



## Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 02:34 PM JST

PDB ID : 5FF1  
Title : Two way mode of binding of antithyroid drug methimazole to mammalian heme peroxidases: Structure of the complex of lactoperoxidase with methimazole at 1.97 Angstrom resolution  
Authors : Singh, R.P.; Singh, A.; Sirohi, H.; Singh, A.K.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2015-12-17  
Resolution : 1.97 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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

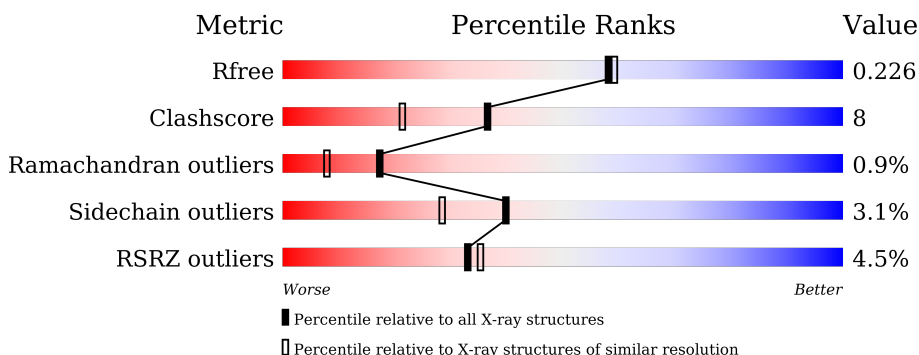
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	595	 3% 89% 10%
1	B	595	 6% 88% 10%
2	C	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MMZ	A	601	-	-	X	-
3	MMZ	A	602	-	-	X	-
3	MMZ	B	601	-	-	X	-
3	MMZ	B	613	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10608 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 Lactoperoxidase.

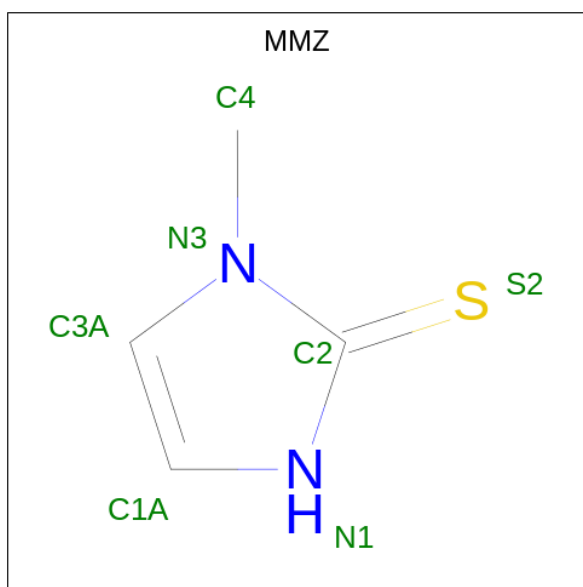
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4754	3021	844	863	26	0	0	0
1	B	595	4753	3021	844	862	26	0	0	0

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



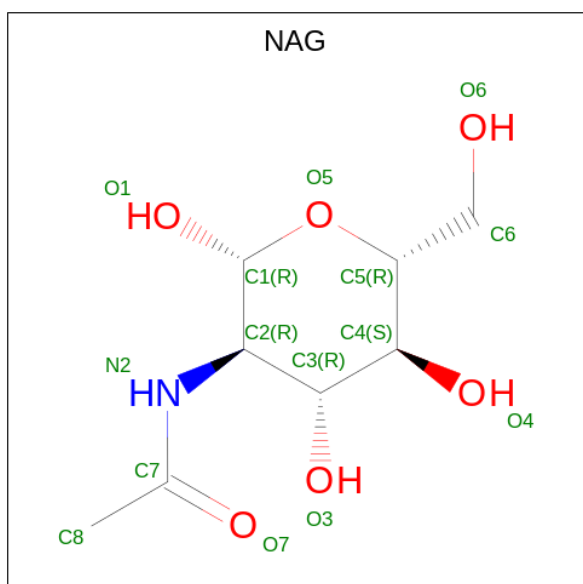
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is 1-METHYL-1,3-DIHYDRO-2H-IMIDAZOLE-2-THIONE (three-letter code: MMZ) (formula: C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>S).



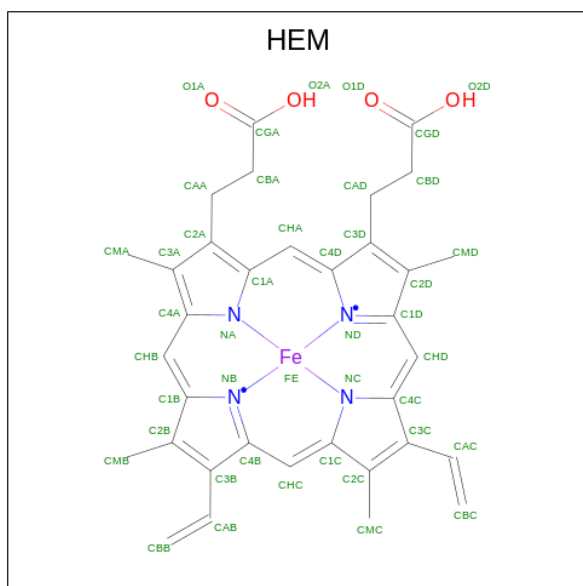
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
3	A	1	7	4	2	1	0	0
3	A	1	7	4	2	1	0	0
3	B	1	7	4	2	1	0	0
3	B	1	7	4	2	1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

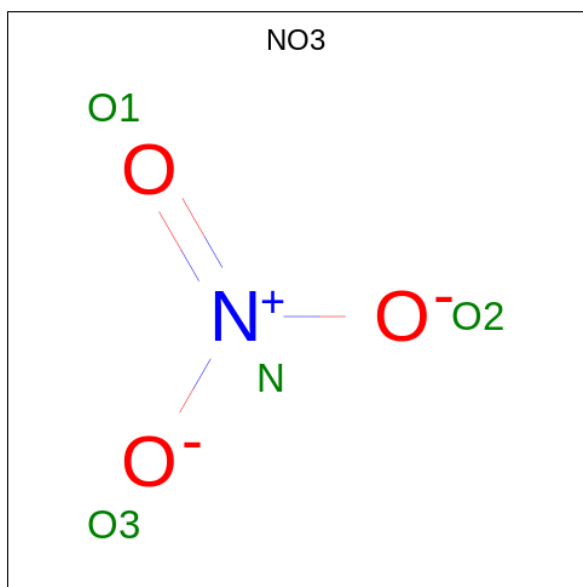


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0

- Molecule 7 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	A	1	Total N O 4 1 3	0	0
7	B	1	Total N O 4 1 3	0	0
7	B	1	Total N O 4 1 3	0	0
7	B	1	Total N O 4 1 3	0	0
7	B	1	Total N O 4 1 3	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





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

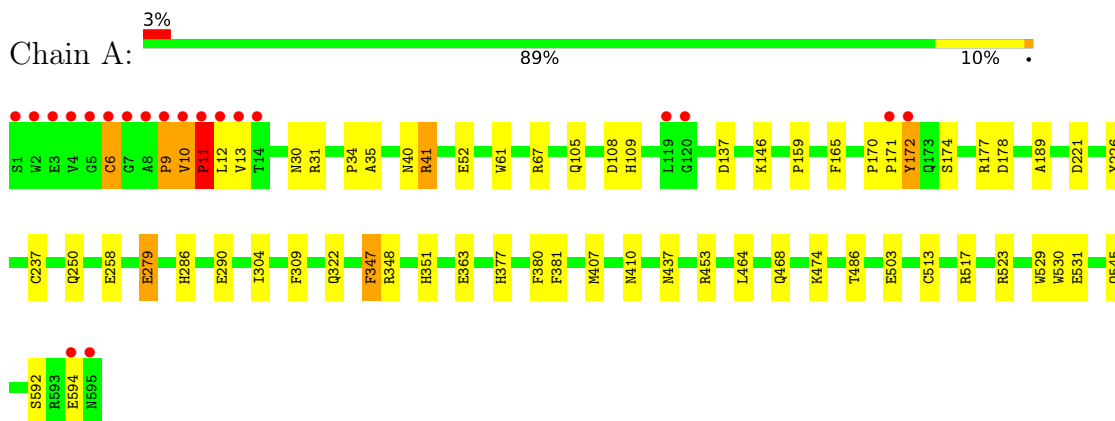
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	415	Total O 415 415	0	0
9	B	360	Total O 360 360	0	0

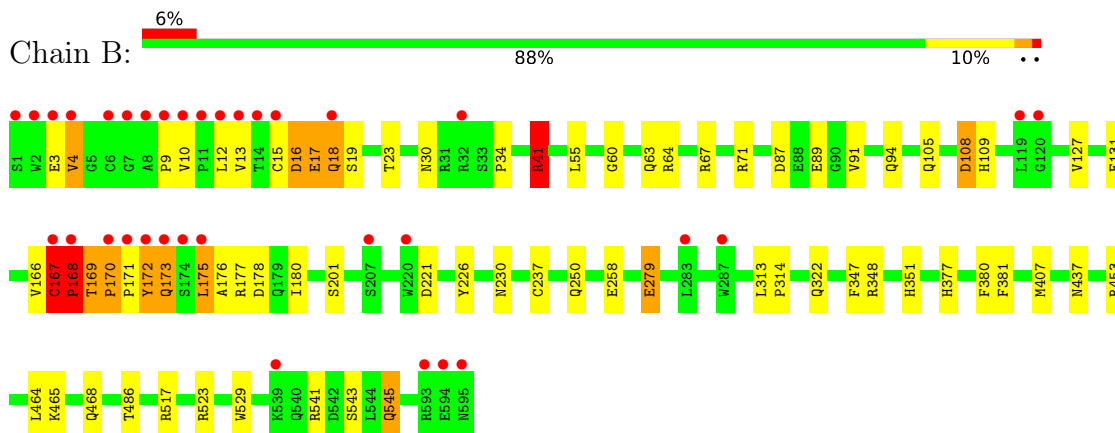
### 3 Residue-property plots [i](#)

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.

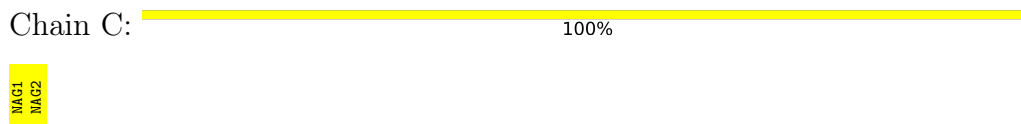
- Molecule 1: Lactoperoxidase



- Molecule 1: Lactoperoxidase



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.31Å 93.02Å 81.53Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	40.43 – 1.97 40.40 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.8 (40.43-1.97) 94.9 (40.40-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.177 , 0.226 0.183 , 0.226	Depositor DCC
$R_{free}$ test set	2415 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtrriage
Anisotropy	0.510	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.019 for -l,k,h 0.176 for h,-k,-l 0.028 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: GOL, MMZ, CA, HEM, NAG, NO3

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	0.90	2/4883 (0.0%)	0.92	9/6632 (0.1%)
1	B	0.86	1/4882 (0.0%)	0.90	10/6632 (0.2%)
All	All	0.88	3/9765 (0.0%)	0.91	19/13264 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	ASP	CA-CB	-7.42	1.37	1.53
1	A	177	ARG	CD-NE	-5.78	1.36	1.46
1	A	137	ASP	C-N	-5.03	1.22	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-14.47	113.06	120.30
1	A	177	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	B	177	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	B	177	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	B	178	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	67	ARG	NE-CZ-NH1	6.17	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	167	CYS	N-CA-C	-5.88	95.13	111.00
1	A	347	PHE	CB-CG-CD1	5.76	124.83	120.80
1	A	178	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	453	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	348	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	67	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	541	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	453	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	11	PRO	N-CA-C	5.53	126.47	112.10
1	A	67	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	41	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	348	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	PRO	Peptide
1	B	167	CYS	Peptide
1	B	168	PRO	Peptide

## 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	4754	0	4644	64	0
1	B	4753	0	4645	83	0
2	C	28	0	25	0	0
3	A	14	0	6	21	0
3	B	14	0	7	26	0
4	A	56	0	52	0	0
4	B	42	0	39	0	0
5	A	43	0	30	14	0
5	B	43	0	30	12	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	20	0	0	0	0
7	B	16	0	0	0	0
8	A	24	0	32	3	0
8	B	24	0	32	1	0
9	A	415	0	0	5	0
9	B	360	0	0	3	0
All	All	10608	0	9542	153	0

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

All (153) 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:108:ASP:OD2	5:A:607:HEM:CMD	1.64	1.45
1:B:108:ASP:OD2	5:B:607:HEM:CMD	1.67	1.42
1:B:258:GLU:OE2	5:B:607:HEM:CMB	1.68	1.41
1:A:258:GLU:OE2	5:A:607:HEM:CMB	1.76	1.32
1:A:258:GLU:OE2	5:A:607:HEM:HMB1	0.93	1.11
1:B:169:THR:HG22	1:B:170:PRO:HD2	1.36	1.07
1:B:108:ASP:OD2	5:B:607:HEM:HMD1	0.83	1.00
1:B:258:GLU:OE2	5:B:607:HEM:HMB1	0.82	0.99
1:B:169:THR:HG22	1:B:170:PRO:CD	1.92	0.98
1:A:258:GLU:CG	3:A:601:MMZ:H42	1.94	0.98
1:A:108:ASP:CG	5:A:607:HEM:HMD1	1.88	0.94
1:A:250:GLN:HG3	9:A:1039:HOH:O	1.71	0.90
1:A:108:ASP:OD2	5:A:607:HEM:HMD1	0.73	0.90
1:B:258:GLU:CG	3:B:613:MMZ:H42	2.03	0.88
1:B:258:GLU:CD	3:B:613:MMZ:H42	1.93	0.88
1:B:230:ASN:HB2	1:B:250:GLN:HG2	1.57	0.83
1:B:258:GLU:CD	5:B:607:HEM:HMB1	2.01	0.81
1:A:258:GLU:CD	3:A:601:MMZ:H42	2.02	0.80
1:B:258:GLU:HB3	3:B:601:MMZ:H41	1.63	0.80
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.26	0.80
1:B:105:GLN:NE2	3:B:613:MMZ:H41	2.02	0.75
1:B:351:HIS:HD1	1:B:437:ASN:HD21	1.31	0.74
1:B:41:ARG:HH21	1:B:41:ARG:HG3	1.51	0.73
1:B:105:GLN:NE2	3:B:601:MMZ:H43	2.03	0.73
1:A:258:GLU:HG3	3:A:601:MMZ:H42	1.71	0.71
5:A:607:HEM:HMC2	5:A:607:HEM:HBC2	1.71	0.71
1:B:105:GLN:NE2	3:B:601:MMZ:C4	2.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HD12	1:B:176:ALA:H	1.59	0.68
1:A:108:ASP:CG	5:A:607:HEM:CMD	2.57	0.68
1:B:279:GLU:HA	1:B:279:GLU:OE1	1.93	0.68
1:B:109:HIS:HE2	3:B:613:MMZ:C3A	2.07	0.68
1:A:279:GLU:HA	1:A:279:GLU:OE1	1.93	0.67
1:B:258:GLU:CB	3:B:601:MMZ:H41	2.24	0.67
1:B:169:THR:HG22	1:B:170:PRO:HD3	1.77	0.66
1:B:13:VAL:HG11	1:B:23:THR:HG21	1.78	0.65
1:B:41:ARG:HH21	1:B:41:ARG:CG	2.10	0.65
1:A:464:LEU:O	1:A:468:GLN:HG3	1.97	0.65
1:A:105:GLN:NE2	3:A:602:MMZ:C4	2.60	0.64
1:B:94:GLN:HG2	9:B:982:HOH:O	1.96	0.64
1:B:169:THR:CG2	1:B:170:PRO:HD2	2.23	0.64
1:A:52:GLU:OE2	8:A:614:GOL:O1	2.16	0.63
1:B:258:GLU:CD	5:B:607:HEM:CMB	2.64	0.63
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.34	0.63
1:A:11:PRO:HB3	1:A:41:ARG:CZ	2.29	0.63
1:A:105:GLN:NE2	3:A:602:MMZ:H43	2.14	0.63
1:A:109:HIS:HE2	3:A:601:MMZ:C3A	2.13	0.61
1:B:169:THR:HG23	9:B:860:HOH:O	2.00	0.61
1:A:258:GLU:CB	3:A:601:MMZ:H42	2.32	0.60
1:A:258:GLU:CB	3:A:601:MMZ:C4	2.79	0.60
1:A:109:HIS:HE1	3:A:602:MMZ:H42	1.68	0.59
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.85	0.59
1:B:523:ARG:HG3	1:B:529:TRP:CE2	2.38	0.58
1:A:171:PRO:O	1:A:172:TYR:HB2	2.03	0.58
1:A:258:GLU:HB3	3:A:602:MMZ:H41	1.84	0.58
1:B:3:GLU:O	1:B:4:VAL:O	2.21	0.57
1:B:109:HIS:NE2	3:B:613:MMZ:C3A	2.67	0.57
1:B:87:ASP:OD1	1:B:89:GLU:HB2	2.05	0.57
1:B:464:LEU:O	1:B:468:GLN:HG3	2.04	0.57
1:A:105:GLN:NE2	3:A:601:MMZ:H41	2.18	0.57
1:B:258:GLU:CB	3:B:613:MMZ:C4	2.81	0.57
5:A:607:HEM:HBB2	5:A:607:HEM:HMB2	1.86	0.56
1:B:258:GLU:HB3	3:B:613:MMZ:H43	1.87	0.56
1:A:290:GLU:HG2	1:B:10:VAL:HG13	1.86	0.56
1:A:12:LEU:HD13	1:A:35:ALA:HB2	1.88	0.56
1:A:258:GLU:HB3	3:A:601:MMZ:C4	2.35	0.55
3:A:601:MMZ:C1A	5:A:607:HEM:C1A	2.89	0.55
1:B:258:GLU:OE1	3:B:613:MMZ:H42	2.05	0.54
5:A:607:HEM:HBC2	5:A:607:HEM:CMC	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:HIS:HE1	3:B:601:MMZ:H42	1.72	0.54
1:B:258:GLU:CB	3:B:613:MMZ:H42	2.38	0.53
1:A:109:HIS:CE1	3:A:602:MMZ:H42	2.43	0.53
1:B:169:THR:CG2	1:B:170:PRO:CD	2.77	0.53
1:B:166:VAL:HG13	1:B:180:ILE:HG12	1.89	0.53
1:A:170:PRO:HA	1:A:171:PRO:C	2.29	0.53
1:A:170:PRO:HA	1:A:172:TYR:N	2.24	0.53
1:A:9:PRO:HB2	1:A:40:ASN:HB3	1.91	0.53
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.53
1:B:166:VAL:CG1	1:B:180:ILE:HG12	2.38	0.53
1:B:16:ASP:O	1:B:17:GLU:C	2.47	0.53
1:B:16:ASP:OD1	1:B:19:SER:HB2	2.09	0.51
1:B:105:GLN:NE2	3:B:601:MMZ:H42	2.23	0.51
1:B:258:GLU:CB	3:B:613:MMZ:H43	2.40	0.51
1:B:377:HIS:HA	1:B:380:PHE:CE2	2.45	0.51
1:A:12:LEU:HD12	1:A:13:VAL:H	1.75	0.51
1:B:105:GLN:HE21	3:B:601:MMZ:C4	2.22	0.50
1:A:468:GLN:OE1	1:A:474:LYS:HG3	2.10	0.50
1:B:230:ASN:CB	1:B:250:GLN:HG2	2.35	0.50
1:B:109:HIS:CE1	3:B:613:MMZ:C3A	2.95	0.50
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.46	0.49
1:A:468:GLN:NE2	1:A:474:LYS:HD2	2.27	0.49
1:A:105:GLN:NE2	3:A:602:MMZ:H42	2.28	0.49
1:A:108:ASP:OD2	5:A:607:HEM:C2D	2.54	0.49
1:A:30:ASN:O	1:A:34:PRO:HA	2.13	0.48
1:A:258:GLU:CG	3:A:601:MMZ:C4	2.81	0.48
1:A:109:HIS:NE2	3:A:601:MMZ:C3A	2.76	0.48
1:B:108:ASP:OD2	5:B:607:HEM:C2D	2.58	0.48
5:B:607:HEM:HMB2	5:B:607:HEM:HBB2	1.94	0.48
1:A:159:PRO:O	8:A:617:GOL:H12	2.14	0.48
1:A:258:GLU:OE2	5:A:607:HEM:HMB2	1.99	0.48
1:B:170:PRO:HB2	1:B:171:PRO:CD	2.44	0.48
1:A:237:CYS:HA	1:A:381:PHE:O	2.14	0.47
1:B:60:GLY:H	8:B:615:GOL:H2	1.78	0.47
1:A:105:GLN:HE21	3:A:602:MMZ:C4	2.28	0.47
1:B:175:LEU:HD12	1:B:176:ALA:N	2.26	0.47
1:A:10:VAL:HG23	1:B:171:PRO:HD3	1.96	0.47
1:B:105:GLN:HE21	3:B:601:MMZ:H43	1.77	0.47
1:B:172:TYR:HA	9:B:776:HOH:O	2.15	0.47
1:B:545:GLN:HE21	1:B:545:GLN:HB2	1.52	0.46
5:A:607:HEM:CMB	5:A:607:HEM:HBB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASN:O	1:B:34:PRO:HA	2.15	0.46
1:A:258:GLU:CB	3:A:601:MMZ:H43	2.46	0.46
1:A:530:TRP:CE2	1:A:531:GLU:HG2	2.51	0.46
1:B:3:GLU:O	1:B:4:VAL:C	2.53	0.46
1:A:279:GLU:HG2	9:A:1083:HOH:O	2.14	0.46
1:B:63:GLN:O	1:B:71:ARG:CZ	2.63	0.46
5:B:607:HEM:HBC2	5:B:607:HEM:HMC2	1.97	0.46
1:A:61:TRP:CH2	8:A:616:GOL:H2	2.51	0.45
1:A:286:HIS:NE2	1:A:592:SER:O	2.48	0.45
5:B:607:HEM:CMB	5:B:607:HEM:HBB2	2.46	0.45
1:A:9:PRO:CB	1:A:40:ASN:HB3	2.46	0.45
1:B:258:GLU:HG3	3:B:613:MMZ:H42	1.90	0.45
1:B:258:GLU:HG3	3:B:613:MMZ:S2	2.57	0.45
1:B:237:CYS:HA	1:B:381:PHE:O	2.16	0.45
1:B:407:MET:C	1:B:407:MET:SD	2.96	0.44
1:A:258:GLU:CD	5:A:607:HEM:CMB	2.72	0.44
1:B:41:ARG:HB3	1:B:41:ARG:CZ	2.48	0.44
1:B:258:GLU:OE2	5:B:607:HEM:C2B	2.61	0.44
9:A:1071:HOH:O	1:B:171:PRO:HD3	2.18	0.44
1:B:105:GLN:HE22	3:B:601:MMZ:H43	1.82	0.44
1:B:15:CYS:O	1:B:16:ASP:C	2.55	0.44
1:B:170:PRO:CB	1:B:171:PRO:HD3	2.47	0.43
1:A:6:CYS:HB3	1:A:165:PHE:CE2	2.53	0.43
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.53	0.43
1:A:468:GLN:HB3	9:A:1075:HOH:O	2.17	0.43
1:A:6:CYS:HB3	1:A:165:PHE:CZ	2.53	0.43
1:B:41:ARG:NH2	1:B:41:ARG:CB	2.82	0.43
1:B:127:VAL:HG13	1:B:131:GLU:HG3	2.00	0.42
1:A:407:MET:C	1:A:407:MET:SD	2.97	0.42
1:A:513:CYS:O	1:A:517:ARG:HG3	2.19	0.42
1:B:109:HIS:NE2	3:B:601:MMZ:S2	2.86	0.42
1:B:109:HIS:CE1	3:B:601:MMZ:H42	2.53	0.42
1:A:545:GLN:HG3	9:A:911:HOH:O	2.19	0.42
1:B:258:GLU:CG	3:B:613:MMZ:C4	2.86	0.41
1:B:18:GLN:O	1:B:19:SER:C	2.59	0.41
1:A:309:PHE:CD1	1:A:529:TRP:HH2	2.37	0.41
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
1:B:41:ARG:CG	1:B:41:ARG:NH2	2.74	0.41
1:B:313:LEU:N	1:B:314:PRO:CD	2.83	0.41
1:A:258:GLU:HB3	3:A:601:MMZ:H43	2.02	0.40
1:A:258:GLU:OE1	3:A:601:MMZ:H42	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:OE1	3:B:613:MMZ:C4	2.69	0.40
1:B:55:LEU:HD13	1:B:173:GLN:O	2.22	0.40
1:B:258:GLU:OE2	5:B:607:HEM:HMB2	1.98	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	593/595 (100%)	572 (96%)	19 (3%)	2 (0%)	41	29
1	B	593/595 (100%)	561 (95%)	23 (4%)	9 (2%)	10	2
All	All	1186/1190 (100%)	1133 (96%)	42 (4%)	11 (1%)	17	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	B	168	PRO
1	B	170	PRO
1	B	175	LEU
1	B	9	PRO
1	A	9	PRO
1	B	4	VAL
1	B	173	GLN
1	B	17	GLU
1	B	169	THR
1	B	167	CYS

### 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	517/517 (100%)	502 (97%)	15 (3%)	42	31
1	B	517/517 (100%)	500 (97%)	17 (3%)	38	26
All	All	1034/1034 (100%)	1002 (97%)	32 (3%)	40	28

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	10	VAL
1	A	31	ARG
1	A	41	ARG
1	A	146	LYS
1	A	172	TYR
1	A	174	SER
1	A	279	GLU
1	A	322	GLN
1	A	347	PHE
1	A	363	GLU
1	A	410	ASN
1	A	486	THR
1	A	503	GLU
1	A	594	GLU
1	B	12	LEU
1	B	16	ASP
1	B	18	GLN
1	B	41	ARG
1	B	64	ARG
1	B	91	VAL
1	B	168	PRO
1	B	172	TYR
1	B	201	SER
1	B	279	GLU
1	B	322	GLN
1	B	347	PHE

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Mol	Chain	Res	Type
1	B	465	LYS
1	B	486	THR
1	B	517	ARG
1	B	543	SER
1	B	545	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	329	GLN
1	A	568	GLN
1	B	128	GLN
1	B	329	GLN
1	B	364	ASN
1	B	423	GLN
1	B	545	GLN
1	B	558	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](#)

2 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	0.58	0	17,19,21	2.67	5 (29%)
2	NAG	C	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.67	2 (11%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	-2.79	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	8.50	123.71	112.19
2	C	2	NAG	C1-C2-N2	-5.62	100.89	110.49
2	C	1	NAG	O7-C7-C8	-3.76	115.07	122.06
2	C	1	NAG	C6-C5-C4	-2.95	106.09	113.00
2	C	1	NAG	O5-C5-C6	2.79	111.58	107.20
2	C	2	NAG	O4-C4-C5	2.26	114.91	109.30
2	C	1	NAG	O7-C7-N2	2.05	125.72	121.95

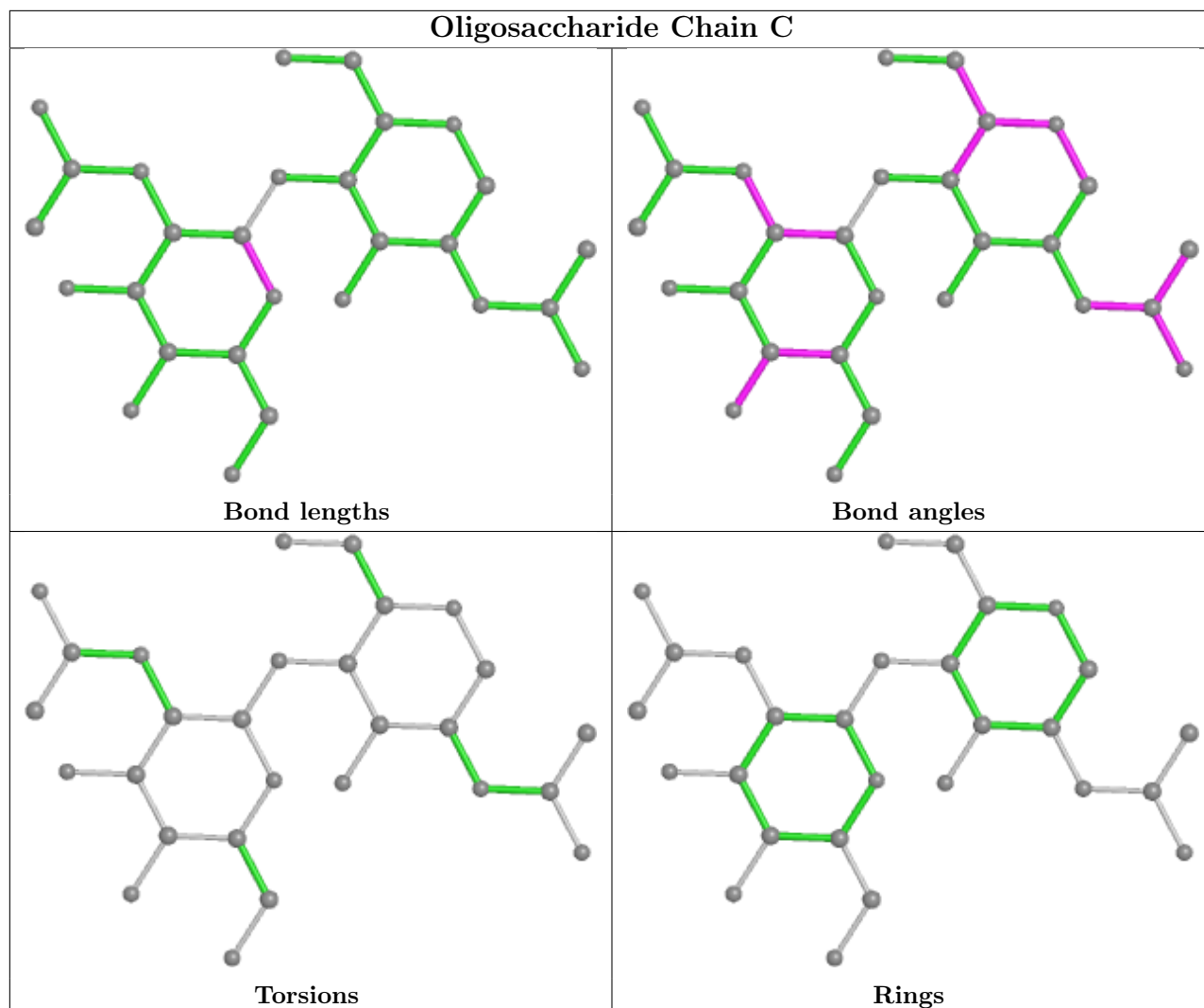
There are no chirality outliers.

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 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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$
3	MMZ	A	602	5,3	5,7,7	1.12	1 (20%)	4,9,9	4.00	2 (50%)
4	NAG	A	605	1	14,14,15	0.65	0	17,19,21	2.47	6 (35%)
7	NO3	B	612	-	1,3,3	0.07	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	603	1	14,14,15	0.69	0	17,19,21	1.65	5 (29%)
4	NAG	A	604	1	14,14,15	0.75	0	17,19,21	2.19	8 (47%)
8	GOL	B	617	-	5,5,5	0.77	0	5,5,5	0.82	0
7	NO3	A	611	-	1,3,3	0.17	0	0,3,3	-	-
4	NAG	B	604	1	14,14,15	0.52	0	17,19,21	1.73	1 (5%)
8	GOL	A	615	-	5,5,5	0.27	0	5,5,5	1.25	0
7	NO3	A	612	-	1,3,3	0.07	0	0,3,3	-	-
8	GOL	A	614	-	5,5,5	0.54	0	5,5,5	1.58	2 (40%)
8	GOL	B	614	-	5,5,5	0.48	0	5,5,5	0.60	0
5	HEM	A	607	1,3	41,50,50	1.67	6 (14%)	45,82,82	2.27	14 (31%)
4	NAG	B	602	1	14,14,15	1.08	1 (7%)	17,19,21	2.42	5 (29%)
7	NO3	B	610	-	1,3,3	0.38	0	0,3,3	-	-
3	MMZ	B	613	3	5,7,7	1.89	1 (20%)	4,9,9	2.82	2 (50%)
8	GOL	A	617	-	5,5,5	1.14	1 (20%)	5,5,5	1.70	1 (20%)
8	GOL	B	616	-	5,5,5	0.45	0	5,5,5	1.00	0
8	GOL	A	616	-	5,5,5	0.48	0	5,5,5	0.75	0
7	NO3	B	611	-	1,3,3	0.27	0	0,3,3	-	-
4	NAG	A	606	1	14,14,15	0.92	1 (7%)	17,19,21	2.01	2 (11%)
3	MMZ	A	601	3	5,7,7	1.84	1 (20%)	4,9,9	2.51	1 (25%)
7	NO3	A	613	-	1,3,3	0.21	0	0,3,3	-	-
4	NAG	A	603	1	14,14,15	1.32	1 (7%)	17,19,21	2.02	6 (35%)
8	GOL	B	615	-	5,5,5	0.72	0	5,5,5	0.77	0
7	NO3	A	609	-	1,3,3	1.23	0	0,3,3	-	-
3	MMZ	B	601	5,3	5,7,7	1.32	1 (20%)	4,9,9	4.78	3 (75%)
7	NO3	A	610	-	1,3,3	0.48	0	0,3,3	-	-
5	HEM	B	607	1,3	41,50,50	1.69	5 (12%)	45,82,82	2.24	15 (33%)
7	NO3	B	609	-	1,3,3	0.21	0	0,3,3	-	-

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	MMZ	A	602	5,3	-	-	0/1/1/1
4	NAG	A	605	1	-	0/6/23/26	0/1/1/1
4	NAG	B	603	1	-	0/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
8	GOL	B	617	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
8	GOL	A	615	-	-	2/4/4/4	-
8	GOL	A	614	-	-	2/4/4/4	-
8	GOL	B	614	-	-	0/4/4/4	-
5	HEM	A	607	1,3	-	4/12/54/54	-
4	NAG	B	602	1	-	2/6/23/26	0/1/1/1
3	MMZ	B	613	3	-	-	0/1/1/1
8	GOL	A	617	-	-	0/4/4/4	-
8	GOL	B	616	-	-	2/4/4/4	-
8	GOL	A	616	-	-	0/4/4/4	-
4	NAG	A	606	1	-	0/6/23/26	0/1/1/1
3	MMZ	A	601	3	-	-	0/1/1/1
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1
8	GOL	B	615	-	-	1/4/4/4	-
3	MMZ	B	601	5,3	-	-	0/1/1/1
5	HEM	B	607	1,3	-	4/12/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	607	HEM	C1B-NB	-5.82	1.30	1.40
5	B	607	HEM	C4D-ND	-5.01	1.31	1.40
5	A	607	HEM	C1B-NB	-4.57	1.32	1.40
5	A	607	HEM	C4D-ND	-4.23	1.33	1.40
3	B	613	MMZ	C3A-N3	-4.13	1.30	1.37
3	A	601	MMZ	C3A-N3	-4.01	1.30	1.37
4	A	603	NAG	O5-C1	-3.73	1.37	1.43
5	A	607	HEM	C4B-NB	-3.51	1.31	1.38
3	B	601	MMZ	C3A-N3	-2.81	1.32	1.37
5	B	607	HEM	FE-NB	2.81	2.10	1.96
4	A	606	NAG	O5-C1	-2.63	1.39	1.43
4	B	602	NAG	O5-C1	-2.53	1.39	1.43
5	A	607	HEM	C3D-C2D	-2.44	1.31	1.36
5	B	607	HEM	CBD-CGD	2.36	1.56	1.50
8	A	617	GOL	O2-C2	2.35	1.50	1.43
3	A	602	MMZ	C3A-N3	-2.31	1.33	1.37
5	A	607	HEM	FE-NB	2.23	2.07	1.96
5	A	607	HEM	O1D-CGD	2.18	1.29	1.22
5	B	607	HEM	C4B-NB	-2.00	1.34	1.38

All (73) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	NAG	C1-O5-C5	7.95	122.96	112.19
5	A	607	HEM	C1B-NB-C4B	7.61	112.94	105.07
3	B	601	MMZ	C4-N3-C2	-6.96	115.09	125.43
4	A	606	NAG	C1-O5-C5	6.44	120.92	112.19
5	B	607	HEM	CHC-C4B-NB	5.77	130.70	124.43
4	B	604	NAG	C1-O5-C5	5.70	119.92	112.19
3	A	602	MMZ	C3A-N3-C2	5.68	114.28	108.51
3	B	601	MMZ	C3A-N3-C2	5.68	114.28	108.51
5	B	607	HEM	C1B-NB-C4B	5.65	110.91	105.07
3	A	602	MMZ	C4-N3-C2	-5.20	117.70	125.43
4	B	602	NAG	C1-C2-N2	-5.02	101.91	110.49
5	B	607	HEM	CHD-C1D-ND	4.94	129.80	124.43
4	B	602	NAG	C4-C3-C2	4.87	118.16	111.02
3	A	601	MMZ	C3A-N3-C2	4.68	113.26	108.51
4	A	603	NAG	O5-C1-C2	-4.46	104.24	111.29
3	B	613	MMZ	C3A-N3-C2	4.43	113.00	108.51
4	A	604	NAG	C1-C2-N2	4.32	117.87	110.49
4	B	602	NAG	O3-C3-C4	-4.29	100.44	110.35
5	A	607	HEM	CHC-C4B-NB	4.28	129.08	124.43
5	A	607	HEM	CMD-C2D-C1D	4.10	131.28	125.04
4	A	603	NAG	C3-C4-C5	-3.93	103.22	110.24
5	B	607	HEM	CHD-C1D-C2D	-3.80	119.05	124.98
5	B	607	HEM	C4B-C3B-C2B	-3.79	104.10	107.11
5	A	607	HEM	CHB-C1B-NB	3.70	128.95	124.38
4	B	603	NAG	O5-C1-C2	-3.68	105.48	111.29
5	A	607	HEM	C4B-CHC-C1C	3.64	127.36	122.56
5	B	607	HEM	CBA-CAA-C2A	-3.57	106.52	112.62
4	A	604	NAG	C4-C3-C2	-3.43	106.00	111.02
5	A	607	HEM	CAD-C3D-C4D	3.34	130.49	124.66
5	A	607	HEM	CHD-C1D-ND	3.30	128.02	124.43
5	B	607	HEM	CMD-C2D-C1D	3.29	130.04	125.04
4	A	604	NAG	O3-C3-C2	3.19	116.06	109.47
5	A	607	HEM	C2B-C1B-NB	-3.09	106.18	109.84
5	A	607	HEM	CBA-CAA-C2A	-3.09	107.35	112.62
8	A	617	GOL	C3-C2-C1	-3.08	99.72	111.70
4	A	605	NAG	C4-C3-C2	3.04	115.47	111.02
5	A	607	HEM	C4B-C3B-C2B	-3.04	104.70	107.11
5	B	607	HEM	C2C-C3C-C4C	-3.03	104.78	106.90
3	B	601	MMZ	C4-N3-C3A	3.01	130.61	124.89
3	B	613	MMZ	C4-N3-C3A	-2.89	119.39	124.89
5	A	607	HEM	C3B-C2B-C1B	2.89	108.63	106.49
4	A	604	NAG	O6-C6-C5	-2.87	101.46	111.29
5	B	607	HEM	C4B-CHC-C1C	2.86	126.33	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	NAG	C3-C4-C5	-2.83	105.19	110.24
4	A	604	NAG	O7-C7-C8	-2.81	116.83	122.06
5	A	607	HEM	CHD-C1D-C2D	-2.78	120.63	124.98
8	A	614	GOL	C3-C2-C1	-2.76	100.98	111.70
4	A	604	NAG	O5-C1-C2	-2.71	107.01	111.29
5	B	607	HEM	C3B-C2B-C1B	2.55	108.38	106.49
4	B	602	NAG	O7-C7-C8	-2.55	117.32	122.06
4	A	605	NAG	O3-C3-C4	-2.55	104.46	110.35
5	A	607	HEM	CAD-C3D-C2D	-2.48	123.27	127.88
4	B	603	NAG	O5-C5-C6	2.47	111.08	107.20
4	A	605	NAG	O4-C4-C5	2.47	115.42	109.30
4	A	605	NAG	O3-C3-C2	-2.43	104.44	109.47
4	B	602	NAG	C1-O5-C5	-2.43	108.91	112.19
5	B	607	HEM	O2D-CGD-CBD	2.39	121.72	114.03
4	A	606	NAG	O7-C7-C8	-2.34	117.71	122.06
4	A	603	NAG	O5-C5-C4	-2.34	105.13	110.83
4	A	604	NAG	C8-C7-N2	2.33	120.04	116.10
4	B	603	NAG	O4-C4-C3	-2.30	105.03	110.35
5	B	607	HEM	CHA-C4D-C3D	-2.27	121.06	125.33
5	B	607	HEM	CHC-C4B-C3B	-2.19	121.22	124.57
4	A	605	NAG	O5-C5-C6	2.18	110.62	107.20
4	A	603	NAG	O5-C5-C6	2.15	110.57	107.20
4	A	603	NAG	C8-C7-N2	-2.09	112.56	116.10
8	A	614	GOL	O2-C2-C1	2.09	118.32	109.12
5	B	607	HEM	C2B-C1B-NB	-2.08	107.38	109.84
4	B	603	NAG	O5-C5-C4	-2.05	105.83	110.83
5	A	607	HEM	O2A-CGA-O1A	-2.04	118.20	123.30
5	B	607	HEM	CHB-C1B-NB	2.04	126.90	124.38
4	B	603	NAG	C4-C3-C2	2.03	113.99	111.02
4	A	603	NAG	C6-C5-C4	2.02	117.74	113.00

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	614	GOL	O1-C1-C2-C3
8	A	615	GOL	O1-C1-C2-C3
8	B	615	GOL	O1-C1-C2-C3
8	B	617	GOL	O1-C1-C2-C3
4	A	604	NAG	O5-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	602	NAG	C4-C5-C6-O6
8	B	616	GOL	O1-C1-C2-C3
8	A	615	GOL	O1-C1-C2-O2
8	B	617	GOL	O1-C1-C2-O2
8	A	614	GOL	O1-C1-C2-O2
8	B	616	GOL	O1-C1-C2-O2
5	A	607	HEM	CAD-CBD-CGD-O2D
5	B	607	HEM	CAD-CBD-CGD-O2D
5	A	607	HEM	CAD-CBD-CGD-O1D
5	A	607	HEM	CAA-CBA-CGA-O2A
5	B	607	HEM	CAA-CBA-CGA-O2A
5	A	607	HEM	CAA-CBA-CGA-O1A
5	B	607	HEM	CAA-CBA-CGA-O1A
5	B	607	HEM	CAD-CBD-CGD-O1D
4	A	603	NAG	C4-C5-C6-O6
4	A	603	NAG	O5-C5-C6-O6

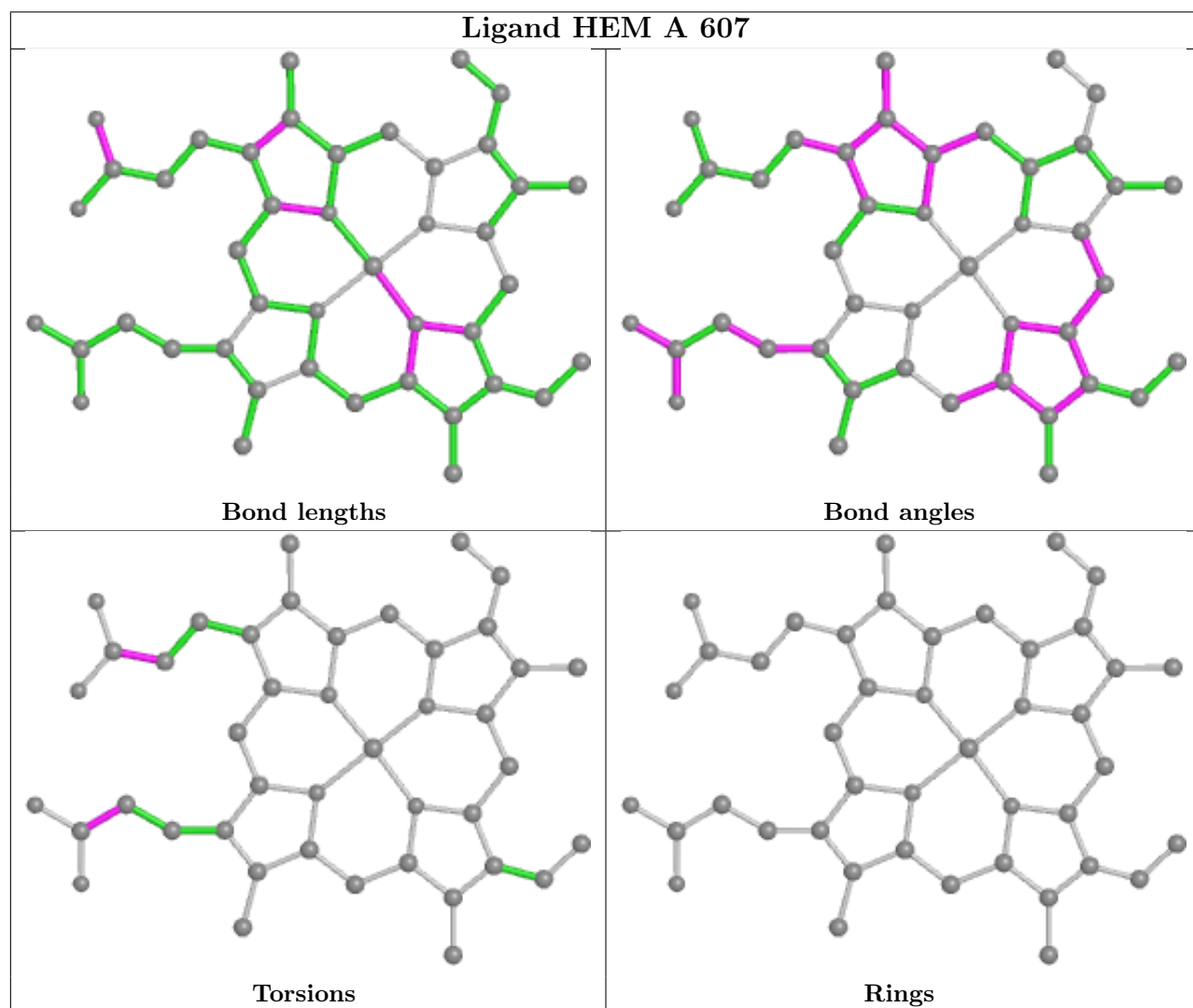
There are no ring outliers.

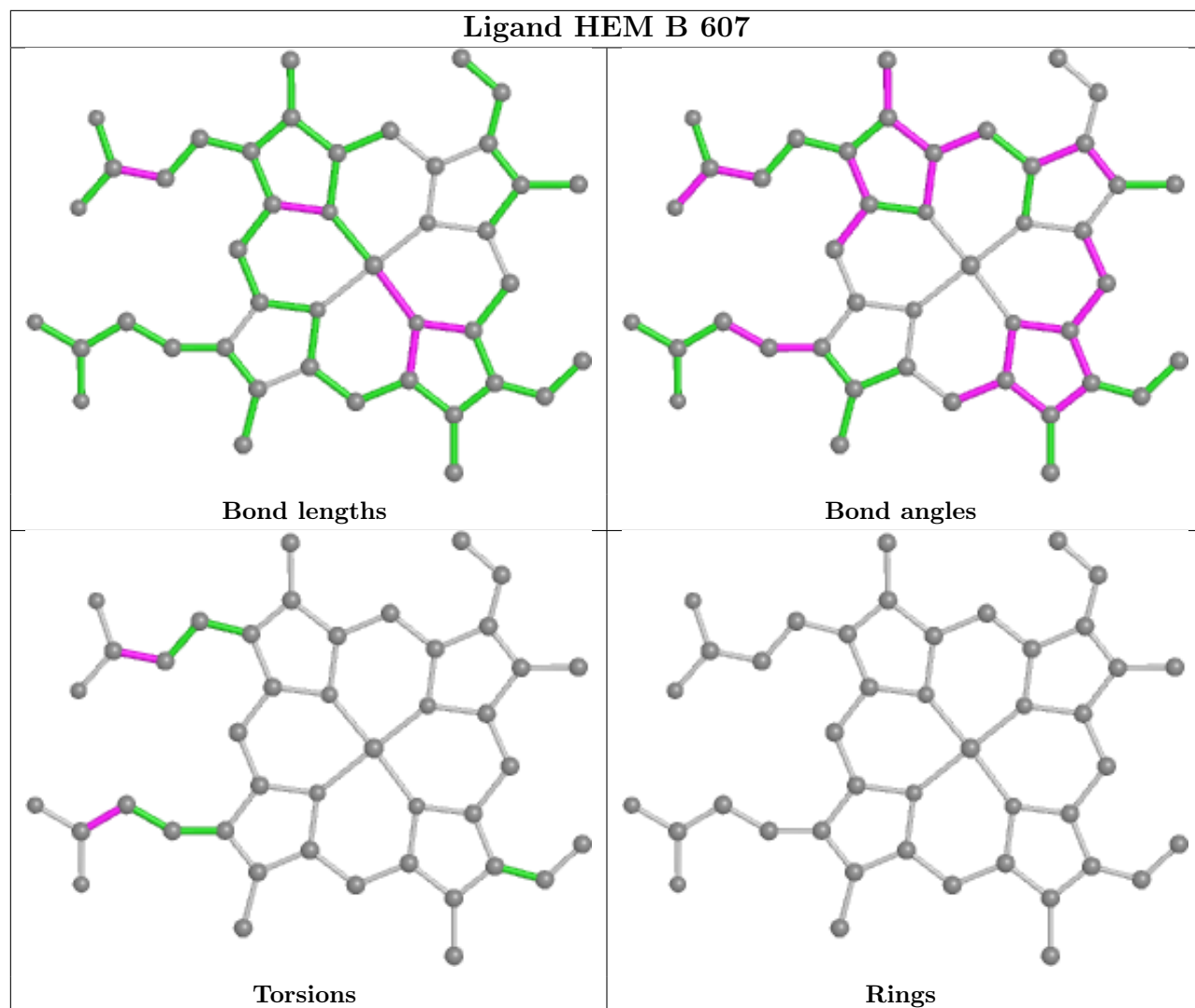
10 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	MMZ	7	0
8	A	614	GOL	1	0
5	A	607	HEM	14	0
3	B	613	MMZ	15	0
8	A	617	GOL	1	0
8	A	616	GOL	1	0
3	A	601	MMZ	14	0
8	B	615	GOL	1	0
3	B	601	MMZ	11	0
5	B	607	HEM	12	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	595/595 (100%)	-0.16	20 (3%) 45 48	13, 24, 59, 137	0
1	B	595/595 (100%)	0.18	34 (5%) 23 25	13, 28, 70, 163	0
All	All	1190/1190 (100%)	0.01	54 (4%) 33 35	13, 26, 66, 163	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	TRP	19.4
1	B	1	SER	17.0
1	A	2	TRP	16.7
1	B	12	LEU	15.7
1	B	11	PRO	14.3
1	B	172	TYR	13.9
1	B	9	PRO	13.8
1	A	10	VAL	11.6
1	B	10	VAL	11.5
1	A	8	ALA	11.3
1	B	174	SER	11.2
1	B	13	VAL	10.8
1	A	12	LEU	10.3
1	B	7	GLY	10.1
1	A	9	PRO	10.1
1	B	171	PRO	9.7
1	A	13	VAL	9.2
1	B	8	ALA	8.7
1	A	1	SER	8.6
1	A	11	PRO	8.6
1	B	170	PRO	8.2
1	B	3	GLU	7.5
1	B	594	GLU	7.4
1	B	595	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	14	THR	6.4
1	A	14	THR	6.3
1	B	4	VAL	6.1
1	A	5	GLY	6.1
1	A	4	VAL	5.9
1	A	3	GLU	5.6
1	B	173	GLN	5.6
1	A	594	GLU	4.9
1	B	6	CYS	4.9
1	B	119	LEU	4.9
1	A	119	LEU	4.4
1	A	7	GLY	3.9
1	B	593	ARG	3.7
1	A	171	PRO	3.6
1	A	172	TYR	3.4
1	B	15	CYS	3.3
1	A	6	CYS	3.2
1	A	595	ASN	3.0
1	B	287	TRP	2.8
1	A	120	GLY	2.5
1	B	539	LYS	2.5
1	B	120	GLY	2.5
1	B	32	ARG	2.4
1	B	283	LEU	2.4
1	B	220	TRP	2.3
1	B	167	CYS	2.2
1	B	168	PRO	2.1
1	B	18	GLN	2.1
1	B	207	SER	2.0
1	B	175	LEU	2.0

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

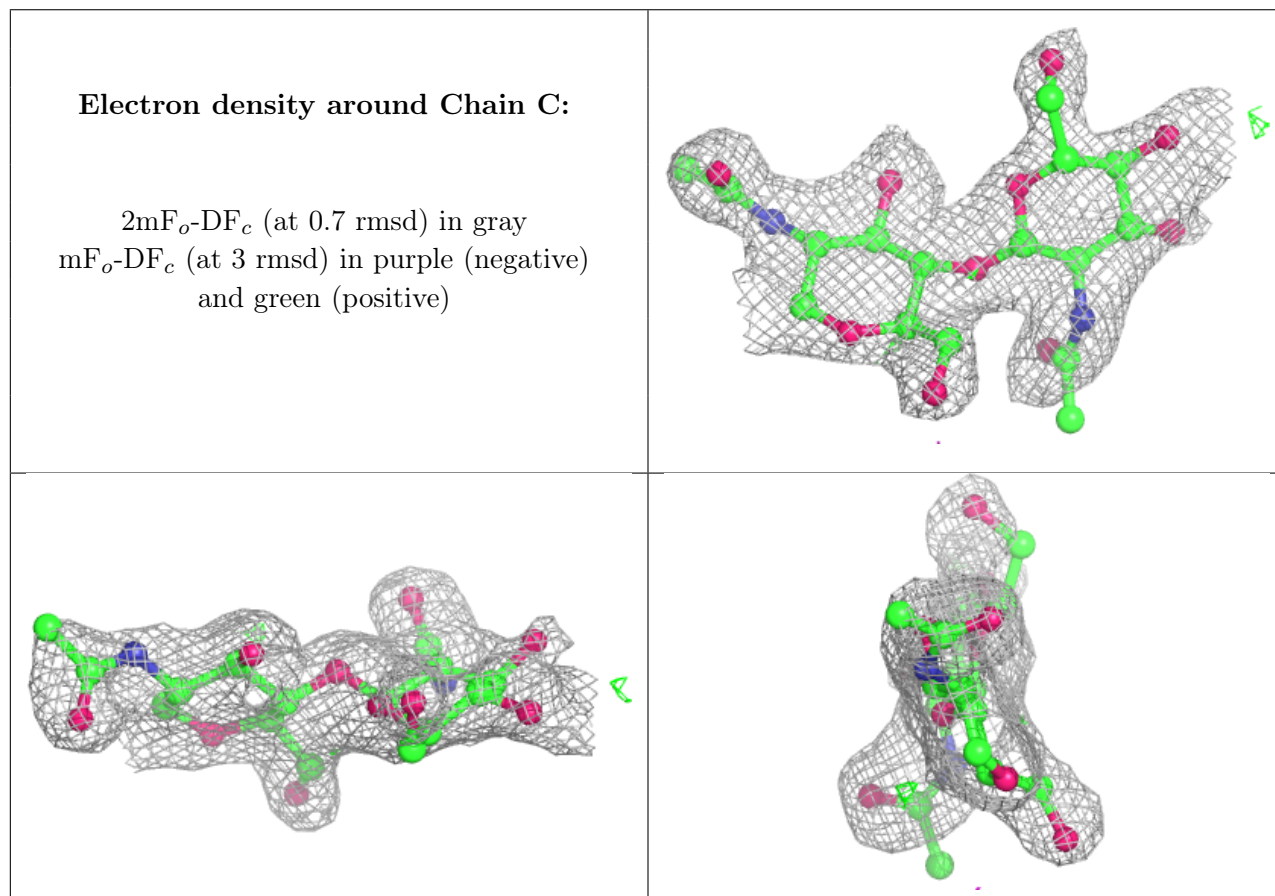
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	2	14/15	0.83	0.17	49,57,66,67	0
2	NAG	C	1	14/15	0.92	0.10	41,54,56,56	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.



## 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	605	14/15	0.73	0.18	54,60,65,65	0
4	NAG	B	604	14/15	0.77	0.17	57,67,69,72	0
8	GOL	A	617	6/6	0.80	0.30	36,47,54,58	0
7	NO3	A	613	4/4	0.81	0.26	65,70,72,74	0
7	NO3	B	611	4/4	0.83	0.18	55,61,62,69	0
8	GOL	B	617	6/6	0.83	0.13	51,56,58,59	0

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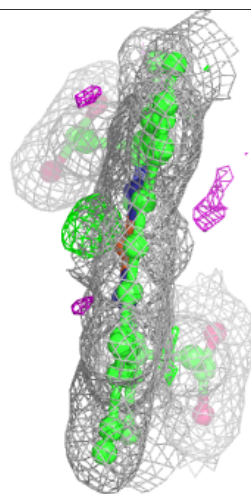
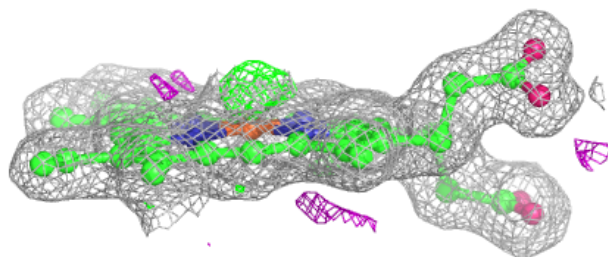
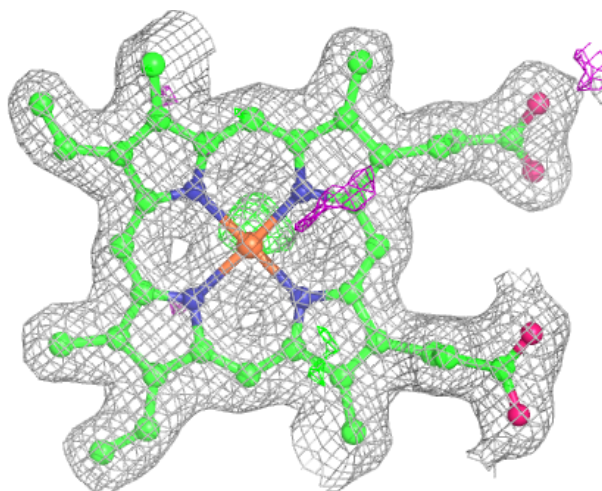
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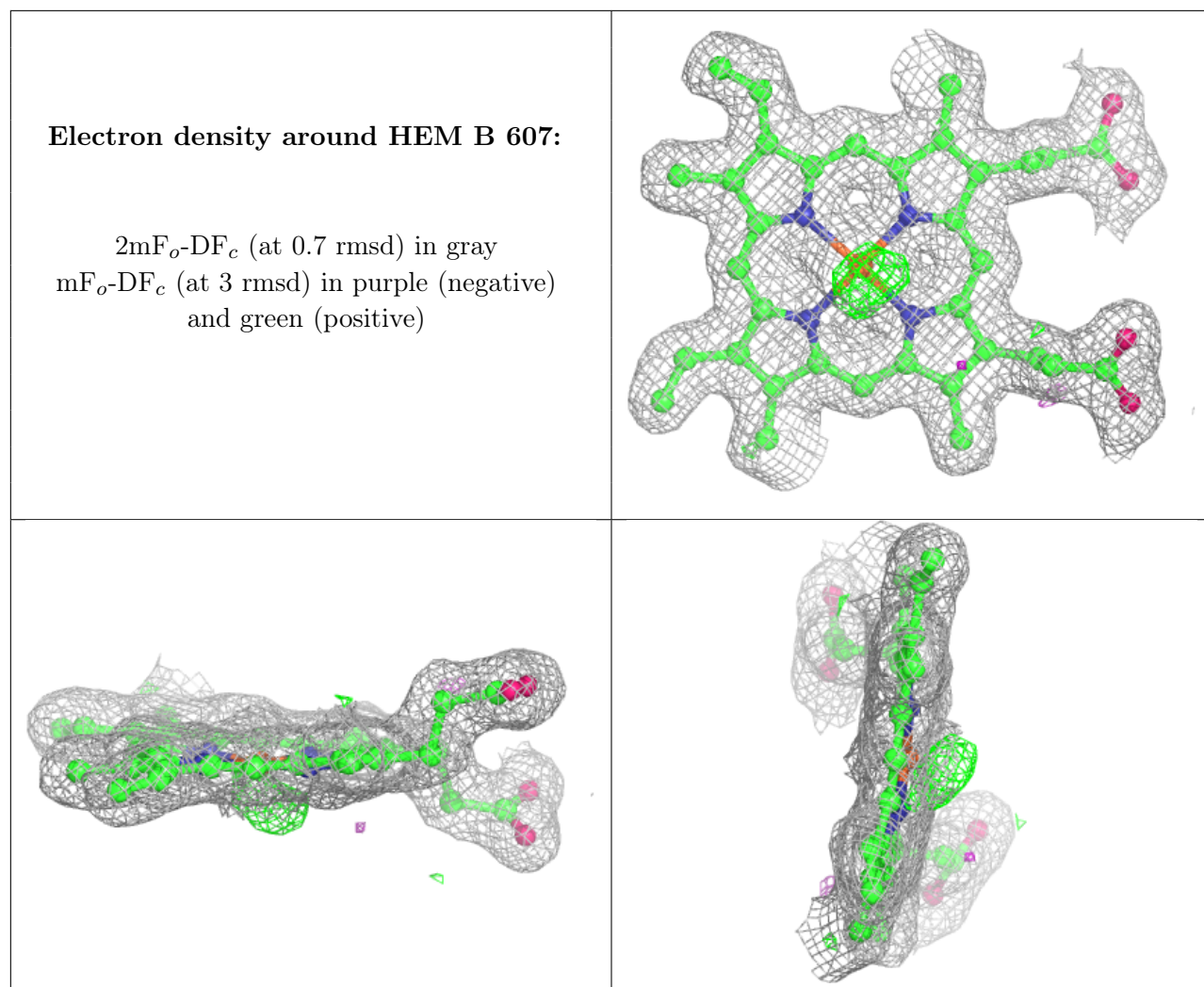
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	604	14/15	0.87	0.17	53,59,62,62	0
4	NAG	B	602	14/15	0.88	0.13	47,60,68,73	0
7	NO3	A	610	4/4	0.91	0.15	51,51,52,54	0
7	NO3	A	612	4/4	0.91	0.19	40,45,47,53	0
8	GOL	A	615	6/6	0.92	0.20	35,39,42,47	0
4	NAG	B	603	14/15	0.93	0.10	22,31,41,48	0
7	NO3	A	611	4/4	0.93	0.14	36,36,40,44	0
8	GOL	B	616	6/6	0.94	0.18	31,34,35,37	0
4	NAG	A	606	14/15	0.94	0.10	27,32,40,45	0
8	GOL	A	614	6/6	0.95	0.09	25,30,31,32	0
4	NAG	A	603	14/15	0.95	0.09	27,36,43,49	0
3	MMZ	A	602	7/7	0.95	0.17	28,29,31,31	7
8	GOL	B	614	6/6	0.95	0.11	26,28,34,39	0
3	MMZ	B	601	7/7	0.95	0.15	27,28,30,31	7
3	MMZ	B	613	7/7	0.95	0.16	25,27,29,31	7
7	NO3	B	612	4/4	0.96	0.12	30,36,37,42	0
8	GOL	B	615	6/6	0.96	0.10	24,26,27,28	0
8	GOL	A	616	6/6	0.96	0.11	22,24,31,38	0
3	MMZ	A	601	7/7	0.96	0.20	34,35,37,41	7
7	NO3	B	609	4/4	0.98	0.09	24,29,32,32	0
7	NO3	B	610	4/4	0.98	0.10	24,25,29,31	0
5	HEM	A	607	43/43	0.98	0.09	14,16,17,19	0
6	CA	B	608	1/1	0.99	0.08	25,25,25,25	0
7	NO3	A	609	4/4	0.99	0.07	18,18,19,22	0
5	HEM	B	607	43/43	0.99	0.09	12,14,16,19	0
6	CA	A	608	1/1	1.00	0.06	19,19,19,19	0

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

**Electron density around HEM A 607:**

$2mF_o-DF_c$  (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.