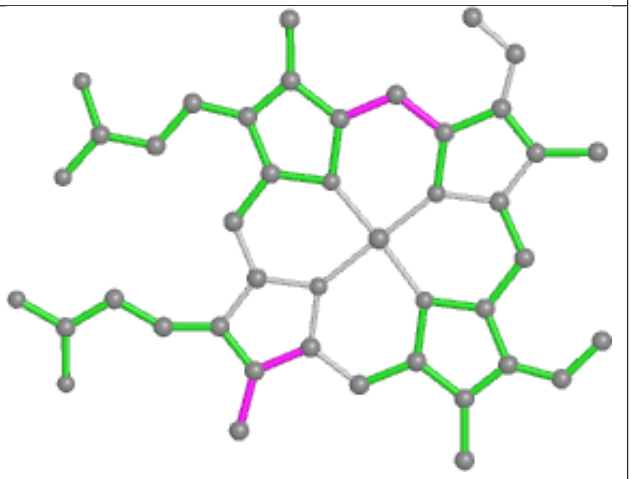


Rings

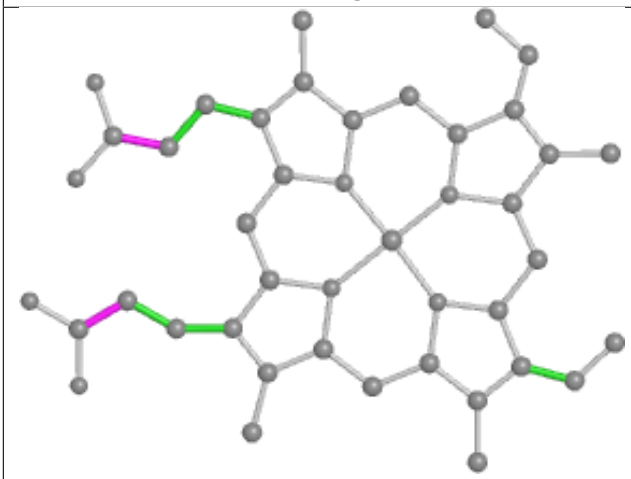
Ligand HEM D 3601



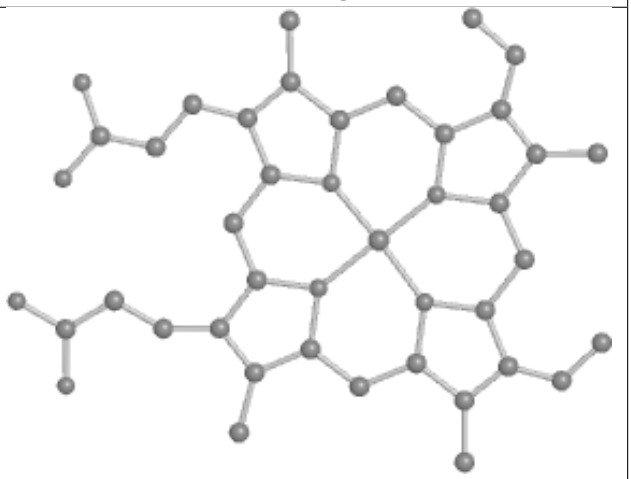
Bond lengths



Bond angles

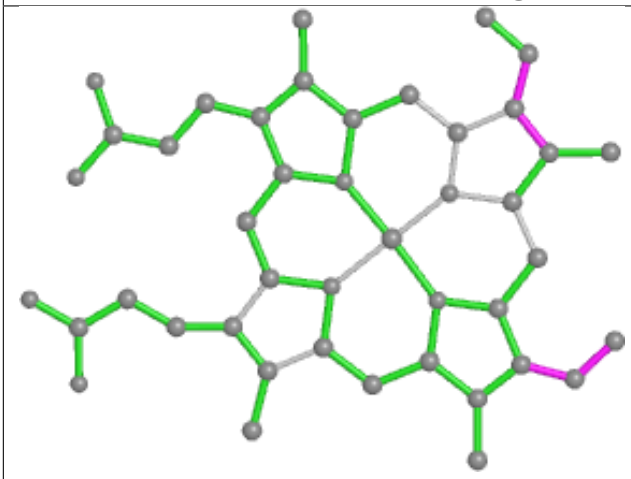


Torsions

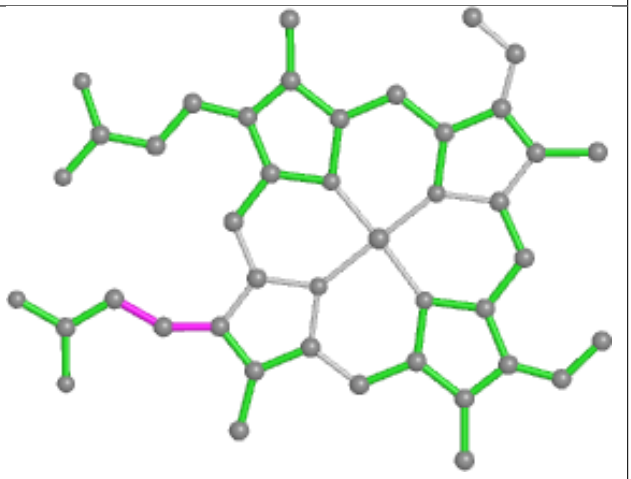


Rings

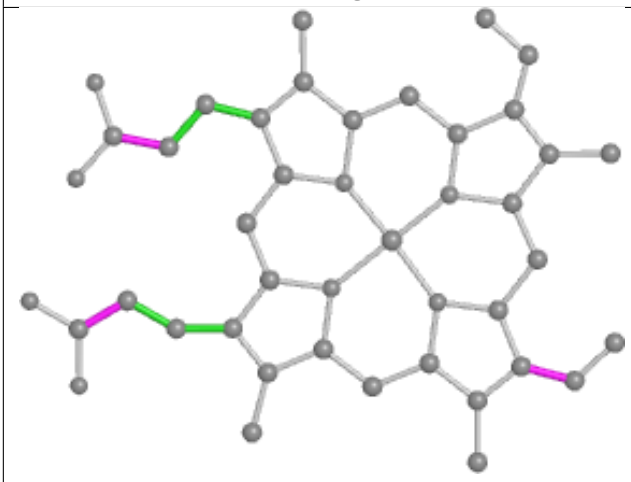
Ligand HEM B 1601



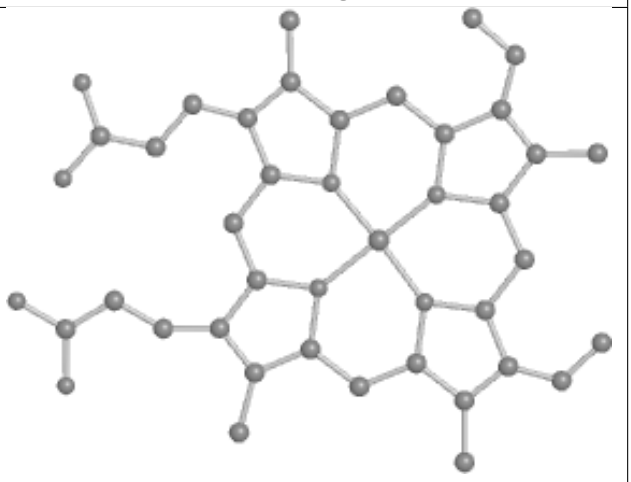
Bond lengths



Bond angles

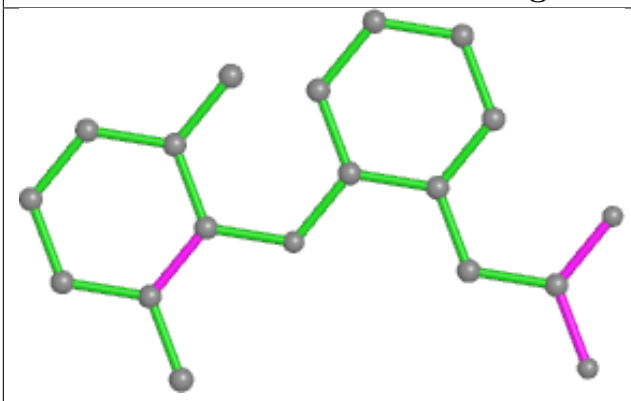


Torsions

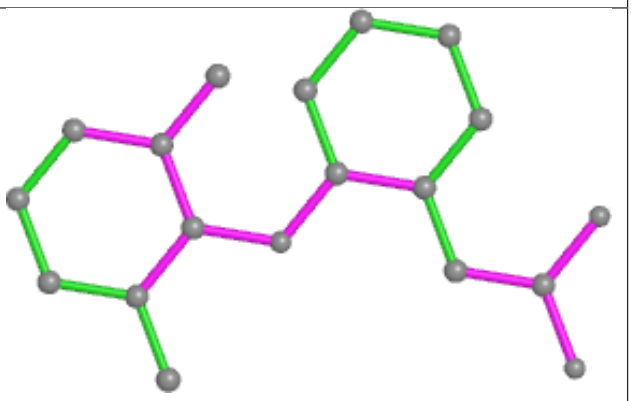


Rings

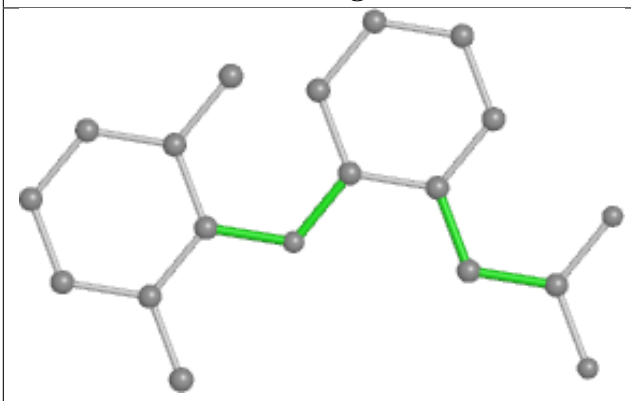
Ligand DIF A 701



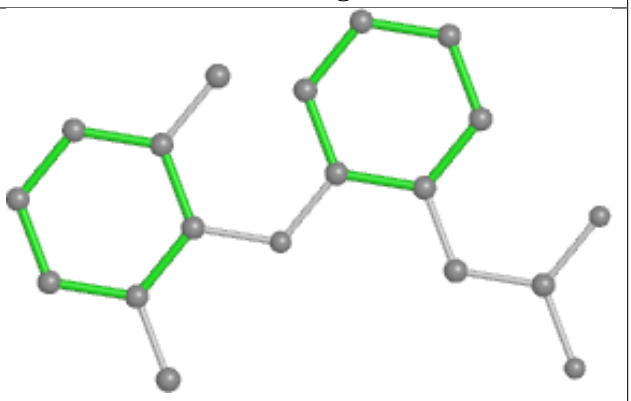
Bond lengths



Bond angles

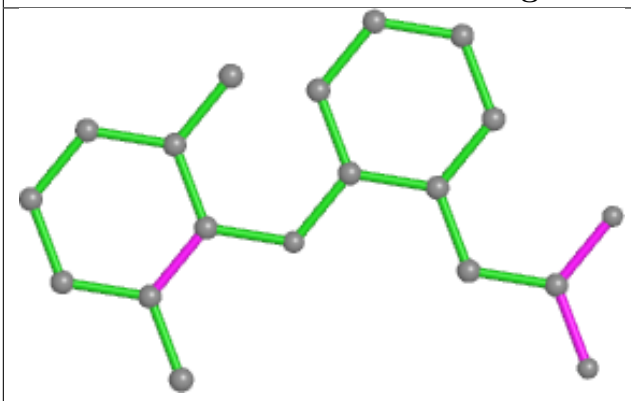


Torsions

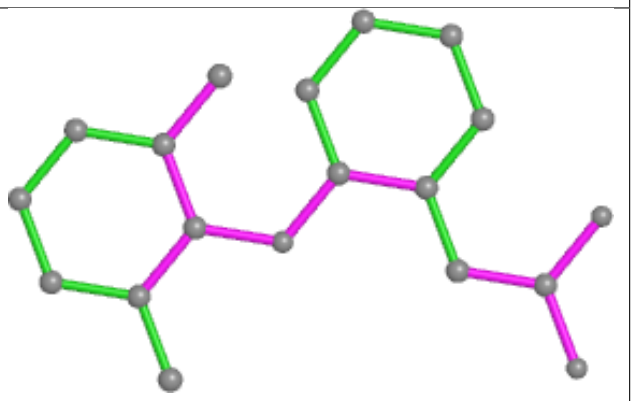


Rings

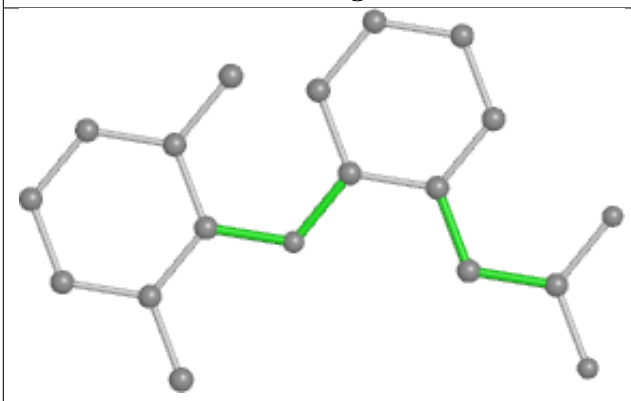
Ligand DIF B 1701



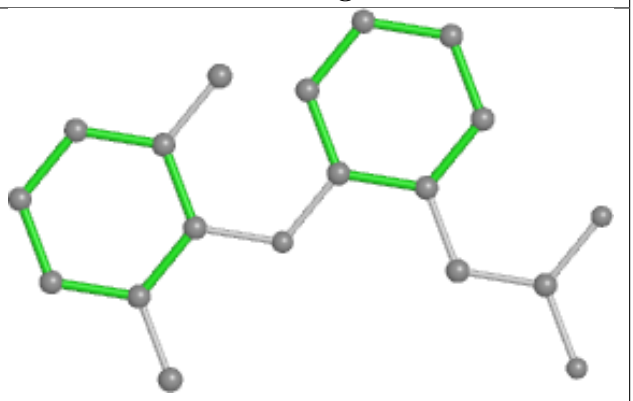
Bond lengths



Bond angles

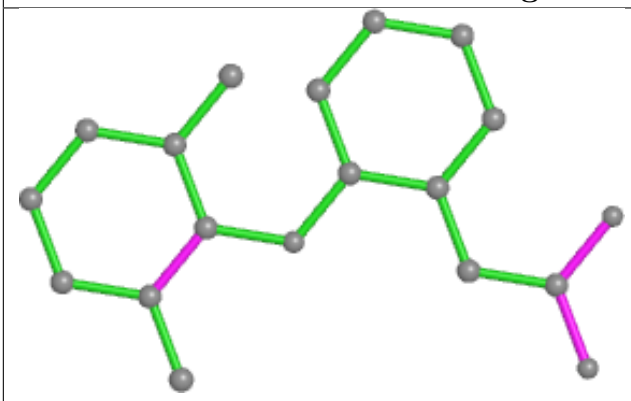


Torsions

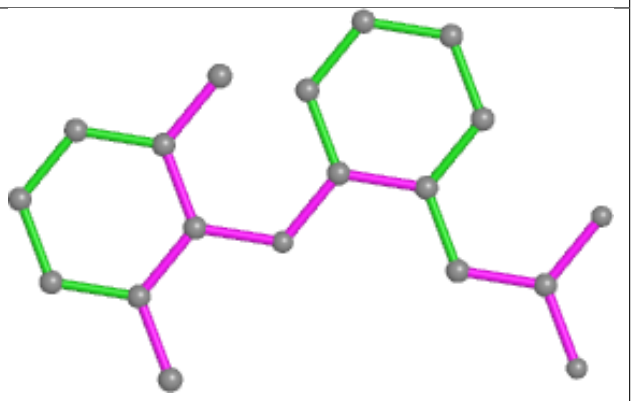


Rings

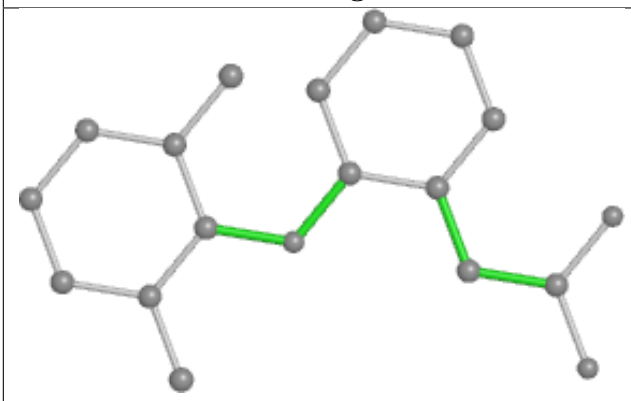
Ligand DIF C 2701



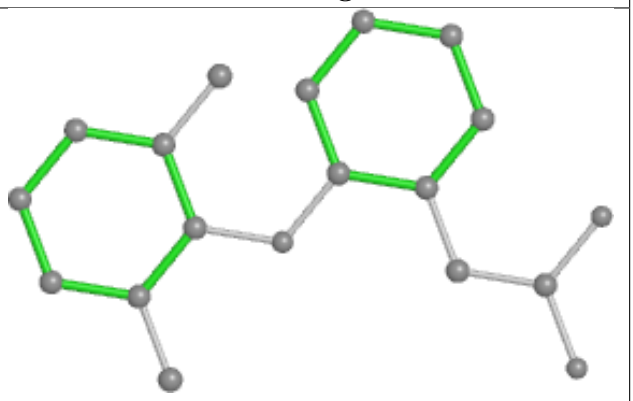
Bond lengths



Bond angles

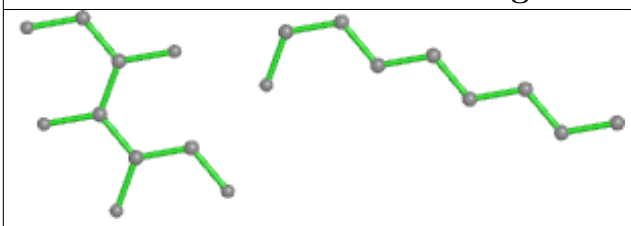


Torsions

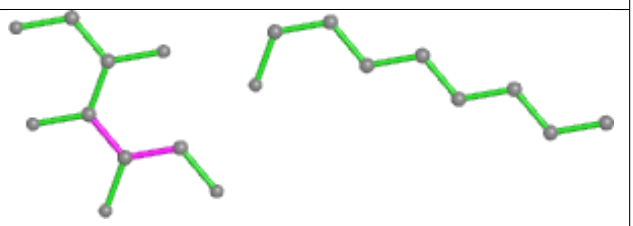


Rings

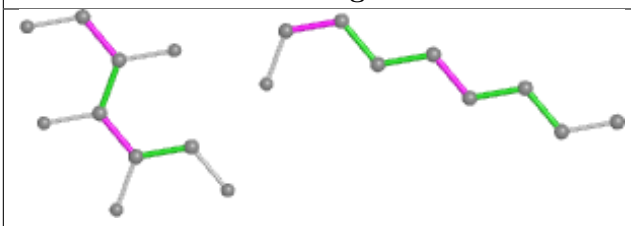
Ligand BOG D 3703



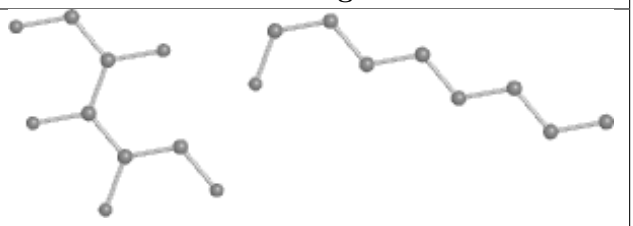
Bond lengths



Bond angles

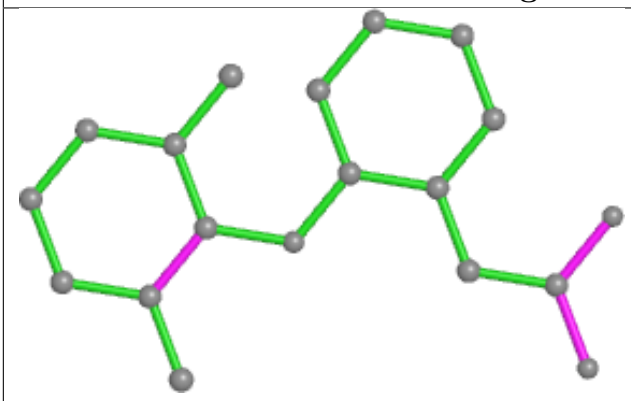


Torsions

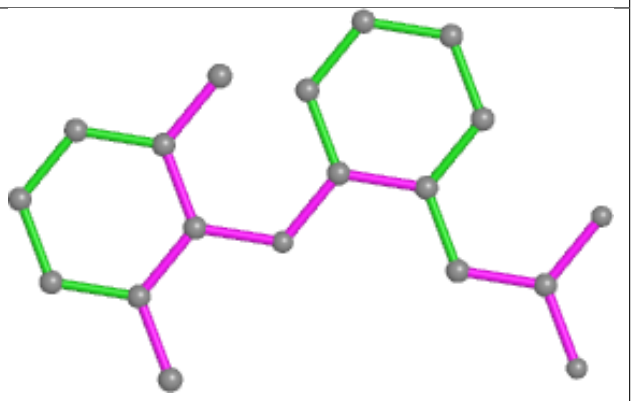


Rings

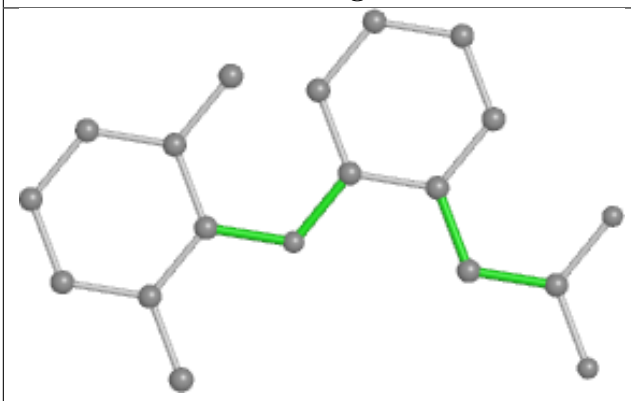
Ligand DIF D 3701



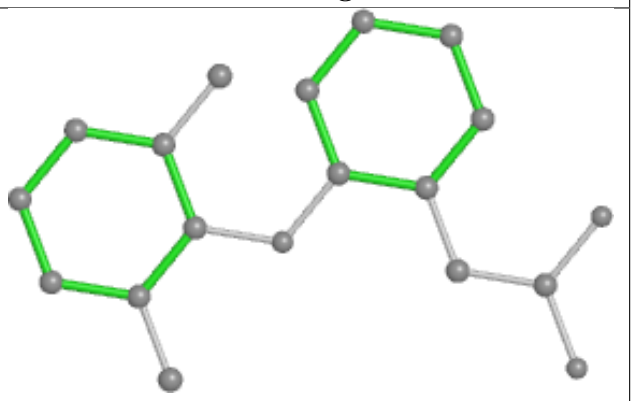
Bond lengths



Bond angles

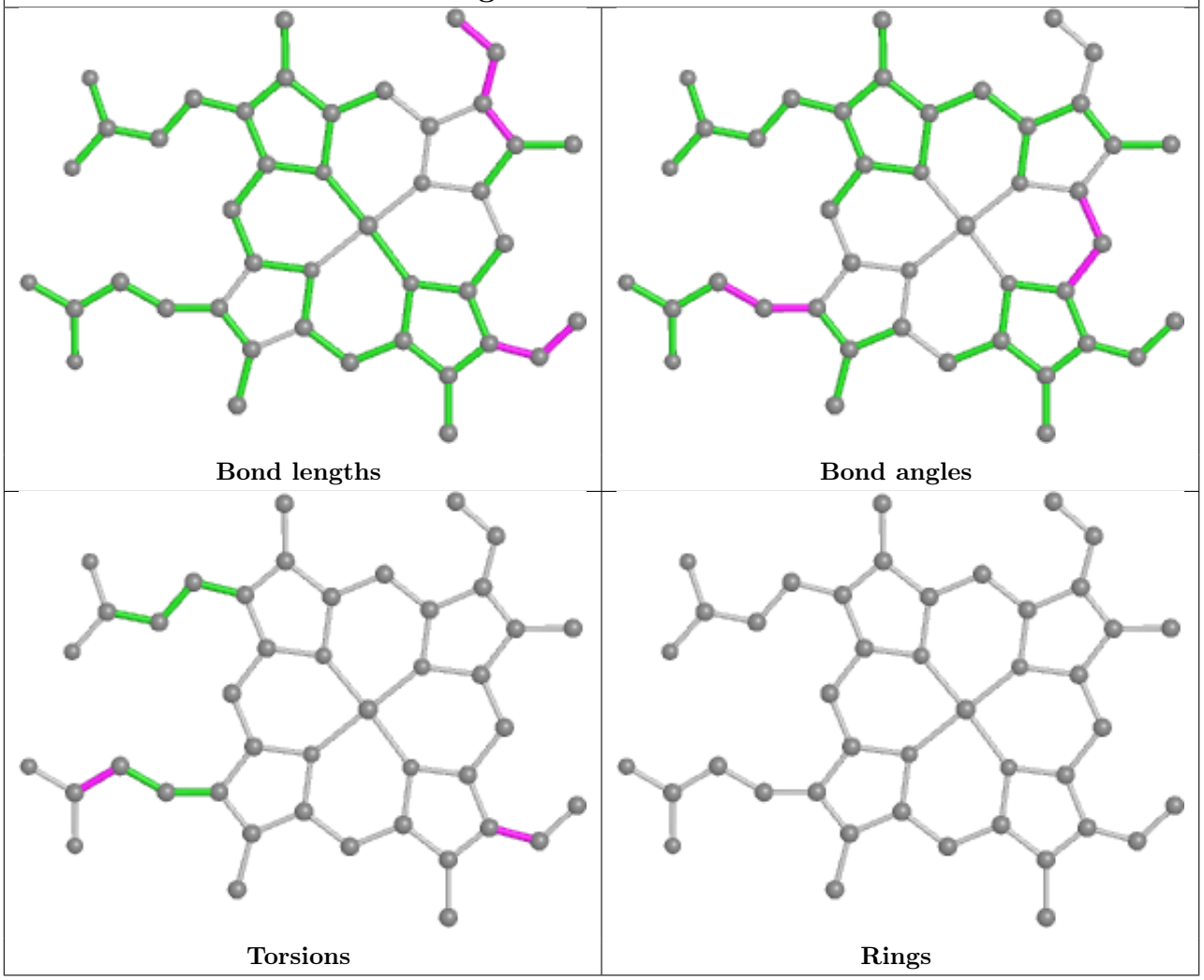


Torsions



Rings

Ligand HEM C 2601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	552/604 (91%)	0.07	13 (2%)	59	56	5, 21, 42, 53	0
1	B	552/604 (91%)	0.11	14 (2%)	57	55	5, 21, 42, 58	0
1	C	552/604 (91%)	0.03	8 (1%)	75	75	3, 21, 41, 62	0
1	D	552/604 (91%)	0.16	11 (1%)	65	63	5, 21, 42, 55	0
All	All	2208/2416 (91%)	0.09	46 (2%)	63	61	3, 21, 42, 62	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1583	GLN	5.4
1	C	2583	GLN	4.7
1	D	3368	ASN	3.3
1	D	3401	GLU	2.9
1	A	82	LEU	2.8

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	3	14/15	0.34	0.51	51,66,71,72	0
2	NAG	G	3	14/15	0.37	0.66	66,71,73,74	0

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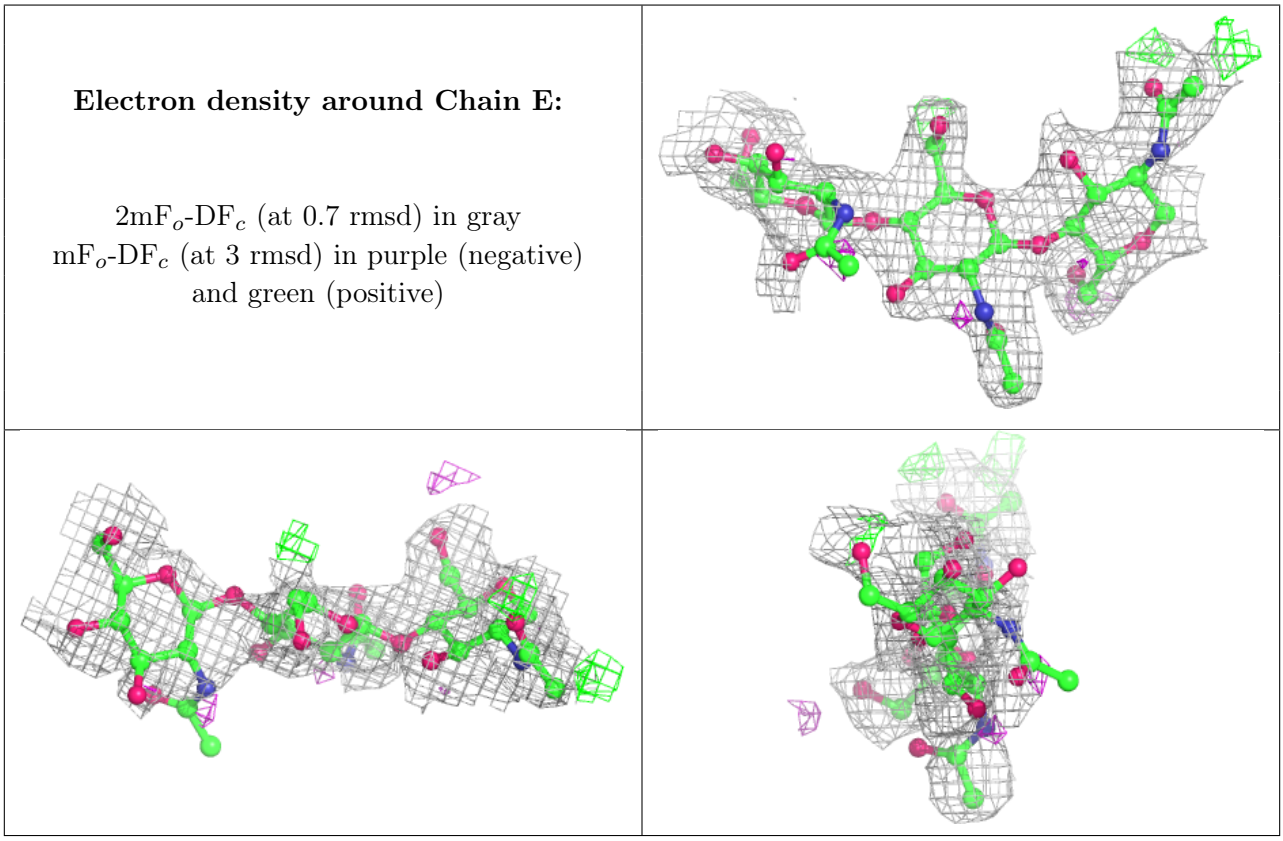
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	3	14/15	0.42	0.61	41,65,67,69	0
2	NAG	E	3	14/15	0.56	0.53	58,64,72,73	0
2	NAG	E	2	14/15	0.74	0.38	44,51,56,57	0
2	NAG	G	2	14/15	0.75	0.34	50,55,62,65	0
2	NAG	F	2	14/15	0.81	0.31	51,57,61,61	0
2	NAG	H	2	14/15	0.82	0.31	44,50,55,59	0
2	NAG	F	1	14/15	0.85	0.23	17,25,39,43	0
2	NAG	E	1	14/15	0.86	0.20	18,26,30,38	0
2	NAG	H	1	14/15	0.88	0.22	18,23,26,36	0
2	NAG	G	1	14/15	0.91	0.18	22,27,40,46	0

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

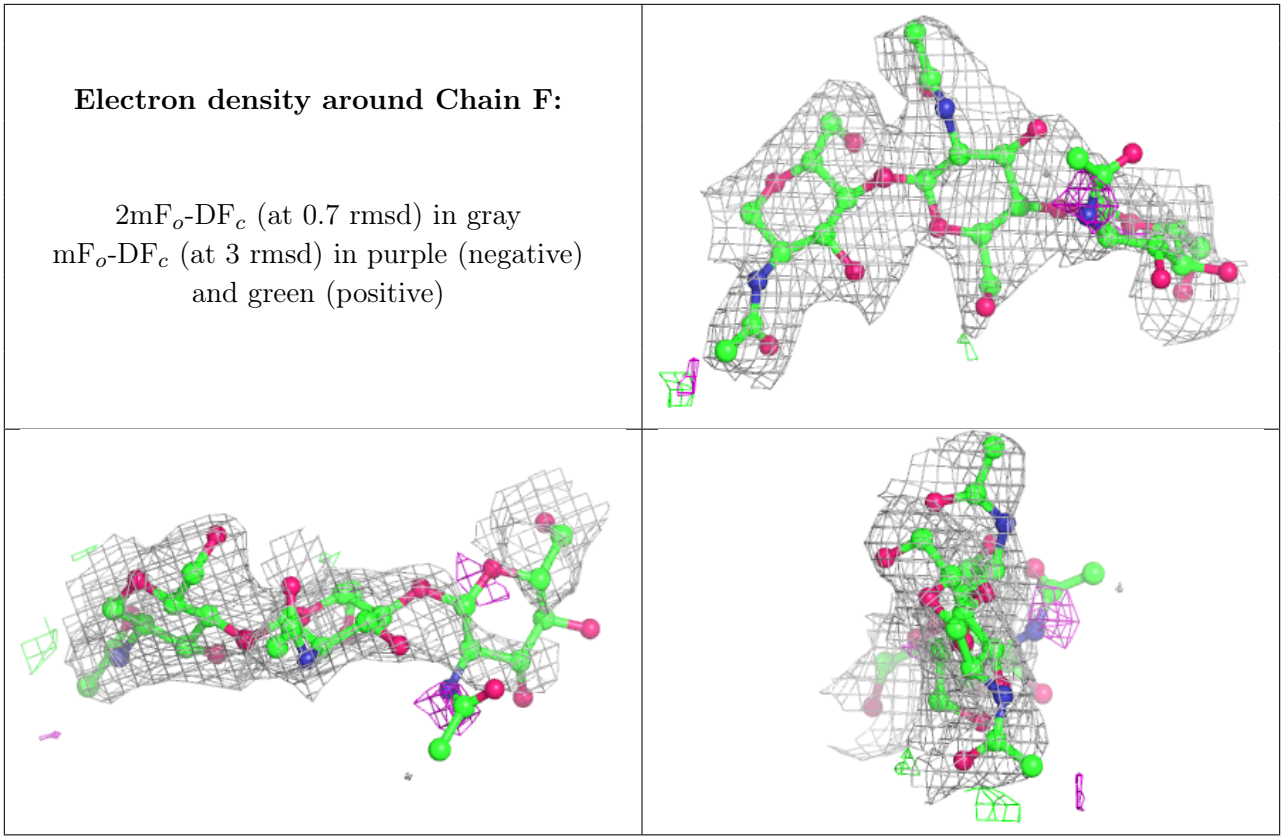
Electron density around Chain E:

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



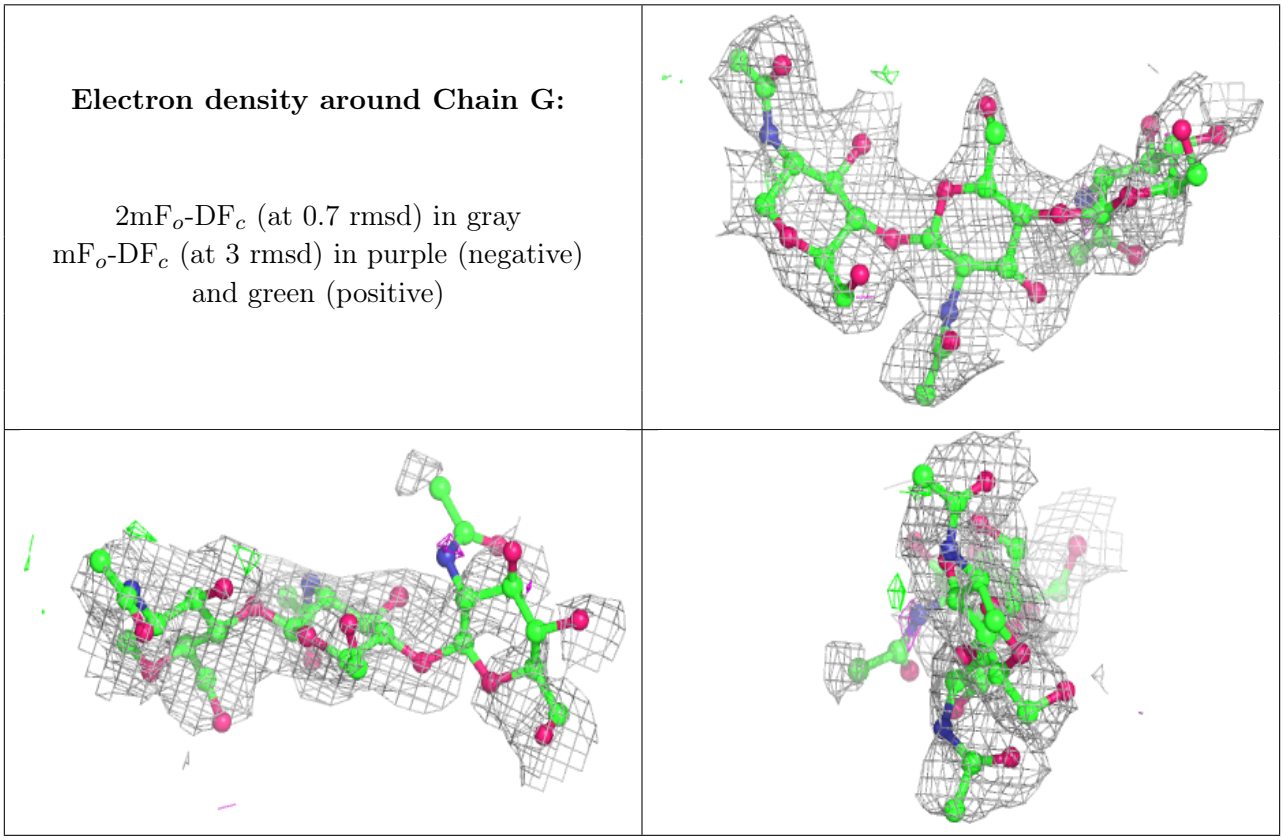
Electron density around Chain F:

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



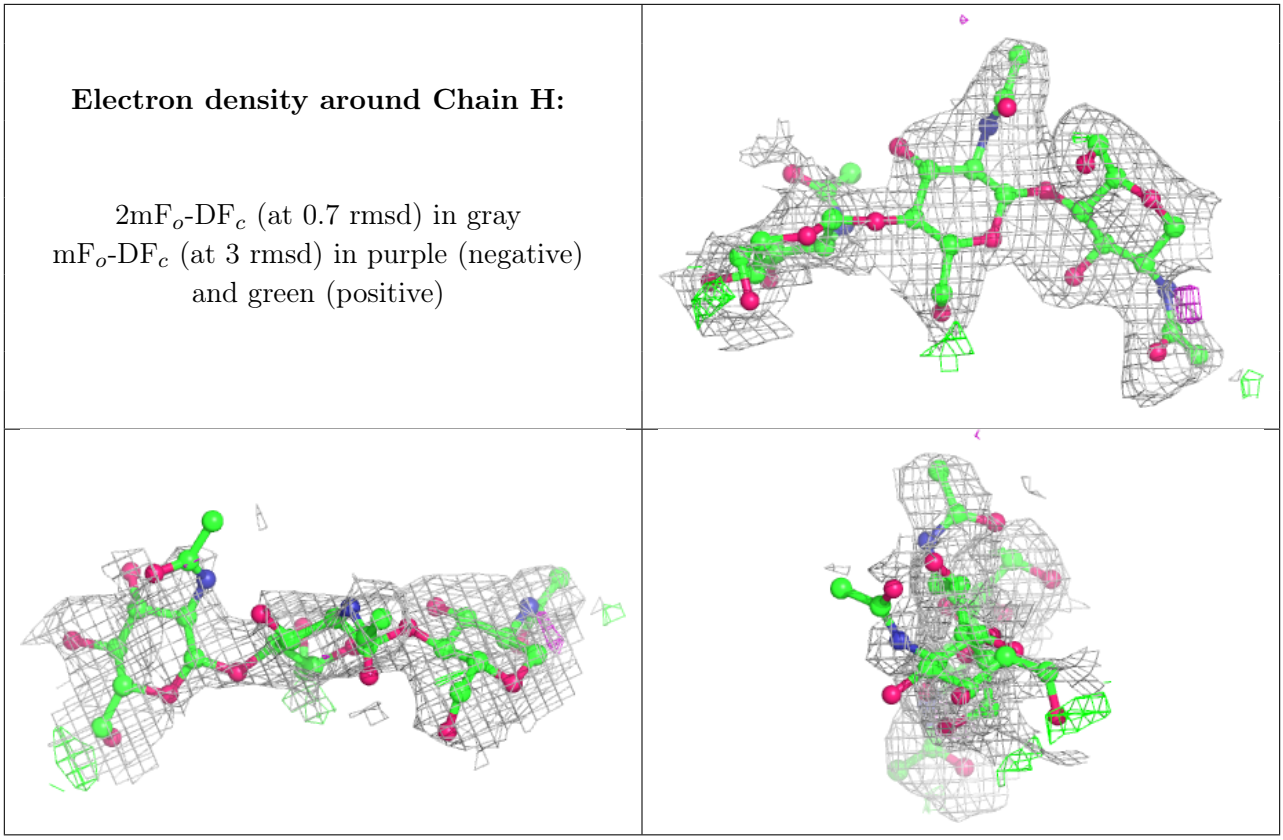
Electron density around Chain G:

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



Electron density around Chain H:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	1661	14/15	0.68	0.35	55,58,61,62	0
3	NAG	C	2661	14/15	0.77	0.32	45,54,61,63	0
3	NAG	B	1681	14/15	0.78	0.38	46,48,56,56	0
3	NAG	D	3661	14/15	0.79	0.46	51,55,59,61	0
3	NAG	A	661	14/15	0.80	0.42	55,57,61,61	0
3	NAG	C	2681	14/15	0.82	0.34	44,46,56,57	0
3	NAG	A	681	14/15	0.84	0.27	44,48,51,52	0
3	NAG	D	3681	14/15	0.84	0.36	47,51,59,62	0
6	DIF	B	1701	19/19	0.88	0.23	13,31,51,52	0
6	DIF	D	3701	19/19	0.88	0.20	17,38,44,55	0
4	BOG	D	3703	19/20	0.89	0.23	19,22,30,30	0
6	DIF	A	701	19/19	0.89	0.24	28,30,46,48	0
5	HEM	D	3601	43/43	0.90	0.21	13,21,41,43	0
6	DIF	C	2701	19/19	0.90	0.24	9,29,57,58	0

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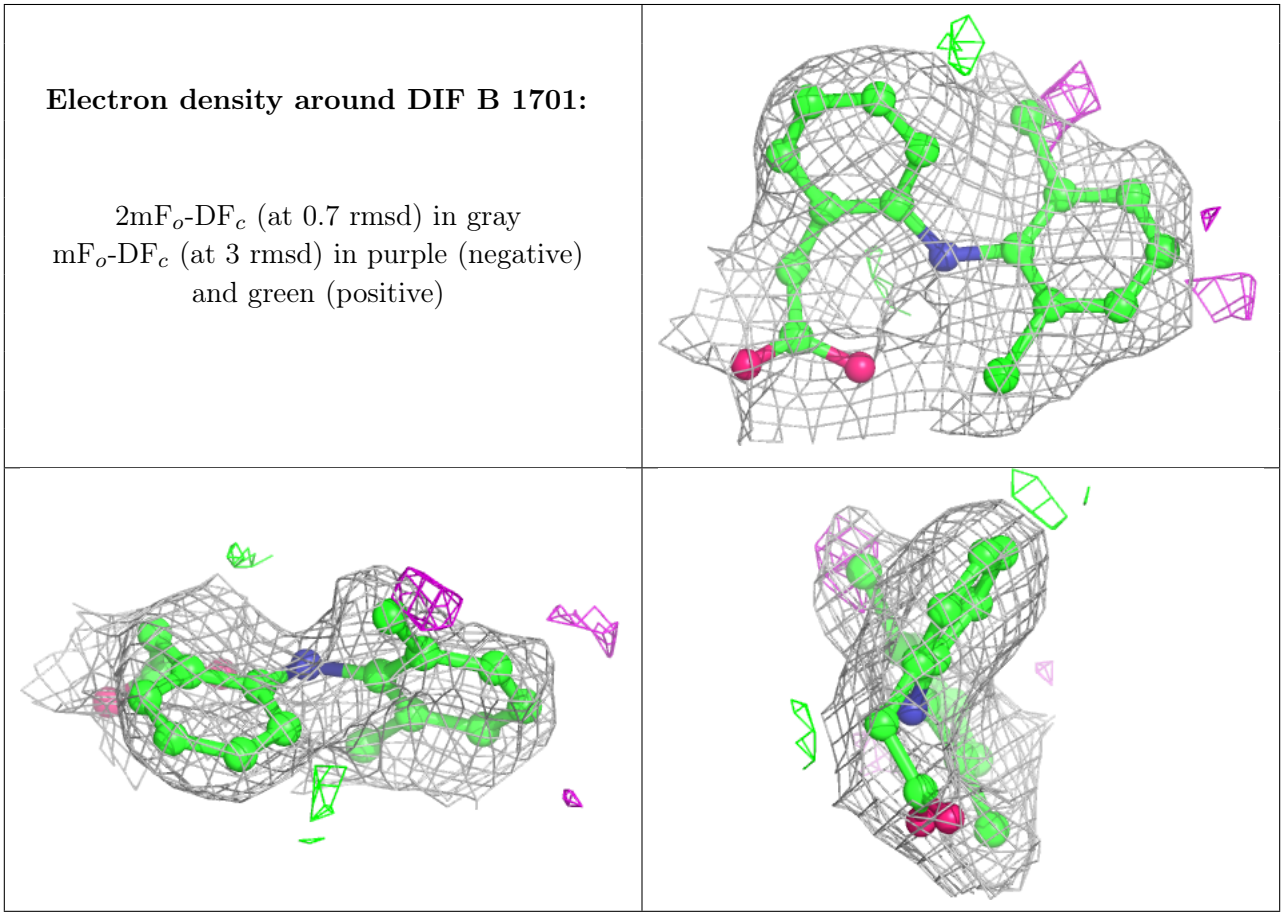
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BOG	A	703	20/20	0.90	0.23	17,20,24,25	0
5	HEM	B	1601	43/43	0.91	0.21	4,22,48,54	0
5	HEM	A	704	43/43	0.94	0.17	2,15,36,43	0
5	HEM	C	2601	43/43	0.95	0.15	8,20,35,40	0

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.

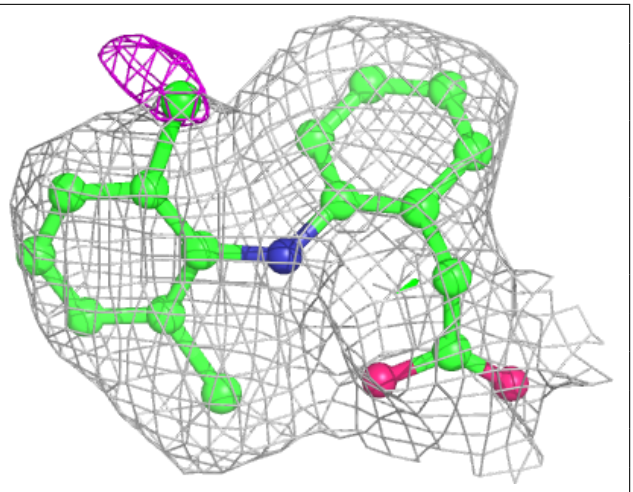
Electron density around DIF B 1701:

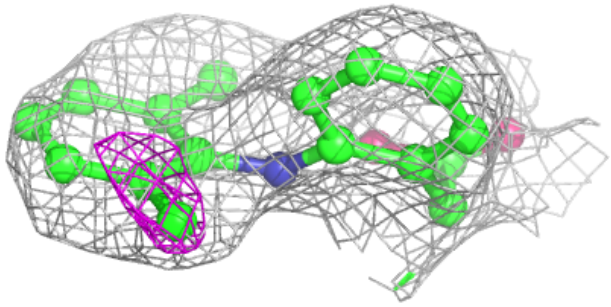
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

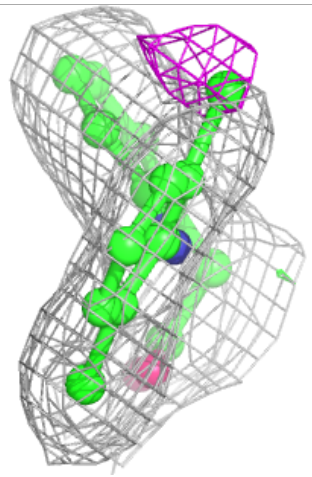


Electron density around DIF D 3701:

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

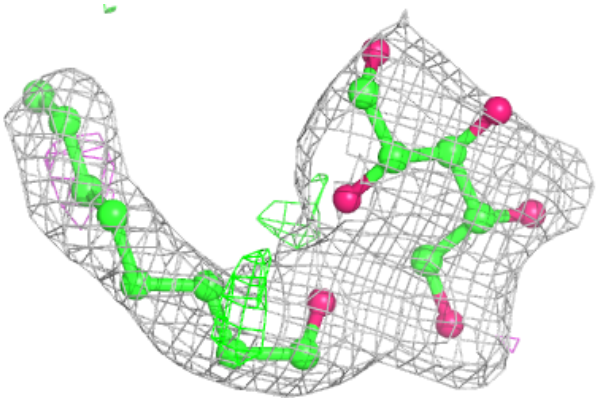


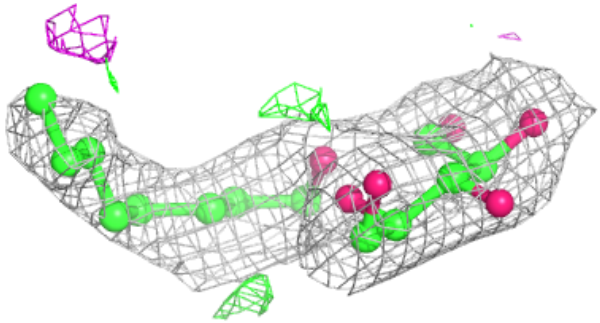


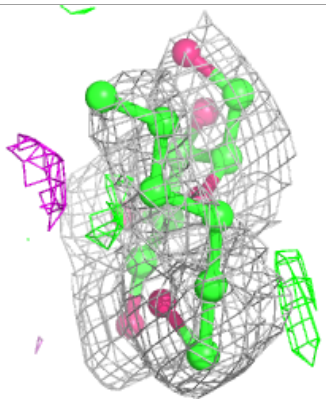


Electron density around BOG D 3703:

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

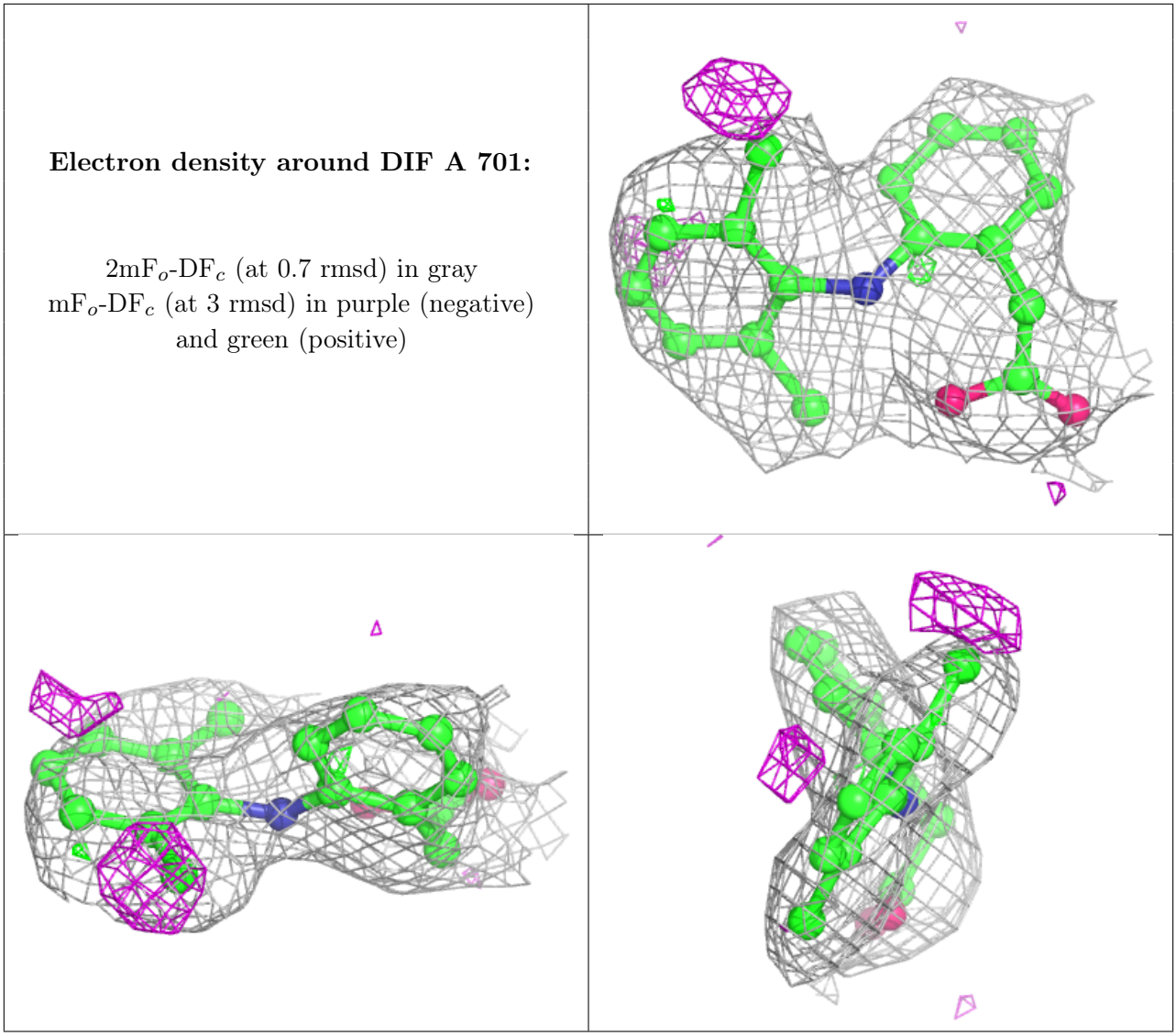






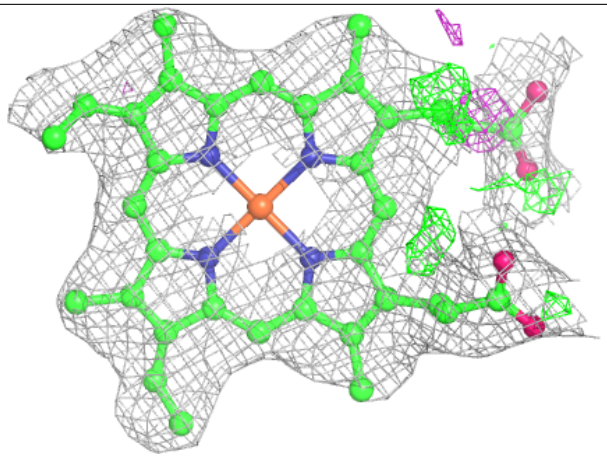
Electron density around DIF A 701:

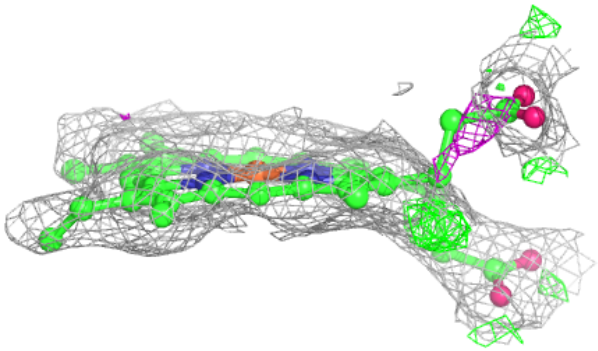
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

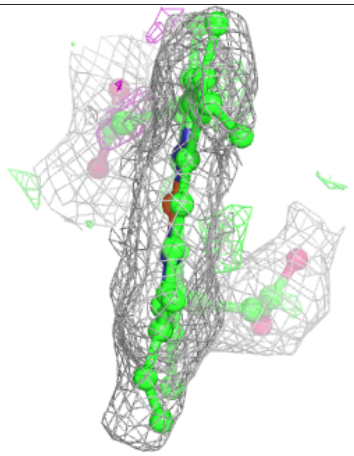


Electron density around HEM D 3601:

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

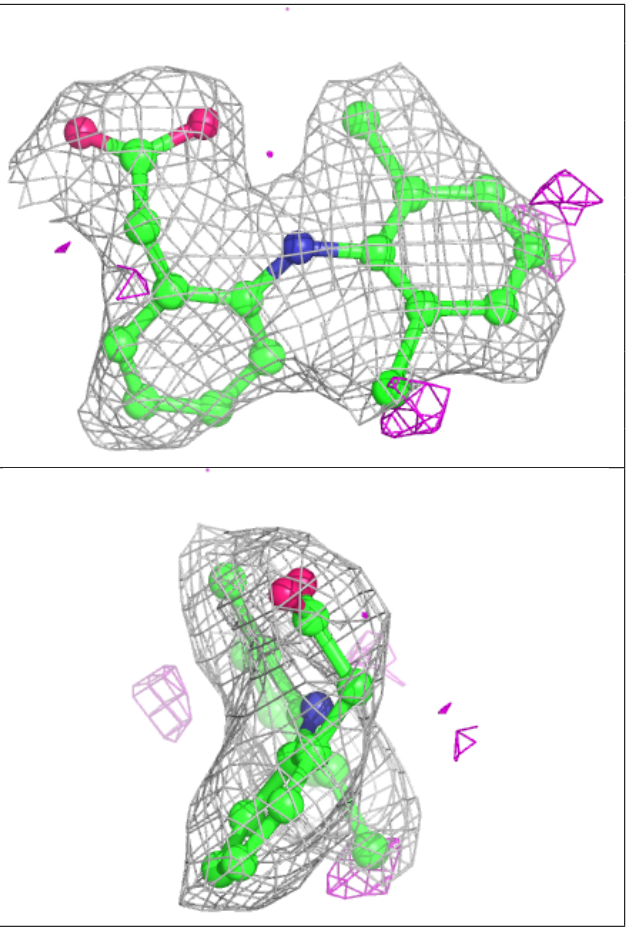






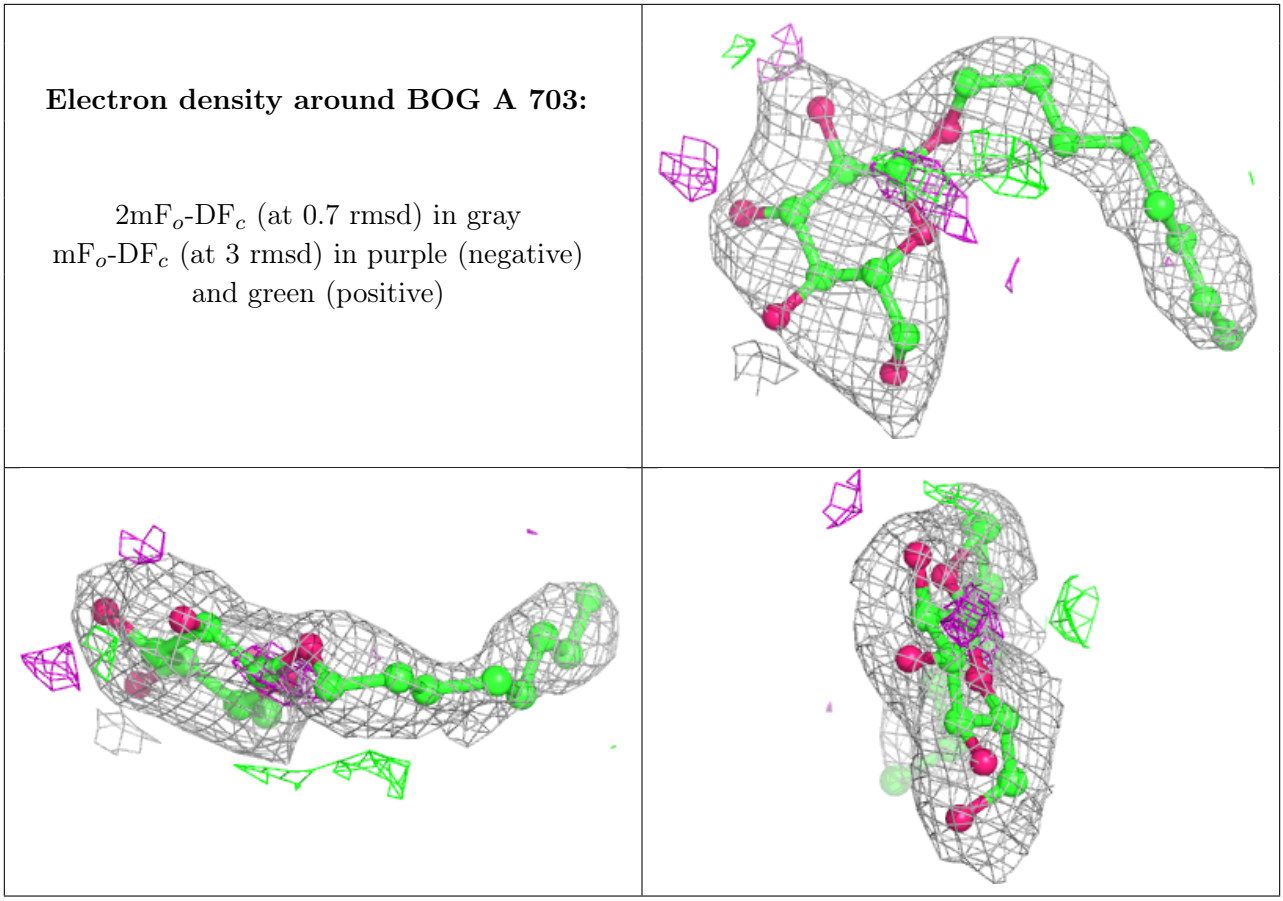
Electron density around DIF C 2701:

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



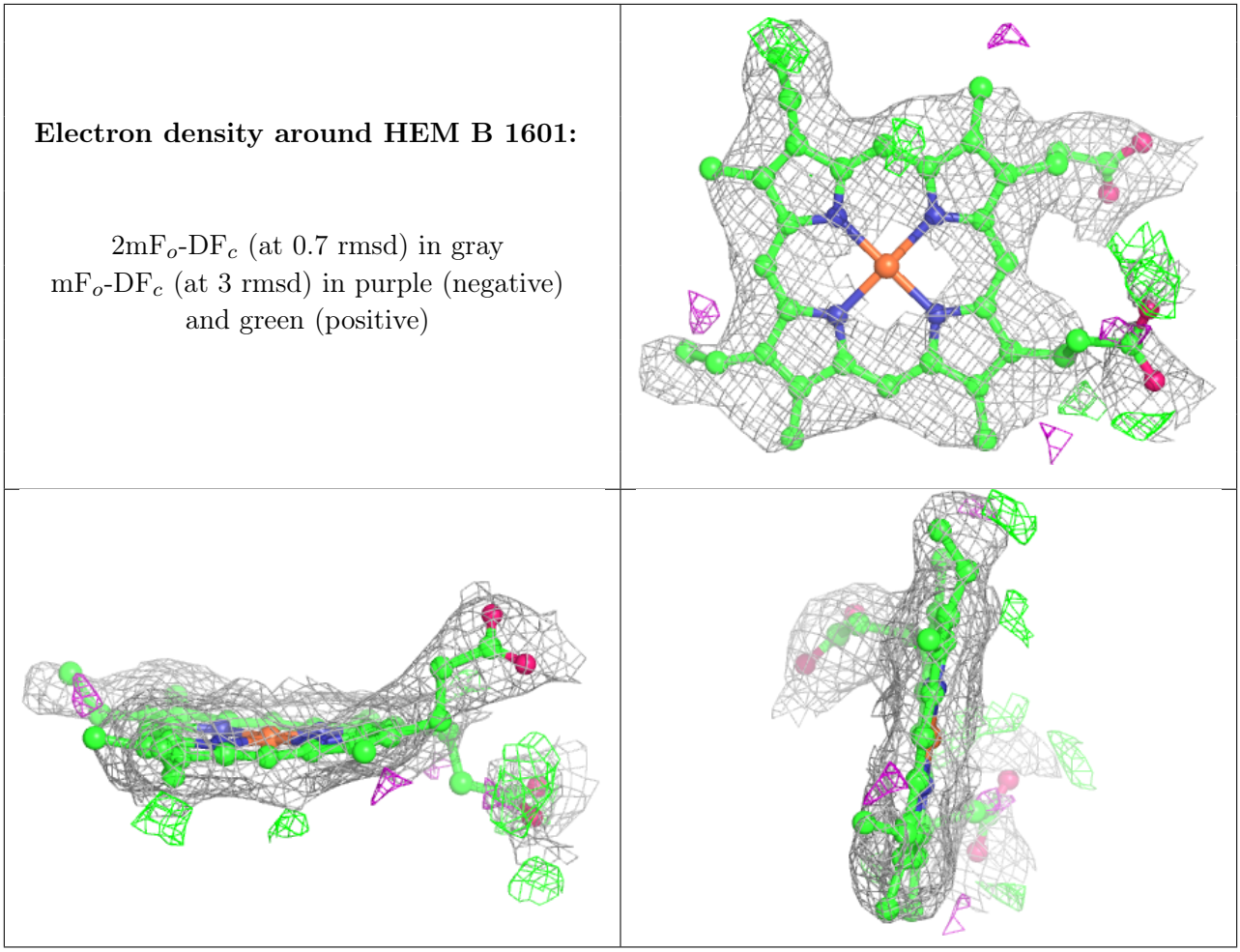
Electron density around BOG A 703:

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



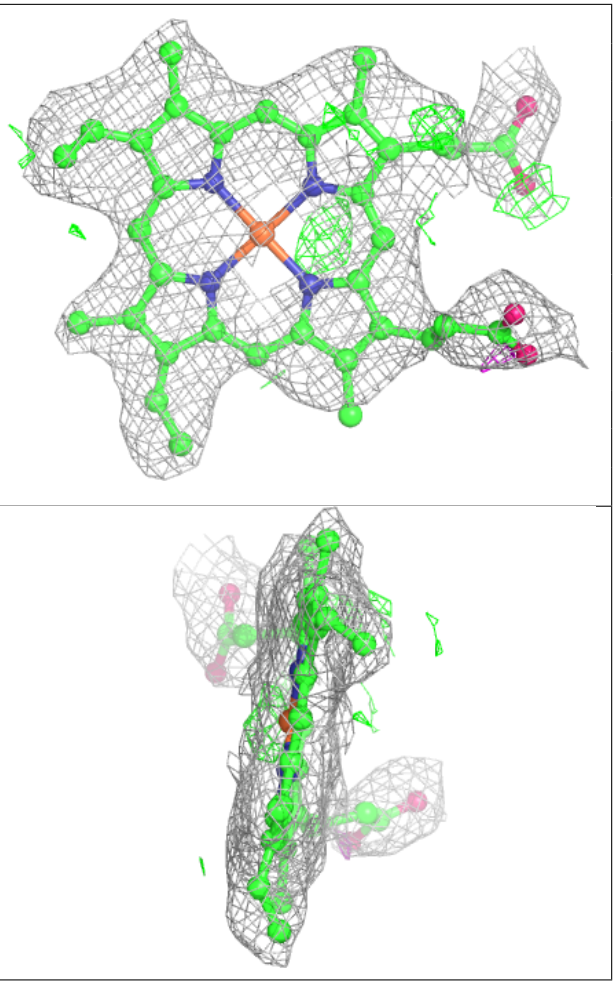
Electron density around HEM B 1601:

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



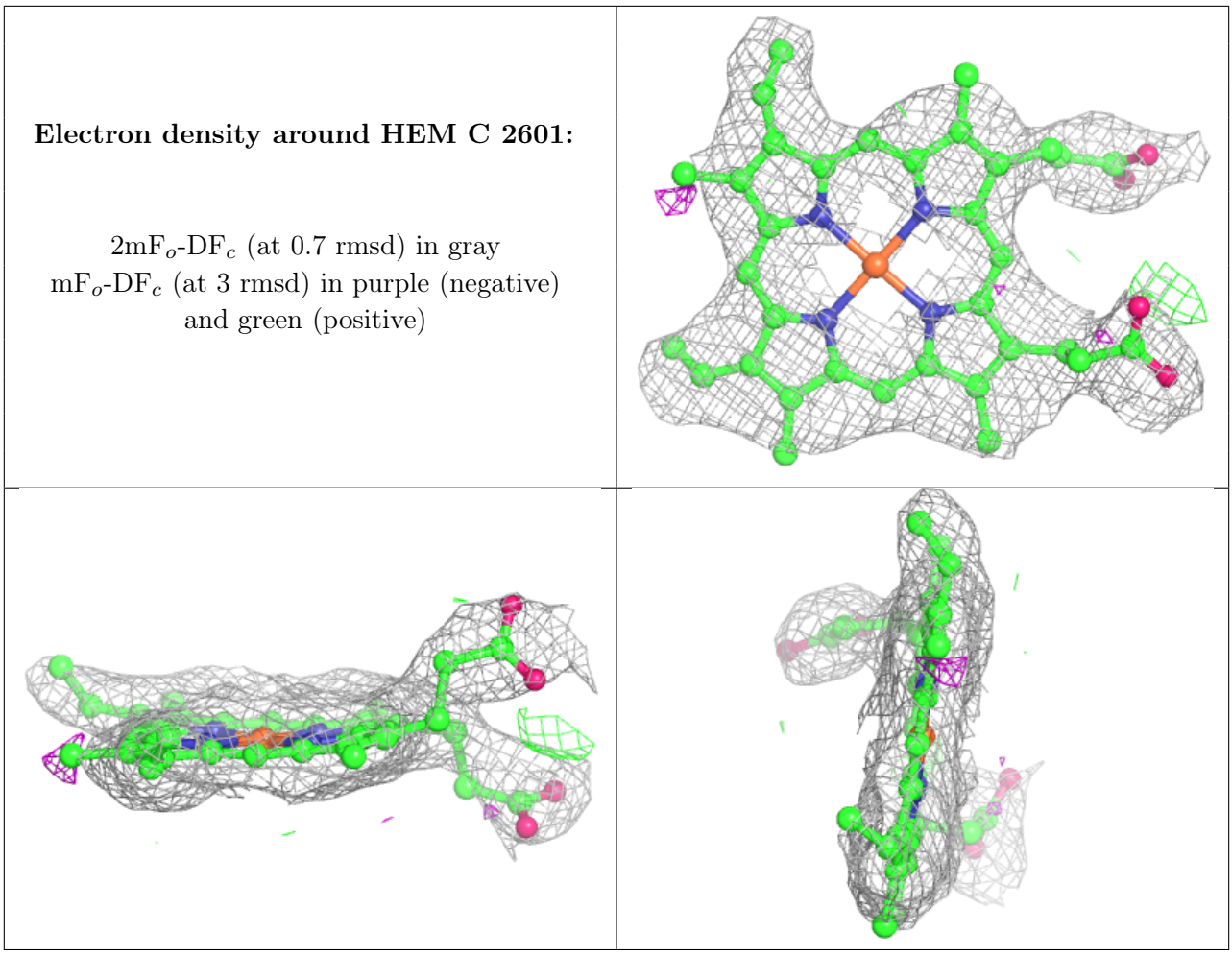
Electron density around HEM A 704:

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



Electron density around HEM C 2601:

$2mF_o$-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.