



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:44 PM EDT

PDB ID : 1DNU  
Title : STRUCTURAL ANALYSES OF HUMAN MYELOPEROXIDASE-THIOCYANATE COMPLEX  
Authors : Blair-Johnson, M.; Fiedler, T.J.; Fenna, R.E.  
Deposited on : 1999-12-16  
Resolution : 1.85 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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

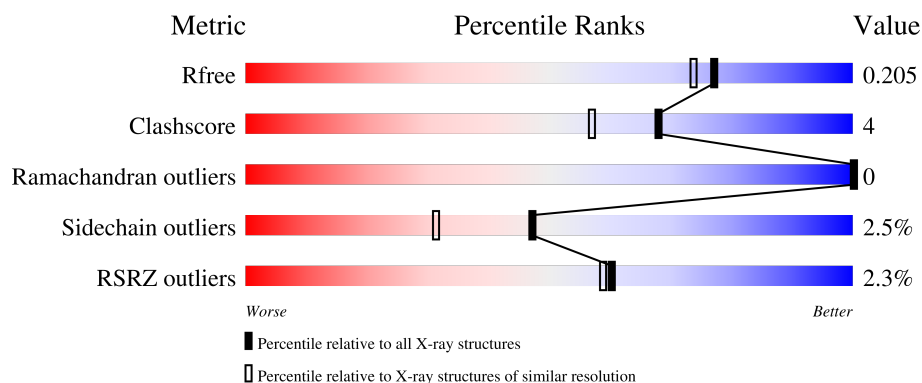
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	104	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	104	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	C	466	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
2	D	466	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>
3	E	6	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	6	<div><div></div><div>50%</div><div></div><div>50%</div></div>

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
9	ACY	C	15	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10318 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 MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	B	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			

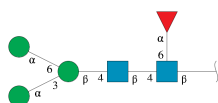
- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			
2	D	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			

There are 2 discrepancies between the modelled and reference sequences:

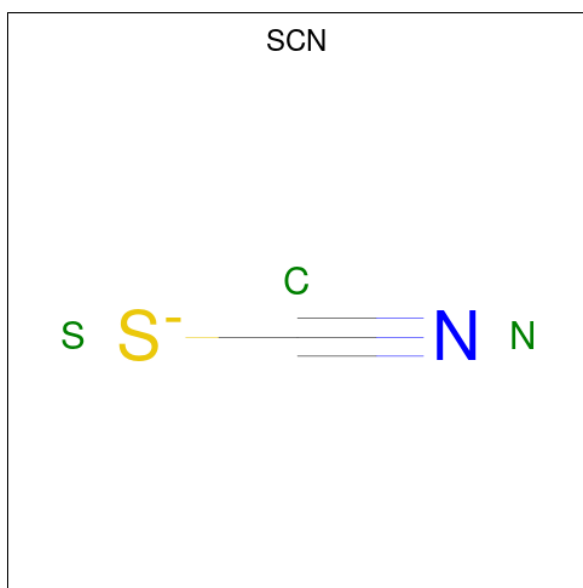
Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	modified residue	UNP P05164
D	150	CSO	CYS	modified residue	UNP P05164

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



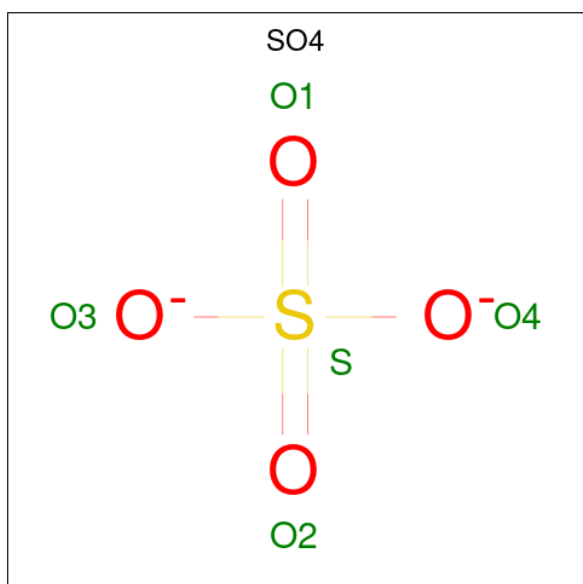
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



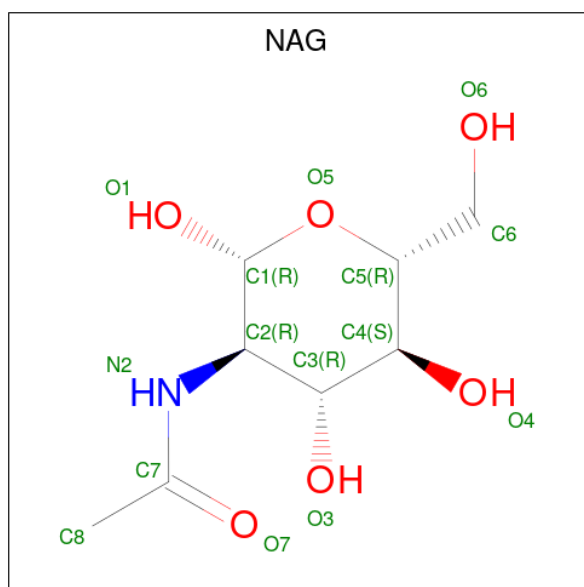
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		

- # HEM

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

- ACY
- 
- The diagram shows the chemical structure of acetic acid (CH<sub>3</sub>COOH). The central carbon atom is labeled 'C' in green. It is bonded to a methyl group (CH<sub>3</sub>) on the left, labeled 'CH3' in green. To the right, the carbon is double-bonded to an oxygen atom labeled 'O' in red, and single-bonded to a hydroxyl group (-OH) where the 'O' is red and the 'H' is green. Above the hydroxyl group, the label 'OXT' is written in green. A small green circle is located below the red oxygen atom of the hydroxyl group.

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

- Molecule 10 is water.

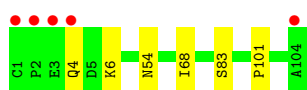
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	92	Total O 92 92	0	0
10	C	334	Total O 334 334	0	0
10	B	103	Total O 103 103	0	0
10	D	310	Total O 310 310	0	0



### 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.

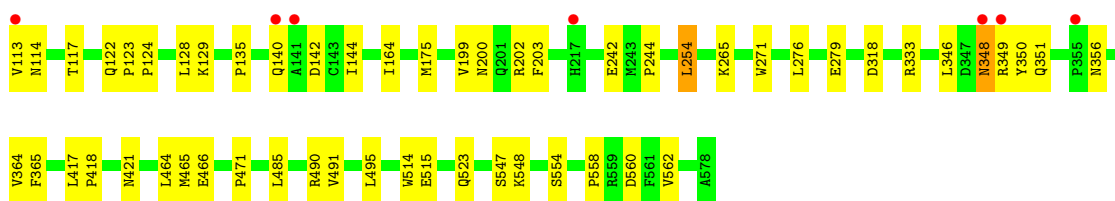
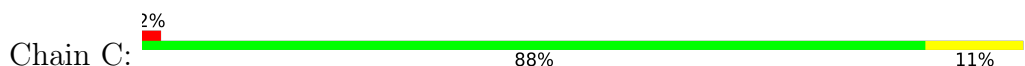
- Molecule 1: MYELOPEROXIDASE



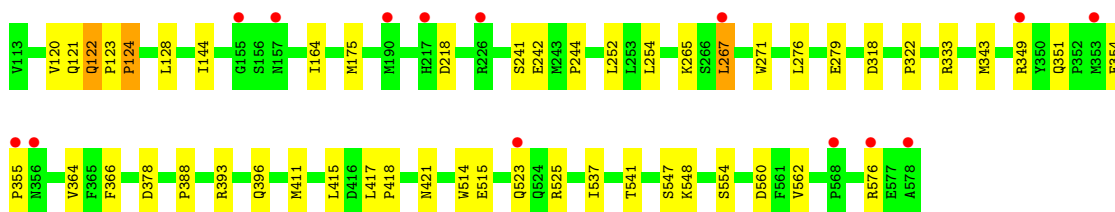
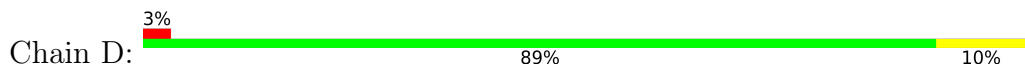
- Molecule 1: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



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

Chain E:  100%



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

Chain F:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.24Å 63.87Å 92.62Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85 48.79 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.7 (10.00-1.85) 98.1 (48.79-1.86)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.51 (at 1.86Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.178 , 0.210 0.173 , 0.205	Depositor DCC
$R_{free}$ test set	5388 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, SCN, FUC, CSO, ACY, CA, SO4, NAG, HEM, 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	0.64	0/863	0.70	0/1174
1	B	0.60	0/863	0.73	0/1174
2	C	0.60	0/3811	0.63	0/5168
2	D	0.57	0/3811	0.61	0/5168
All	All	0.59	0/9348	0.64	0/12684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	838	0	798	4	0
1	B	838	0	798	5	0
2	C	3733	0	3725	37	0
2	D	3733	0	3725	31	0
3	E	71	0	61	0	0
3	F	71	0	61	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	C	28	0	26	0	0
6	D	28	0	26	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	43	0	30	2	0
8	C	43	0	30	2	0
9	C	12	0	9	2	0
9	D	12	0	9	1	0
10	A	92	0	0	1	0
10	B	103	0	0	0	0
10	C	334	0	0	2	0
10	D	310	0	0	0	0
All	All	10318	0	9298	72	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 4.

All (72) 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)
2:C:135:PRO:HG2	10:C:897:HOH:O	1.84	0.77
2:D:525:ARG:HH11	9:D:13:ACY:H2	1.48	0.75
2:C:348:ASN:H	2:C:348:ASN:HD22	1.37	0.71
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.77	0.66
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.33	0.63
2:D:265:LYS:HD3	2:D:276:LEU:HD11	1.80	0.62
10:A:188:HOH:O	2:C:129:LYS:HD3	2.00	0.60
2:C:333:ARG:HH21	2:C:421:ASN:HD22	1.50	0.60
2:C:200:ASN:HD22	2:C:203:PHE:H	1.49	0.59
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.85	0.58
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.85	0.58
2:C:200:ASN:ND2	2:C:202:ARG:H	2.01	0.58
2:C:200:ASN:HD22	2:C:202:ARG:H	1.51	0.57
2:D:411:MET:CE	2:D:415:LEU:HD21	2.34	0.57
2:C:142:ASP:HB3	10:C:928:HOH:O	2.05	0.57
8:B:107:HEM:HMC2	8:B:107:HEM:HBC2	1.87	0.56
2:C:465:MET:HE1	2:C:471:PRO:HD3	1.90	0.55
2:D:354:GLU:HB3	2:D:355:PRO:HA	1.90	0.53
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.92	0.52
2:D:333:ARG:HH21	2:D:421:ASN:HD22	1.57	0.52
2:D:120:VAL:HG12	2:D:122:GLN:CG	2.41	0.51
2:D:244:PRO:HD3	2:D:364:VAL:O	2.09	0.51
2:C:348:ASN:H	2:C:348:ASN:ND2	2.06	0.50
1:A:101:PRO:HD2	2:C:164:ILE:O	2.12	0.50
2:C:548:LYS:HG2	2:C:562:VAL:HG13	1.93	0.50
2:C:265:LYS:HD3	2:C:276:LEU:HD11	1.94	0.49
2:C:333:ARG:HH21	2:C:421:ASN:ND2	2.11	0.48
8:B:107:HEM:HBB2	2:D:242:GLU:OE1	2.13	0.48
2:C:200:ASN:ND2	2:C:203:PHE:H	2.12	0.48
1:B:83:SER:HB3	2:D:554:SER:O	2.13	0.47
2:D:267:LEU:HD13	2:D:576:ARG:NE	2.29	0.47
1:B:1:CYS:SG	1:B:20:PRO:HB3	2.55	0.47
1:A:68:ILE:HD13	2:C:464:LEU:HD23	1.96	0.47
2:D:393:ARG:HB2	2:D:396:GLN:HB2	1.97	0.47
2:D:378:ASP:OD1	2:D:541:THR:HB	2.15	0.46
2:D:333:ARG:HH21	2:D:421:ASN:ND2	2.12	0.46
1:A:83:SER:HB3	2:C:554:SER:O	2.15	0.46
2:C:554:SER:HB3	2:C:560:ASP:HB3	1.97	0.46
2:D:271:TRP:CZ3	2:D:279:GLU:HG3	2.50	0.46
8:C:10:HEM:HBC2	8:C:10:HEM:HMC2	1.98	0.46
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.50	0.46
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.97	0.46
2:C:123:PRO:HB3	9:C:15:ACY:H3	1.98	0.46
2:D:120:VAL:HG12	2:D:122:GLN:HG2	1.96	0.46
2:C:349:ARG:HG3	2:C:351:GLN:HG2	1.98	0.45
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.98	0.44
2:C:485:LEU:HD13	2:C:490:ARG:HA	1.99	0.44
2:D:244:PRO:HB2	2:D:343:MET:SD	2.58	0.44
2:D:349:ARG:HG3	2:D:351:GLN:CG	2.46	0.43
2:C:124:PRO:HA	9:C:15:ACY:CH3	2.49	0.43
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.54	0.43
2:D:554:SER:HB3	2:D:560:ASP:HB3	2.01	0.43
2:D:252:LEU:HD11	2:D:537:ILE:HA	2.02	0.42
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.34	0.42
2:C:417:LEU:HB3	2:C:418:PRO:HD3	2.00	0.42
2:C:244:PRO:HD3	2:C:364:VAL:O	2.19	0.42
1:B:79:ASP:O	2:D:388:PRO:HB3	2.19	0.42
2:D:121:GLN:C	2:D:122:GLN:HG2	2.39	0.42
2:C:346:LEU:HB3	2:C:350:TYR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:CD1	2:C:464:LEU:HD23	2.50	0.42
2:C:123:PRO:HA	2:C:124:PRO:HA	1.84	0.42
1:B:101:PRO:HD2	2:D:164:ILE:O	2.19	0.42
2:D:123:PRO:HA	2:D:124:PRO:HA	1.89	0.41
2:C:242:GLU:OE1	8:C:10:HEM:HBB2	2.21	0.41
2:D:120:VAL:HG12	2:D:122:GLN:HG3	2.03	0.41
2:D:241:SER:O	2:D:366:PHE:HA	2.20	0.41
2:C:113:VAL:HG12	2:C:114:ASN:N	2.35	0.41
2:C:114:ASN:HB3	2:C:117:THR:OG1	2.20	0.41
1:B:6:LYS:HE2	1:B:6:LYS:HB2	1.99	0.41
2:D:128:LEU:HB2	2:D:144:ILE:HB	2.03	0.41
2:C:242:GLU:O	2:C:365:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
1	B	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	450 (97%)	13 (3%)	0	100	100
2	D	463/466 (99%)	453 (98%)	10 (2%)	0	100	100
All	All	1130/1140 (99%)	1101 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/90 (100%)	87 (97%)	3 (3%)	38	21
1	B	90/90 (100%)	89 (99%)	1 (1%)	73	65
2	C	410/410 (100%)	399 (97%)	11 (3%)	44	29
2	D	410/410 (100%)	400 (98%)	10 (2%)	49	33
All	All	1000/1000 (100%)	975 (98%)	25 (2%)	47	31

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	LYS
1	A	54	ASN
2	C	122	GLN
2	C	140	GLN
2	C	175	MET
2	C	254	LEU
2	C	318	ASP
2	C	348	ASN
2	C	356	ASN
2	C	466	GLU
2	C	523	GLN
2	C	547	SER
2	C	558	PRO
1	B	54	ASN
2	D	122	GLN
2	D	124	PRO
2	D	175	MET
2	D	218	ASP
2	D	254	LEU
2	D	267	LEU
2	D	318	ASP
2	D	322	PRO
2	D	523	GLN
2	D	547	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:



Mol	Chain	Res	Type
2	C	200	ASN
2	C	348	ASN
2	C	421	ASN
1	B	54	ASN
2	D	421	ASN
2	D	549	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	CSO	C	150	2	3,6,7	0.76	0	0,6,8	-	-
2	CSO	D	150	2	3,6,7	0.70	0	0,6,8	-	-

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	CSO	C	150	2	-	0/1/5/7	-
2	CSO	D	150	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

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	$\# Z  > 2$
3	NAG	E	1	3,2	14,14,15	0.76	0	17,19,21	0.83	0
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	0.80	0
3	BMA	E	3	3	11,11,12	0.71	0	15,15,17	0.53	0
3	MAN	E	4	3	11,11,12	1.03	0	15,15,17	0.55	0
3	MAN	E	5	3	11,11,12	0.61	0	15,15,17	0.69	0
3	FUC	E	6	3	10,10,11	0.61	0	14,14,16	0.52	0
3	NAG	F	1	3,2	14,14,15	0.60	0	17,19,21	0.84	0
3	NAG	F	2	3	14,14,15	0.57	0	17,19,21	0.79	1 (5%)
3	BMA	F	3	3	11,11,12	0.58	0	15,15,17	0.60	0
3	MAN	F	4	3	11,11,12	0.88	0	15,15,17	0.67	1 (6%)
3	MAN	F	5	3	11,11,12	0.60	0	15,15,17	0.57	1 (6%)
3	FUC	F	6	3	10,10,11	0.55	0	14,14,16	0.45	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C4-C3-C2	-2.21	107.78	111.02
3	F	4	MAN	C1-O5-C5	2.08	115.01	112.19
3	F	5	MAN	C1-O5-C5	2.06	114.98	112.19

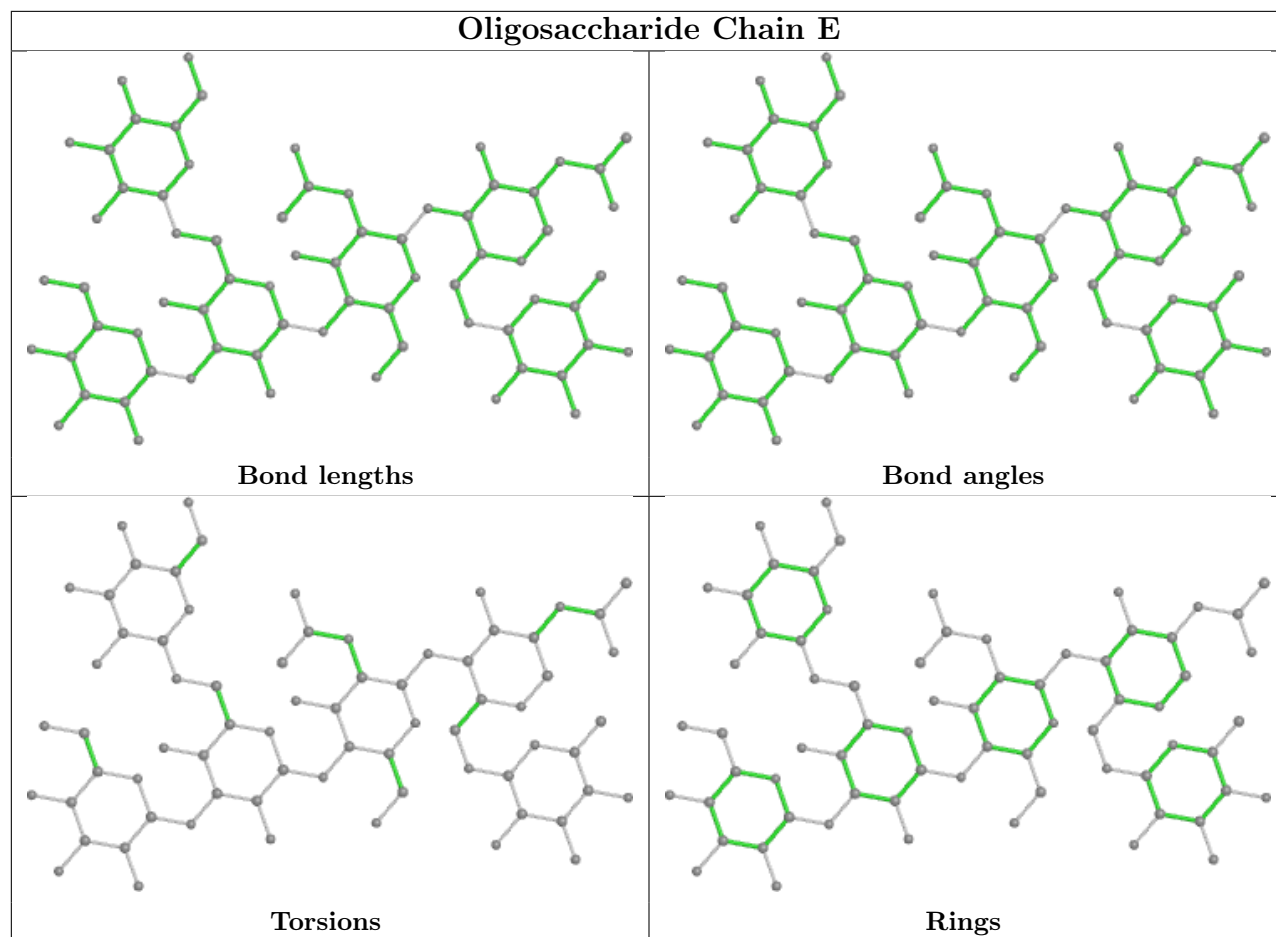
There are no chirality outliers.

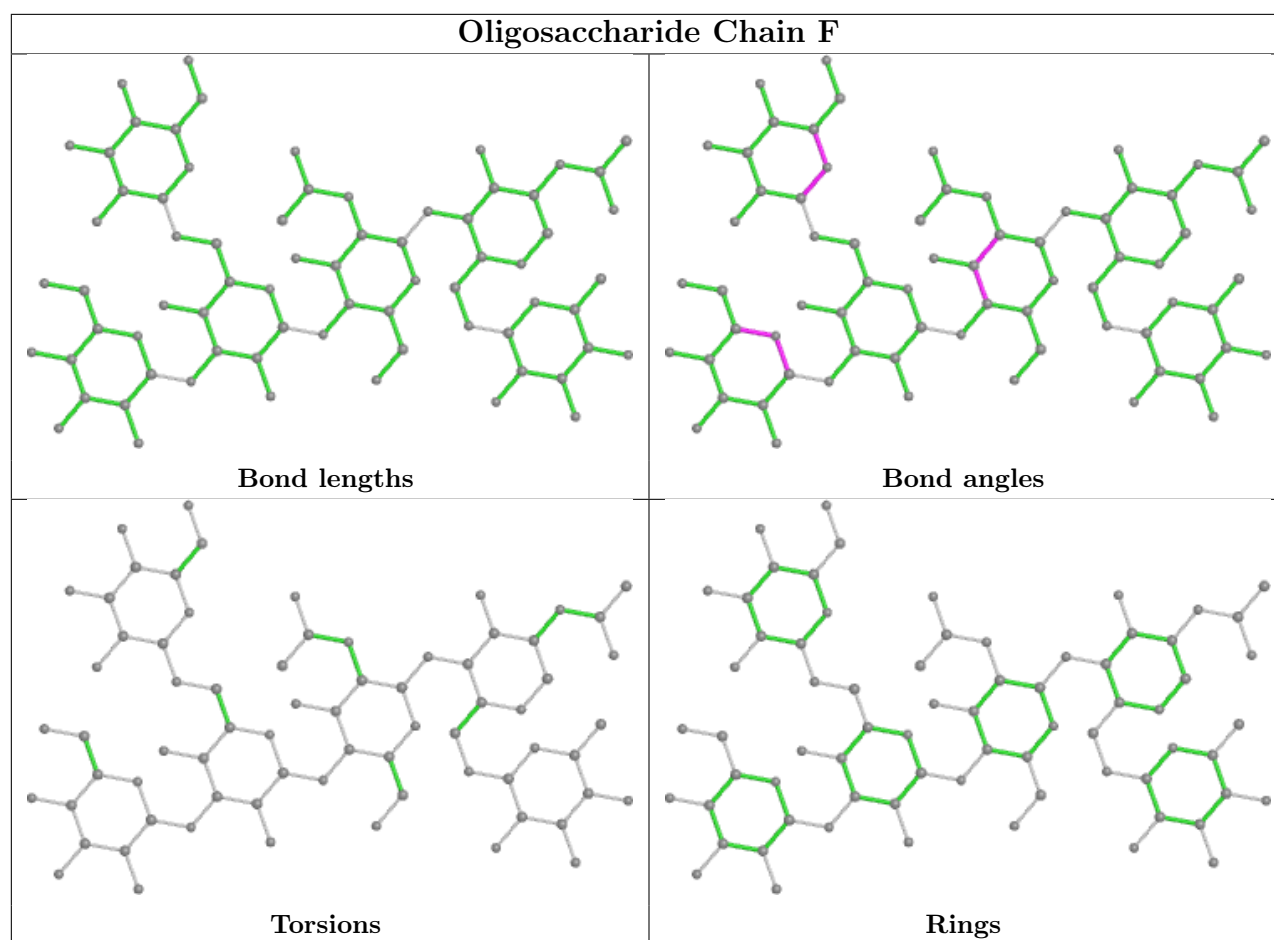
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	ACY	C	17	-	3,3,3	1.04	0	3,3,3	1.71	1 (33%)
8	HEM	B	107	10,2,1	41,50,50	1.22	4 (9%)	45,82,82	1.07	4 (8%)
4	SCN	A	107	-	1,2,2	1.95	0	0,1,1	-	-
4	SCN	B	106	-	1,2,2	2.02	1 (100%)	0,1,1	-	-
6	NAG	D	630	2	14,14,15	0.61	0	17,19,21	0.84	1 (5%)
9	ACY	C	15	-	3,3,3	1.10	0	3,3,3	1.62	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ACY	D	13	-	3,3,3	1.32	1 (33%)	3,3,3	1.72	1 (33%)
5	SO4	C	9	-	4,4,4	0.37	0	6,6,6	0.13	0
8	HEM	C	10	2,1	41,50,50	1.32	4 (9%)	45,82,82	1.11	2 (4%)
6	NAG	D	620	2	14,14,15	0.65	0	17,19,21	0.66	0
6	NAG	C	630	2	14,14,15	0.78	0	17,19,21	0.78	0
9	ACY	C	16	-	3,3,3	1.33	1 (33%)	3,3,3	1.64	1 (33%)
5	SO4	D	7	-	4,4,4	0.35	0	6,6,6	0.09	0
9	ACY	D	12	-	3,3,3	1.22	0	3,3,3	1.69	1 (33%)
4	SCN	A	105	-	1,2,2	1.59	0	0,1,1	-	-
5	SO4	A	106	-	4,4,4	0.16	0	6,6,6	0.07	0
6	NAG	C	620	2	14,14,15	0.78	1 (7%)	17,19,21	0.96	1 (5%)
4	SCN	B	105	-	1,2,2	1.73	0	0,1,1	-	-
9	ACY	D	14	-	3,3,3	1.24	0	3,3,3	1.65	1 (33%)

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	NAG	C	630	2	-	0/6/23/26	0/1/1/1
6	NAG	D	630	2	-	0/6/23/26	0/1/1/1
8	HEM	C	10	2,1	-	5/12/54/54	-
6	NAG	C	620	2	-	0/6/23/26	0/1/1/1
6	NAG	D	620	2	-	0/6/23/26	0/1/1/1
8	HEM	B	107	10,2,1	-	4/12/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	10	HEM	C3C-CAC	-3.37	1.40	1.47
8	B	107	HEM	CBB-CAB	3.24	1.46	1.30
8	C	10	HEM	CBB-CAB	3.17	1.46	1.30
8	B	107	HEM	C3C-CAC	-2.97	1.41	1.47
8	C	10	HEM	CBC-CAC	2.33	1.44	1.29
8	B	107	HEM	CBC-CAC	2.21	1.43	1.29
8	C	10	HEM	C3C-C2C	-2.18	1.37	1.40
9	D	13	ACY	O-C	2.14	1.32	1.22
9	C	16	ACY	O-C	2.05	1.31	1.22
6	C	620	NAG	C1-C2	2.03	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	106	SCN	C-N	2.02	1.22	1.15
8	B	107	HEM	O2A-CGA	-2.02	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	620	NAG	C1-O5-C5	2.82	116.02	112.19
9	D	13	ACY	O-C-CH3	-2.37	113.11	122.33
9	C	17	ACY	O-C-CH3	-2.36	113.13	122.33
9	D	12	ACY	O-C-CH3	-2.33	113.26	122.33
9	D	14	ACY	O-C-CH3	-2.28	113.46	122.33
9	C	16	ACY	O-C-CH3	-2.26	113.54	122.33
8	B	107	HEM	CMC-C2C-C3C	2.23	128.85	124.68
6	D	630	NAG	C1-C2-N2	-2.22	106.69	110.49
8	C	10	HEM	C4C-CHD-C1D	2.21	125.47	122.56
9	C	15	ACY	O-C-CH3	-2.21	113.75	122.33
8	C	10	HEM	C2B-C1B-NB	2.09	112.32	109.84
8	B	107	HEM	C4C-CHD-C1D	2.06	125.28	122.56
8	B	107	HEM	C4B-C3B-C2B	-2.05	105.48	107.11
8	B	107	HEM	C4B-CHC-C1C	2.02	125.23	122.56

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	10	HEM	CAD-CBD-CGD-O2D
8	B	107	HEM	CAD-CBD-CGD-O2D
8	B	107	HEM	CAD-CBD-CGD-O1D
8	C	10	HEM	CAD-CBD-CGD-O1D
8	C	10	HEM	CAA-CBA-CGA-O2A
8	C	10	HEM	CAA-CBA-CGA-O1A
8	B	107	HEM	CAA-CBA-CGA-O2A
8	B	107	HEM	CAA-CBA-CGA-O1A
8	C	10	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

4 monomers are involved in 7 short contacts:

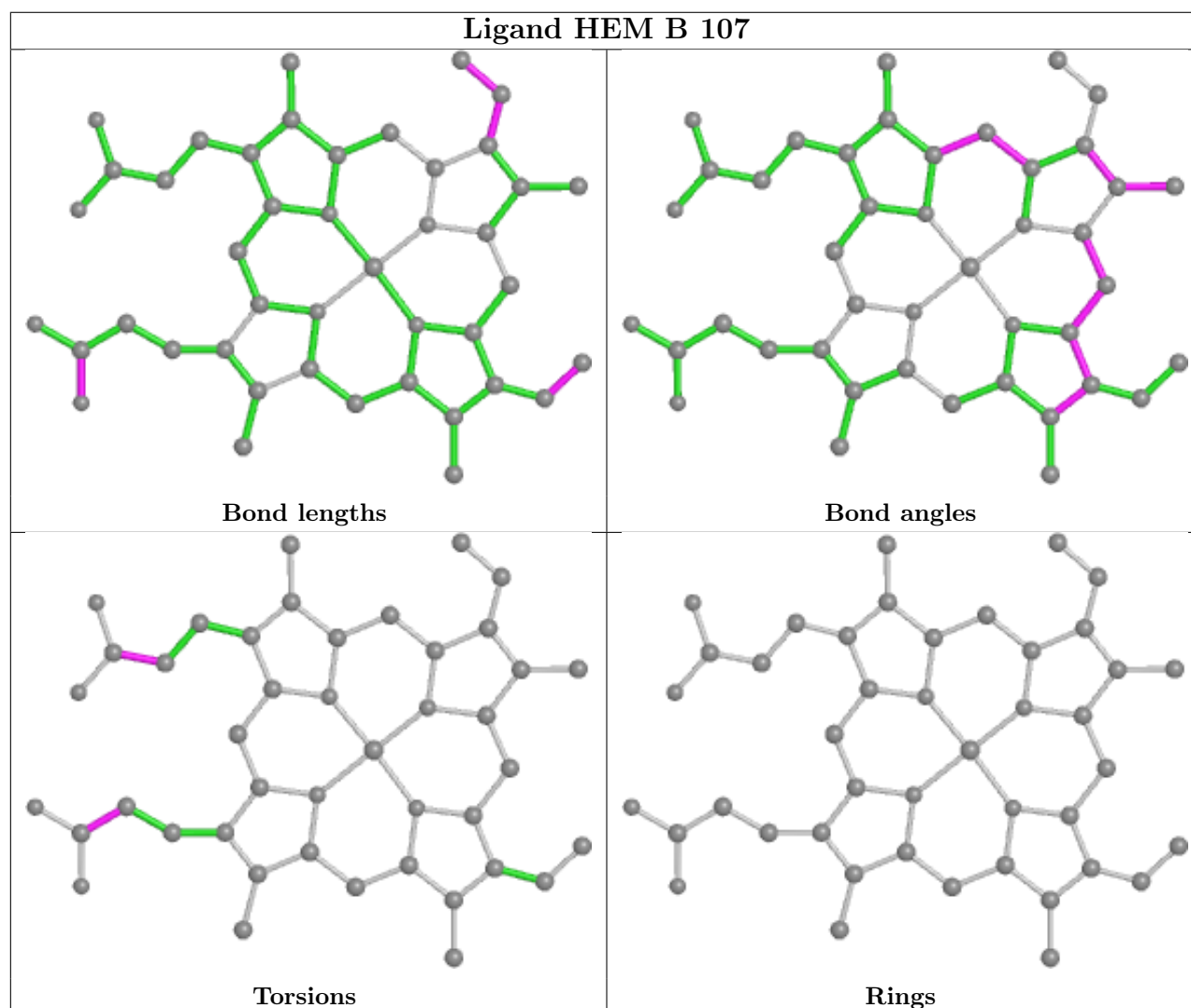
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	107	HEM	2	0
9	C	15	ACY	2	0

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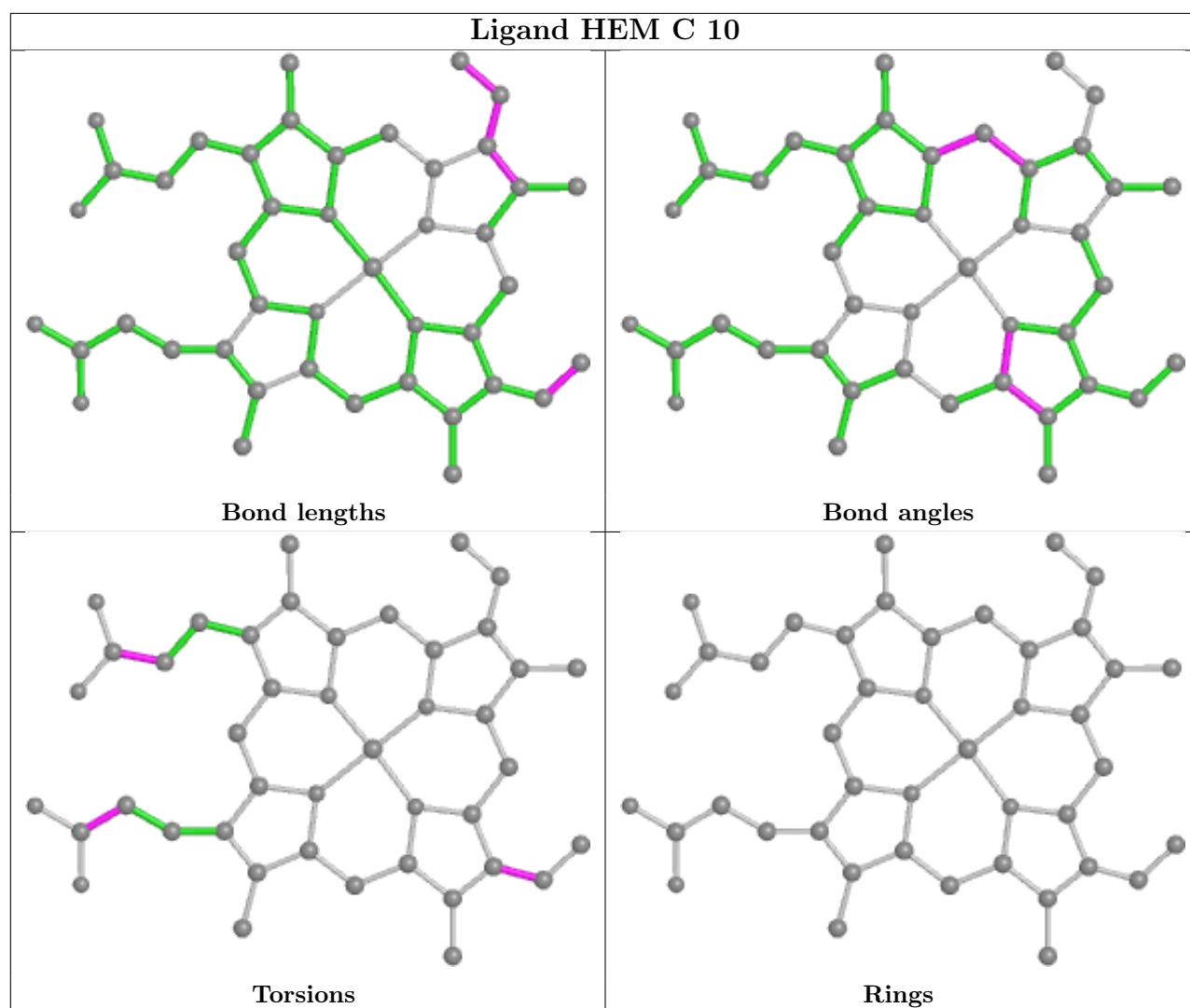
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	13	ACY	1	0
8	C	10	HEM	2	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	104/104 (100%)	0.01	5 (4%) 30 29	6, 9, 23, 46	0
1	B	104/104 (100%)	-0.08	0 100 100	6, 10, 19, 24	0
2	C	465/466 (99%)	-0.10	7 (1%) 73 74	5, 10, 24, 39	0
2	D	465/466 (99%)	0.13	14 (3%) 50 48	6, 12, 27, 43	0
All	All	1138/1140 (99%)	0.01	26 (2%) 60 59	5, 11, 25, 46	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	13.8
2	D	217	HIS	6.0
2	C	355	PRO	5.9
2	D	355	PRO	5.7
2	D	578	ALA	5.6
1	A	1	CYS	4.7
1	A	3	GLU	4.6
1	A	4	GLN	4.4
2	D	267	LEU	3.8
2	C	217	HIS	3.7
2	C	140	GLN	3.5
2	D	576	ARG	3.5
2	D	568	PRO	3.4
2	D	190	MET	2.9
2	D	356	ASN	2.7
2	D	155	GLY	2.7
2	C	349	ARG	2.5
2	C	348	ASN	2.5
2	D	157	ASN	2.5
2	D	226	ARG	2.3
2	D	349	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	353	MET	2.3
1	A	2	PRO	2.2
2	D	523	GLN	2.2
1	A	104	ALA	2.0
2	C	141	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSO	C	150	7/8	0.94	0.09	8,10,11,15	0
2	CSO	D	150	7/8	0.94	0.10	6,8,10,14	0

## 6.3 Carbohydrates [i](#)

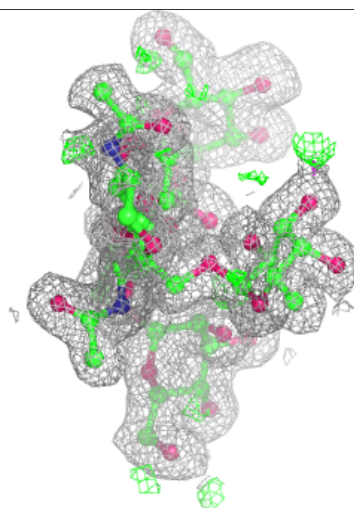
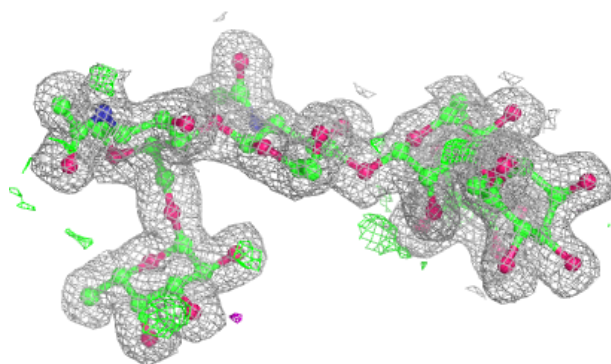
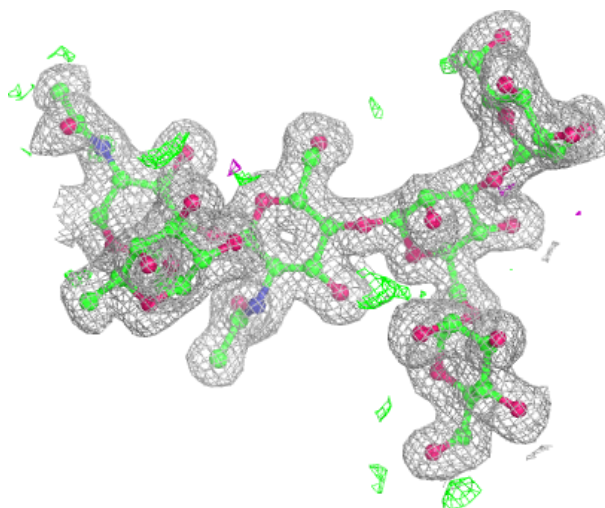
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

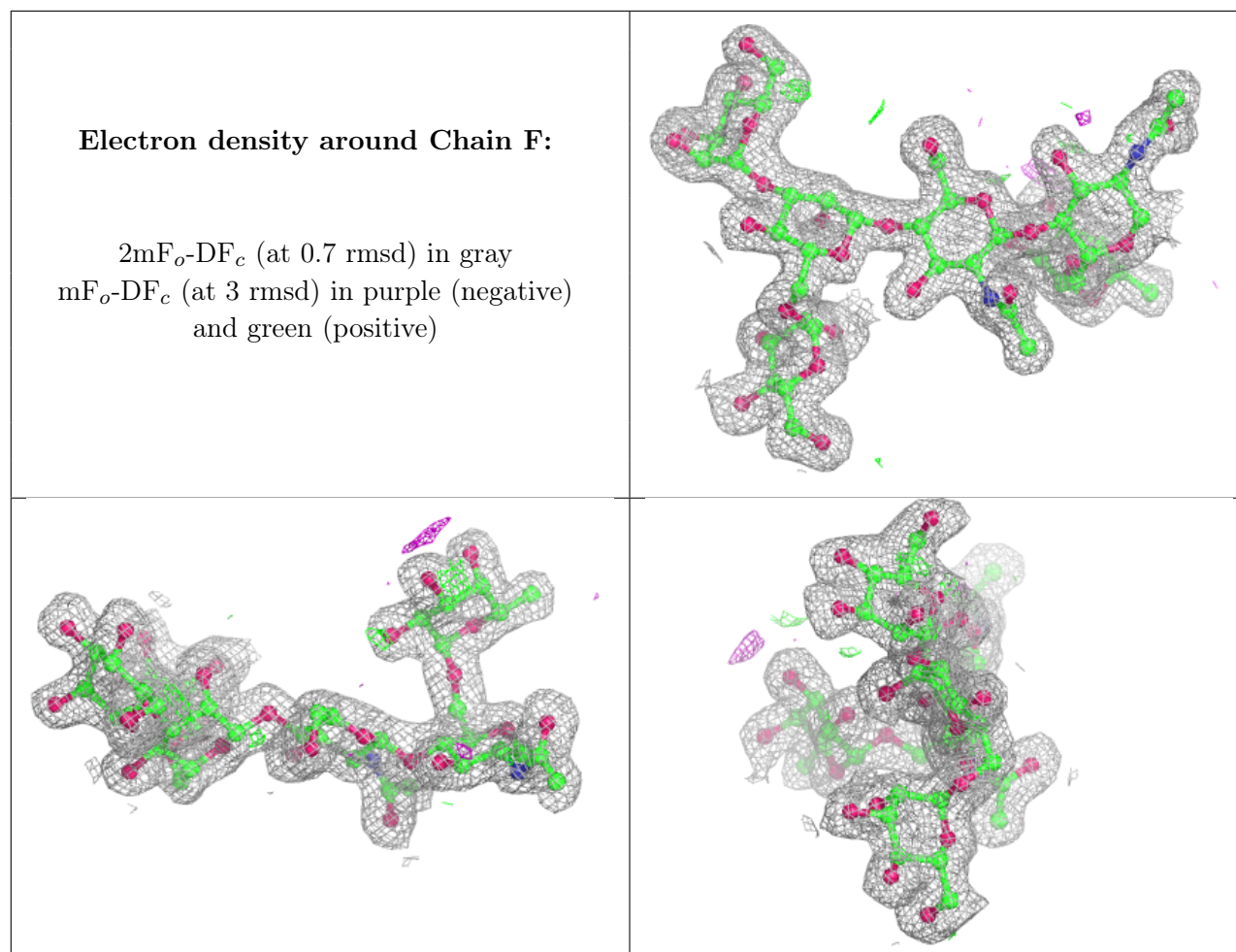
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	F	4	11/12	0.89	0.12	22,24,28,30	0
3	MAN	E	4	11/12	0.90	0.11	24,26,27,27	0
3	MAN	F	5	11/12	0.93	0.12	13,14,16,17	0
3	BMA	E	3	11/12	0.94	0.12	11,13,16,21	0
3	NAG	E	1	14/15	0.94	0.10	8,12,16,17	0
3	MAN	E	5	11/12	0.95	0.14	13,15,17,18	0
3	FUC	E	6	10/11	0.95	0.09	15,16,18,19	0
3	BMA	F	3	11/12	0.96	0.09	10,12,15,19	0
3	NAG	E	2	14/15	0.96	0.11	8,10,11,11	0
3	NAG	F	1	14/15	0.96	0.11	10,12,17,20	0
3	FUC	F	6	10/11	0.96	0.09	14,15,17,18	0
3	NAG	F	2	14/15	0.97	0.11	8,11,12,13	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)





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	ACY	D	13	4/4	0.34	0.39	38,38,38,39	0
5	SO4	D	7	5/5	0.68	0.35	46,47,47,47	5
9	ACY	C	15	4/4	0.79	0.14	27,28,29,30	0
6	NAG	D	630	14/15	0.82	0.19	32,34,37,38	0
6	NAG	C	630	14/15	0.85	0.14	23,28,36,36	0
9	ACY	C	16	4/4	0.88	0.14	27,28,29,29	0
6	NAG	D	620	14/15	0.89	0.17	17,24,28,29	0
9	ACY	D	14	4/4	0.91	0.13	20,21,21,24	0
9	ACY	C	17	4/4	0.92	0.20	17,20,20,21	0
6	NAG	C	620	14/15	0.92	0.11	15,17,21,22	0
9	ACY	D	12	4/4	0.93	0.14	30,31,31,32	0

*Continued on next page...*

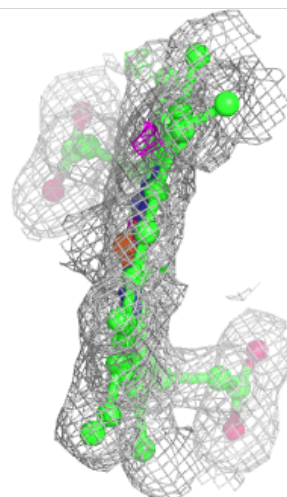
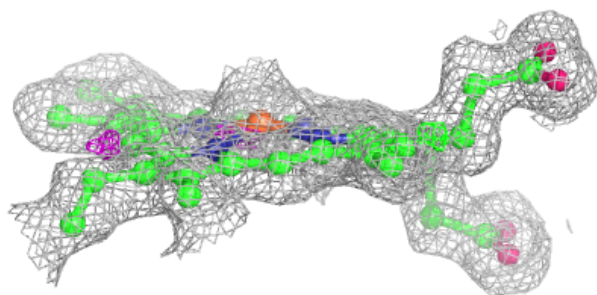
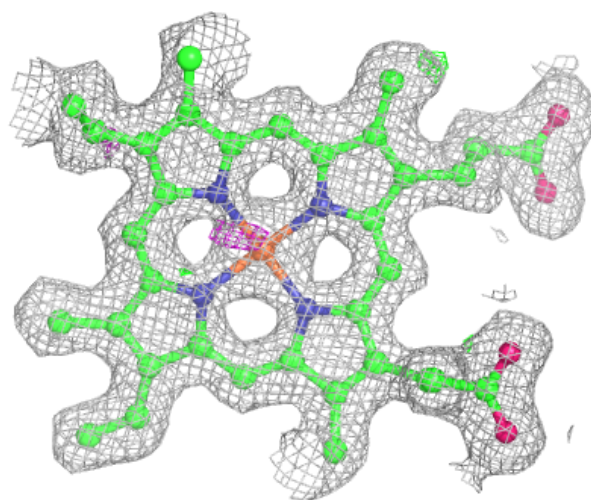
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	C	9	5/5	0.95	0.15	27,29,31,33	0
8	HEM	C	10	43/43	0.96	0.10	4,8,9,10	0
8	HEM	B	107	43/43	0.96	0.11	5,8,10,12	0
4	SCN	B	106	3/3	0.97	0.10	19,19,19,19	0
4	SCN	A	105	3/3	0.98	0.14	12,12,12,17	0
5	SO4	A	106	5/5	0.98	0.08	25,25,28,29	0
4	SCN	A	107	3/3	0.98	0.09	15,15,18,20	0
4	SCN	B	105	3/3	0.98	0.14	11,11,16,17	0
7	CA	C	1	1/1	1.00	0.09	10,10,10,10	0
7	CA	D	2	1/1	1.00	0.11	9,9,9,9	0

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

#### Electron density around HEM C 10:

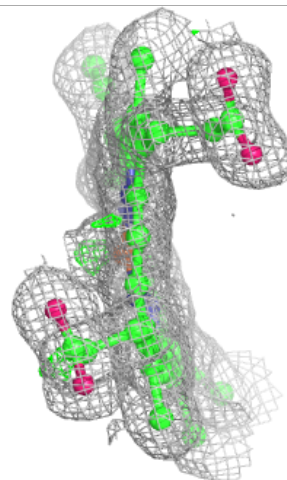
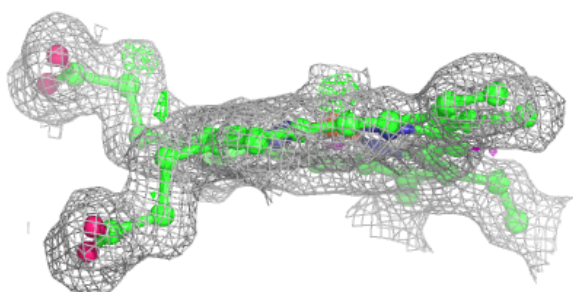
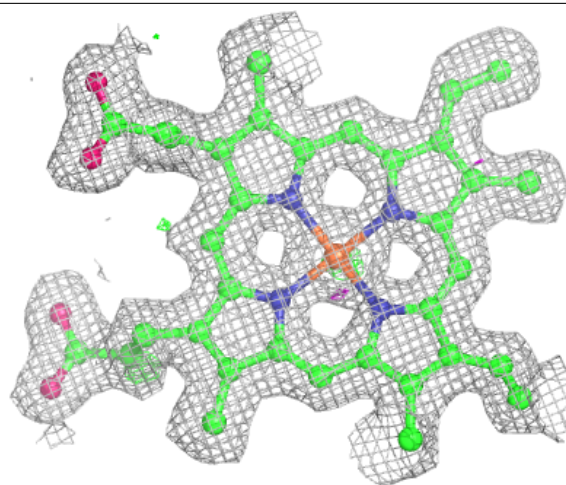
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM B 107:**

$2mF_o-DF_c$  (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.