



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:59 AM BST

PDB ID : 4C1M  
Title : Myeloperoxidase in complex with the reversible inhibitor HX1  
Authors : Forbes, L.V.; Sjogren, T.; Auchere, F.; Jenkins, D.W.; Thong, B.; Laughton, D.; Hemsley, P.; Pairaudeau, G.; Eriksson, H.; Unitt, J.F.; Kettle, A.J.  
Deposited on : 2013-08-13  
Resolution : 2.00 Å(reported)

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

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

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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 : 2.13.1  
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) : 2.13.1

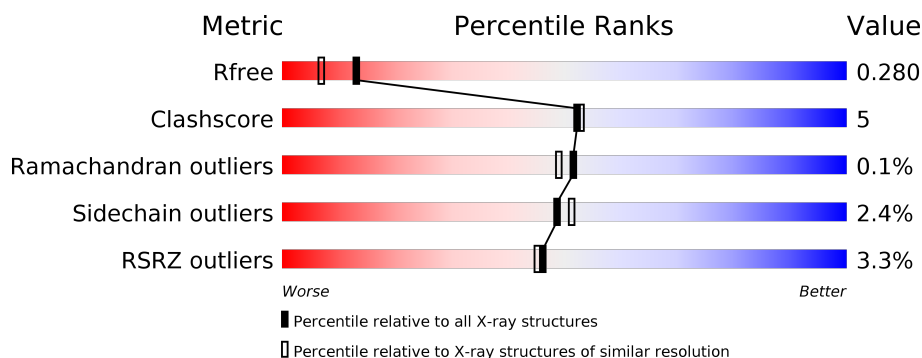
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	108	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	108	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> </div>
2	C	467	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
2	D	467	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
3	E	6	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
3	F	6	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10168 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.

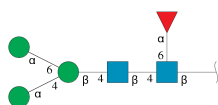
- Molecule 1 is a protein called MYELOPEROXIDASE LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	1
			816	516	146	150	4			
1	B	105	Total	C	N	O	S	0	0	1
			838	529	149	155	5			

- Molecule 2 is a protein called MYELOPEROXIDASE HEAVY CHAIN.

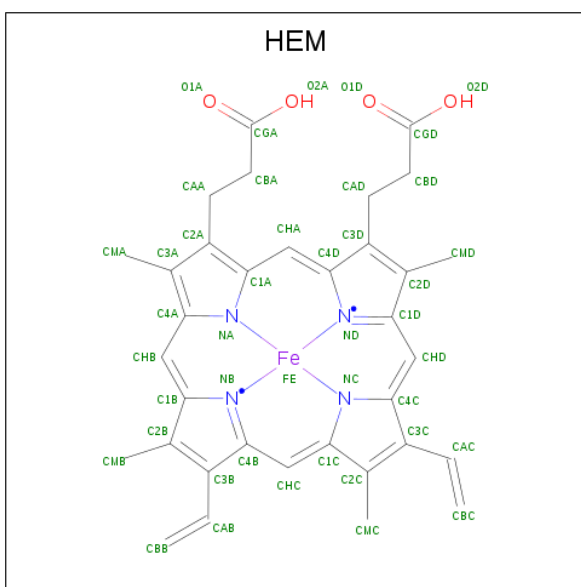
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			
2	D	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-[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.



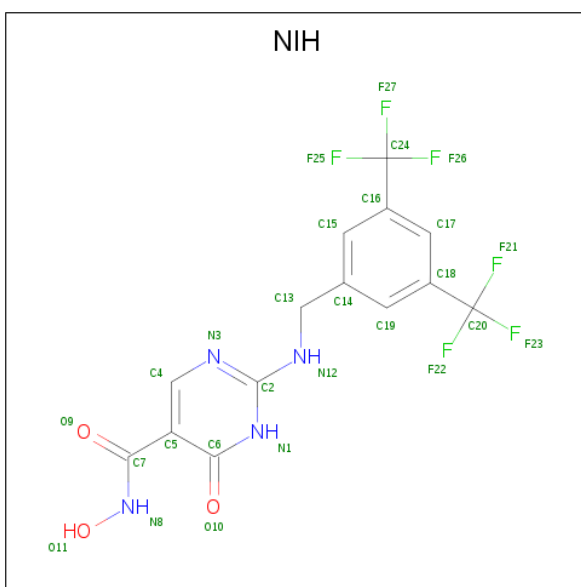
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 5 is 2-[3,5-BIS(TRIFLUOROMETHYL)BENZYL]AMINO}-N-HYDROXY-6-OXO-1,6-DIHYDROPYRIMIDINE-5-CARBOXAMIDE (three-letter code: NIH) (formula: C<sub>14</sub>H<sub>10</sub>F<sub>6</sub>N<sub>4</sub>O<sub>3</sub>).



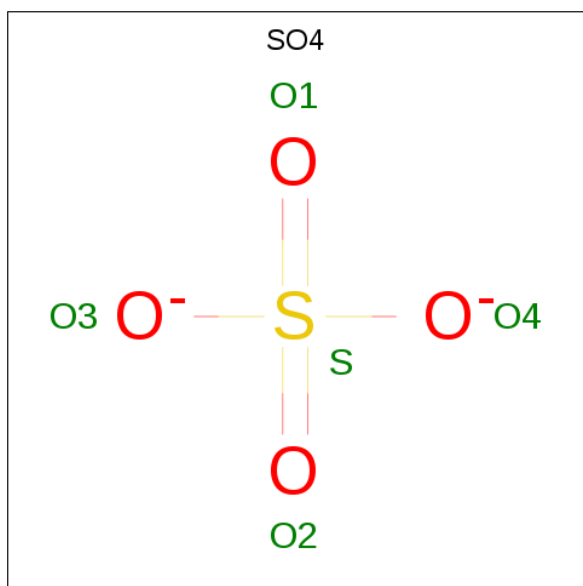
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			27	14	6	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	0	0
			27	14	6	4	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 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
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

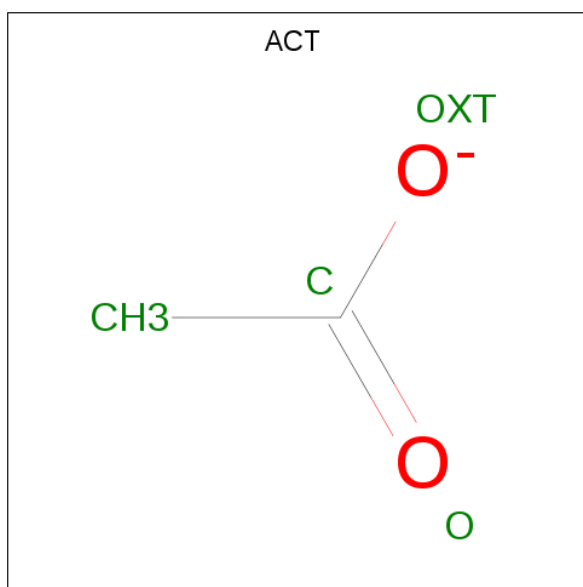
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

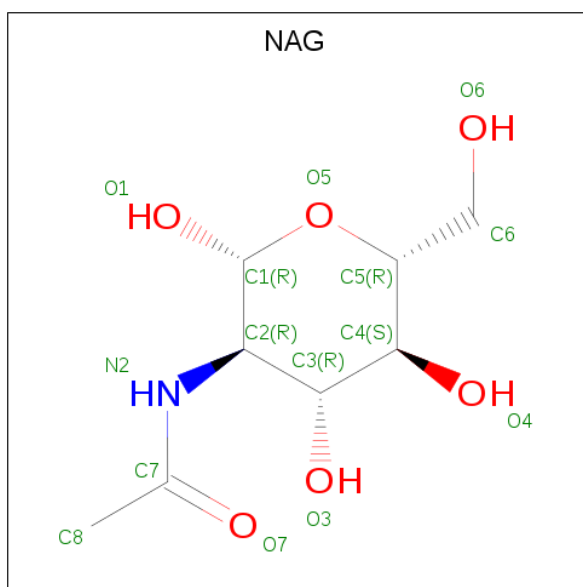
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Cl	0	0
			1	1		
9	C	1	Total	Cl	0	0
			1	1		

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 12 is water.

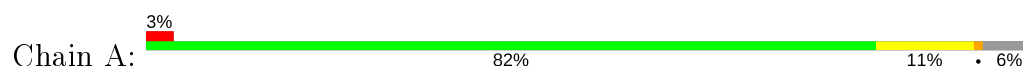
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	103	Total	O	0	0
			103	103		
12	B	108	Total	O	0	0
			108	108		
12	C	254	Total	O	0	0
			254	254		
12	D	199	Total	O	0	0
			199	199		



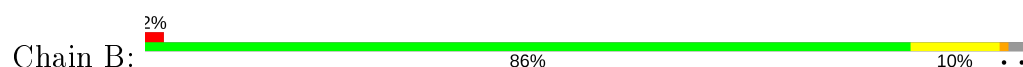
### 3 Residue-property plots [i](#)

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.

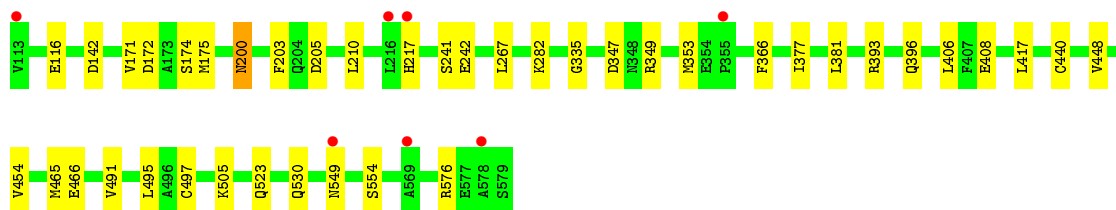
#### • Molecule 1: MYELOPEROXIDASE LIGHT CHAIN



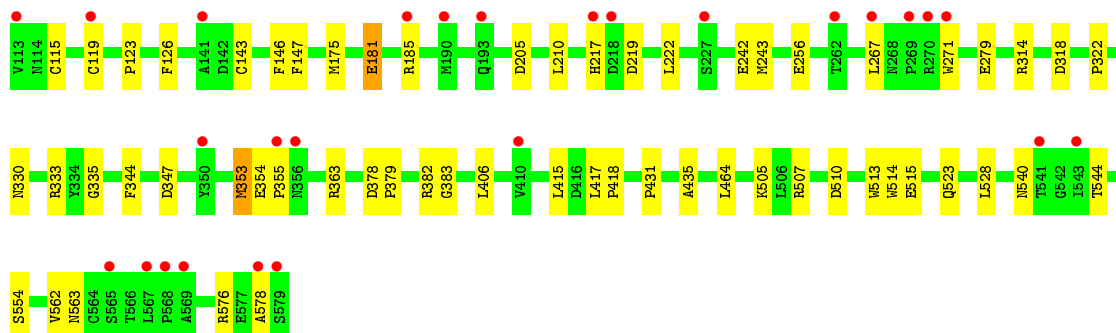
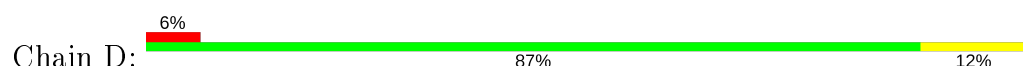
#### • Molecule 1: MYELOPEROXIDASE LIGHT CHAIN



#### • Molecule 2: MYELOPEROXIDASE HEAVY CHAIN



#### • Molecule 2: MYELOPEROXIDASE HEAVY CHAIN



- Molecule 3:  $\alpha$ -D-mannopyranose-(1-4)-[ $\alpha$ -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:  33% 67%

MAG1
MAG2
EMA3
MAN4
MAN5
FUC6

- Molecule 3:  $\alpha$ -D-mannopyranose-(1-4)-[ $\alpha$ -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%

MAG1
MAG2
EMA3
MAN4
MAN5
FUC6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.28Å 63.44Å 92.38Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 55.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.00) 94.0 (55.00-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.222 , 0.278 0.226 , 0.280	Depositor DCC
$R_{free}$ test set	4064 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtriage
Anisotropy	0.945	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, BMA, NAG, CL, SO4, CA, NIH, FUC, ACT, HEM, MAN

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	0.81	1/840 (0.1%)	0.87	1/1144 (0.1%)
1	B	0.73	0/863	0.82	0/1176
2	C	0.76	0/3811	0.79	0/5170
2	D	0.69	0/3811	0.74	1/5170 (0.0%)
All	All	0.73	1/9325 (0.0%)	0.78	2/12660 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ALA	C-N	-5.02	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	510	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	94	ASP	CB-CG-OD2	-5.19	113.63	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	779	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	838	0	800	14	0
2	C	3733	0	3727	31	0
2	D	3733	0	3729	41	0
3	E	71	0	61	6	0
3	F	71	0	61	4	0
4	A	43	0	30	10	0
4	B	43	0	30	17	0
5	A	27	0	10	1	0
5	B	27	0	10	1	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	C	6	0	8	0	0
7	D	6	0	8	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	C	8	0	6	0	0
10	D	12	0	9	0	0
11	C	28	0	26	0	0
11	D	28	0	26	0	0
12	A	103	0	0	4	0
12	B	108	0	0	2	0
12	C	254	0	0	10	0
12	D	199	0	0	7	0
All	All	10168	0	9320	103	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 5.

All (103) 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)
4:B:605:HEM:HBB1	2:D:243:MET:SD	1.57	1.44
1:A:94:ASP:OD2	4:A:605:HEM:CMD	1.64	1.44
4:A:605:HEM:CMB	2:C:242:GLU:OE2	1.69	1.37
4:B:605:HEM:CBB	2:D:243:MET:SD	2.13	1.35
4:A:605:HEM:HMB1	2:C:242:GLU:OE2	1.17	1.33
1:B:94:ASP:OD2	4:B:605:HEM:CMD	1.78	1.31
4:B:605:HEM:HMB1	2:D:242:GLU:OE2	1.45	1.15
4:B:605:HEM:CMB	2:D:242:GLU:OE2	1.98	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:605:HEM:HBB1	2:D:243:MET:CE	1.81	1.10
1:B:94:ASP:OD2	4:B:605:HEM:HMD1	0.87	1.04
1:A:94:ASP:OD2	4:A:605:HEM:HMD1	0.80	0.97
3:E:3:BMA:O3	3:E:5:MAN:H2	1.67	0.93
3:E:3:BMA:H3	3:E:4:MAN:H2	1.52	0.91
1:A:90:GLY:HA2	12:A:2093:HOH:O	1.74	0.88
4:A:605:HEM:HMB2	2:C:242:GLU:OE2	1.76	0.83
2:C:448:VAL:HA	12:C:2194:HOH:O	1.81	0.81
4:B:605:HEM:HBB1	2:D:243:MET:HE3	1.69	0.74
2:D:431:PRO:HB2	12:D:2145:HOH:O	1.86	0.74
4:A:605:HEM:C2B	2:C:242:GLU:OE2	2.39	0.74
1:B:94:ASP:CG	4:B:605:HEM:HMD1	1.99	0.73
1:A:93:LEU:HB3	12:A:2093:HOH:O	1.90	0.72
1:A:94:ASP:OD2	4:A:605:HEM:C2D	2.45	0.67
4:B:605:HEM:C2B	2:D:242:GLU:OE2	2.51	0.62
4:A:605:HEM:CBC	2:C:335:GLY:HA3	2.30	0.62
3:F:3:BMA:H3	3:F:4:MAN:O5	2.02	0.60
3:F:3:BMA:O3	3:F:4:MAN:H3	2.03	0.59
3:F:3:BMA:C3	3:F:4:MAN:O5	2.50	0.59
2:D:382:ARG:NH2	12:D:2130:HOH:O	2.34	0.57
4:B:605:HEM:CBB	2:D:243:MET:CE	2.70	0.57
4:A:605:HEM:HBC2	2:C:335:GLY:HA3	1.87	0.57
1:A:94:ASP:CG	4:A:605:HEM:CMD	2.68	0.57
1:A:83:SER:HB3	2:C:554:SER:O	2.05	0.56
4:B:605:HEM:HMB2	2:D:242:GLU:OE2	2.03	0.54
2:C:440:CYS:HG	2:C:497:CYS:HG	1.54	0.54
2:C:347:ASP:HB2	12:C:2159:HOH:O	2.08	0.53
2:C:205:ASP:HB2	2:C:210:LEU:HD21	1.91	0.53
2:C:200:ASN:HD22	2:C:203:PHE:H	1.55	0.53
2:D:205:ASP:HB2	2:D:210:LEU:HD21	1.90	0.53
1:B:64:VAL:HG13	1:B:68:ILE:HD12	1.91	0.52
4:B:605:HEM:CBB	2:D:243:MET:HE3	2.40	0.51
2:C:116:GLU:HG3	12:C:2015:HOH:O	2.10	0.51
2:D:576:ARG:NH2	12:D:2192:HOH:O	2.43	0.51
2:C:530:GLN:NE2	12:C:2222:HOH:O	2.43	0.50
2:C:454:VAL:HA	12:C:2198:HOH:O	2.10	0.50
1:A:64:VAL:HG13	1:A:68:ILE:HD12	1.92	0.50
1:B:10:ILE:HB	12:B:2019:HOH:O	2.10	0.50
3:E:3:BMA:C3	3:E:4:MAN:H2	2.31	0.50
2:C:377:ILE:HD12	2:C:381:LEU:HD11	1.93	0.49
5:A:606:NIH:O10	5:A:606:NIH:N8	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:H	1:B:6:LYS:HE2	1.78	0.49
2:C:393:ARG:HB2	2:C:396:GLN:HB2	1.94	0.49
1:B:94:ASP:OD2	4:B:605:HEM:C2D	2.62	0.49
2:C:200:ASN:ND2	2:C:203:PHE:H	2.10	0.49
2:D:563:ASN:HB3	12:D:2188:HOH:O	2.13	0.49
4:B:605:HEM:CBC	2:D:335:GLY:HA3	2.44	0.48
2:C:505:LYS:HE3	3:F:5:MAN:O4	2.13	0.48
4:B:605:HEM:HBB2	4:B:605:HEM:HMB2	1.96	0.48
2:D:119:CYS:SG	2:D:143:CYS:SG	3.09	0.47
2:D:435:ALA:HB3	12:D:2145:HOH:O	2.14	0.47
1:B:94:ASP:CG	4:B:605:HEM:CMD	2.71	0.47
1:B:22:LEU:HB3	2:D:322:PRO:HD2	1.96	0.47
1:B:83:SER:HB3	2:D:554:SER:O	2.15	0.47
2:C:142:ASP:HB3	12:C:2038:HOH:O	2.15	0.46
2:D:123:PRO:HA	12:D:2016:HOH:O	2.16	0.46
5:B:606:NIH:H4	2:D:242:GLU:HG3	1.98	0.46
2:C:406:LEU:HD22	2:C:417:LEU:HB2	1.98	0.46
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.51	0.45
2:D:344:PHE:O	2:D:383:GLY:HA3	2.16	0.45
2:D:528:LEU:HD22	12:D:2091:HOH:O	2.16	0.45
2:D:271:TRP:CZ3	2:D:279:GLU:HG3	2.52	0.45
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.99	0.45
1:B:93:LEU:O	1:B:97:LEU:HG	2.16	0.45
2:C:241:SER:O	2:C:366:PHE:HA	2.17	0.45
12:B:2019:HOH:O	2:D:181:GLU:HG3	2.16	0.44
2:D:347:ASP:HB3	2:D:353:MET:HG3	1.99	0.44
1:A:40:GLY:HA3	1:B:20:PRO:HG2	1.99	0.44
2:D:507:ARG:HG3	2:D:513:TRP:CE2	2.51	0.44
2:D:378:ASP:HB2	2:D:379:PRO:HD3	1.99	0.44
1:B:68:ILE:HD13	2:D:464:LEU:HD23	1.99	0.44
1:A:93:LEU:HD23	12:A:2093:HOH:O	2.18	0.44
2:D:505:LYS:HE3	3:E:5:MAN:H61	2.00	0.43
2:C:465:MET:HG2	12:C:2194:HOH:O	2.18	0.43
2:C:172:ASP:OD1	2:C:174:SER:HB3	2.19	0.43
2:C:393:ARG:HB3	2:C:393:ARG:HE	1.62	0.43
2:D:115:CYS:HB2	2:D:147:PHE:CZ	2.53	0.43
12:A:2004:HOH:O	2:C:282:LYS:HE3	2.19	0.43
2:D:267:LEU:HD12	2:D:576:ARG:HB2	2.01	0.42
2:C:465:MET:CG	12:C:2194:HOH:O	2.67	0.42
2:C:491:VAL:HB	2:C:495:LEU:HB2	2.00	0.42
2:C:440:CYS:SG	2:C:497:CYS:SG	3.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:GLU:HB3	2:D:355:PRO:HA	2.00	0.42
2:D:330:ASN:O	2:D:333:ARG:HB2	2.20	0.42
2:C:549:ASN:HB3	12:C:2232:HOH:O	2.20	0.42
2:D:126:PHE:HB3	2:D:146:PHE:CD1	2.55	0.42
1:A:16:ASN:O	1:A:20:PRO:HA	2.19	0.41
2:D:219:ASP:HB3	2:D:222:LEU:HD12	2.02	0.41
1:B:83:SER:O	1:B:86:PHE:HB3	2.20	0.41
2:D:256:GLU:OE1	2:D:540:ASN:ND2	2.43	0.41
1:A:84:LEU:HA	1:A:84:LEU:HD12	1.88	0.40
2:D:406:LEU:HB3	2:D:415:LEU:HB2	2.03	0.40
12:C:2148:HOH:O	3:E:6:FUC:H5	2.20	0.40
1:A:97:LEU:HD21	2:C:171:VAL:HG22	2.03	0.40
3:E:3:BMA:H3	3:E:4:MAN:C2	2.37	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	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
1	B	103/108 (95%)	100 (97%)	3 (3%)	0	100	100
2	C	464/467 (99%)	449 (97%)	15 (3%)	0	100	100
2	D	464/467 (99%)	452 (97%)	11 (2%)	1 (0%)	47	44
All	All	1131/1150 (98%)	1098 (97%)	32 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	578	ALA



### 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	87/93 (94%)	86 (99%)	1 (1%)	73	78
1	B	90/93 (97%)	88 (98%)	2 (2%)	52	55
2	C	410/411 (100%)	400 (98%)	10 (2%)	49	51
2	D	410/411 (100%)	399 (97%)	11 (3%)	44	46
All	All	997/1008 (99%)	973 (98%)	24 (2%)	49	51

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	B	6	LYS
1	B	54	ASN
2	C	175	MET
2	C	200	ASN
2	C	217	HIS
2	C	267	LEU
2	C	349	ARG
2	C	353	MET
2	C	408	GLU
2	C	466	GLU
2	C	523	GLN
2	C	576	ARG
2	D	175	MET
2	D	181	GLU
2	D	185	ARG
2	D	217	HIS
2	D	314	ARG
2	D	318	ASP
2	D	353	MET
2	D	363	ARG
2	D	523	GLN
2	D	544	THR
2	D	562	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	80	GLN
2	C	200	ASN
2	C	421	ASN
2	C	530	GLN

### 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	0.58	0	0,6,8	0.00	-
2	CSO	D	150	2	3,6,7	0.60	0	0,6,8	0.00	-

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 [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$
3	NAG	E	1	3,2	14,14,15	0.94	1 (7%)	17,19,21	2.68	6 (35%)
3	NAG	E	2	3	14,14,15	1.30	2 (14%)	17,19,21	1.94	6 (35%)
3	BMA	E	3	3	11,11,12	0.89	0	15,15,17	1.98	4 (26%)
3	MAN	E	4	3	11,11,12	0.75	0	15,15,17	1.60	3 (20%)
3	MAN	E	5	3	11,11,12	0.88	0	15,15,17	1.46	4 (26%)
3	FUC	E	6	3	10,10,11	0.81	0	14,14,16	1.85	4 (28%)
3	NAG	F	1	3,2	14,14,15	0.57	0	17,19,21	1.62	5 (29%)
3	NAG	F	2	3	14,14,15	1.19	2 (14%)	17,19,21	1.76	5 (29%)
3	BMA	F	3	3	11,11,12	1.34	2 (18%)	15,15,17	2.13	6 (40%)
3	MAN	F	4	3	11,11,12	1.05	2 (18%)	15,15,17	3.21	4 (26%)
3	MAN	F	5	3	11,11,12	0.41	0	15,15,17	1.50	5 (33%)
3	FUC	F	6	3	10,10,11	0.74	0	14,14,16	1.37	2 (14%)

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 Torsions 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	1/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C4-C5	3.18	1.59	1.53
3	E	2	NAG	C2-N2	-3.05	1.41	1.46
3	F	2	NAG	O5-C1	-2.70	1.39	1.43
3	E	2	NAG	O5-C1	-2.44	1.39	1.43
3	F	2	NAG	C2-N2	-2.38	1.42	1.46
3	F	3	BMA	C2-C3	-2.33	1.49	1.52
3	F	4	MAN	C2-C3	2.18	1.55	1.52
3	E	1	NAG	C1-C2	-2.12	1.49	1.52
3	F	4	MAN	C1-C2	2.03	1.56	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	8.09	123.15	112.19
3	F	4	MAN	O5-C5-C6	6.83	117.92	107.20
3	E	1	NAG	C1-C2-N2	6.44	121.48	110.49
3	E	1	NAG	O5-C1-C2	-5.90	101.97	111.29
3	F	4	MAN	C1-C2-C3	4.63	115.36	109.67
3	E	2	NAG	C1-O5-C5	4.58	118.40	112.19
3	E	3	BMA	O2-C2-C3	-4.00	102.12	110.14
3	E	4	MAN	C1-O5-C5	3.99	117.60	112.19
3	F	2	NAG	C4-C3-C2	-3.95	105.23	111.02
3	F	3	BMA	O3-C3-C2	-3.88	102.57	109.99
3	F	3	BMA	C6-C5-C4	3.81	121.92	113.00
3	E	6	FUC	O5-C5-C4	3.79	116.32	109.52
3	E	1	NAG	C1-O5-C5	3.65	117.14	112.19
3	F	3	BMA	O4-C4-C5	3.61	118.25	109.30
3	F	1	NAG	C1-O5-C5	3.55	117.01	112.19
3	E	6	FUC	C3-C4-C5	3.35	114.99	109.77
3	E	4	MAN	C1-C2-C3	3.31	113.74	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	C1-O5-C5	3.28	116.63	112.19
3	E	1	NAG	O7-C7-N2	3.18	127.80	121.95
3	E	2	NAG	O4-C4-C5	-3.05	101.73	109.30
3	F	6	FUC	C3-C4-C5	3.04	114.50	109.77
3	E	1	NAG	C2-N2-C7	3.03	127.22	122.90
3	E	2	NAG	O7-C7-N2	3.01	127.48	121.95
3	E	6	FUC	C6-C5-C4	-2.98	107.57	113.07
3	E	2	NAG	C2-N2-C7	2.86	126.97	122.90
3	E	5	MAN	C1-C2-C3	2.77	113.08	109.67
3	F	1	NAG	O4-C4-C3	-2.75	104.00	110.35
3	F	3	BMA	O5-C5-C6	-2.65	103.05	107.20
3	F	2	NAG	O3-C3-C2	2.65	114.94	109.47
3	E	4	MAN	O5-C5-C6	2.58	111.25	107.20
3	E	6	FUC	O4-C4-C3	-2.57	104.41	110.35
3	F	5	MAN	C1-O5-C5	2.53	115.62	112.19
3	F	5	MAN	O2-C2-C1	2.48	114.22	109.15
3	F	2	NAG	C2-N2-C7	2.45	126.39	122.90
3	F	1	NAG	C1-C2-N2	2.41	114.61	110.49
3	E	3	BMA	O2-C2-C1	2.41	114.08	109.15
3	E	3	BMA	C1-C2-C3	2.40	112.61	109.67
3	E	5	MAN	O5-C1-C2	-2.38	107.10	110.77
3	F	6	FUC	C2-C3-C4	-2.36	106.82	110.89
3	F	3	BMA	O4-C4-C3	-2.34	104.95	110.35
3	E	1	NAG	O7-C7-C8	-2.30	117.79	122.06
3	E	2	NAG	O7-C7-C8	-2.25	117.87	122.06
3	E	2	NAG	C4-C3-C2	-2.17	107.84	111.02
3	E	5	MAN	C1-O5-C5	2.17	115.13	112.19
3	F	5	MAN	C1-C2-C3	-2.16	107.01	109.67
3	F	2	NAG	O4-C4-C5	-2.12	104.02	109.30
3	F	1	NAG	C8-C7-N2	2.12	119.69	116.10
3	E	5	MAN	O3-C3-C2	-2.10	105.98	109.99
3	F	5	MAN	O3-C3-C4	2.08	115.17	110.35
3	F	4	MAN	C2-C3-C4	2.08	114.49	110.89
3	F	3	BMA	O5-C5-C4	2.07	115.86	110.83
3	F	5	MAN	O5-C1-C2	-2.04	107.63	110.77
3	F	1	NAG	O5-C1-C2	-2.02	108.10	111.29
3	F	2	NAG	O5-C5-C6	2.02	110.37	107.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4	MAN	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6

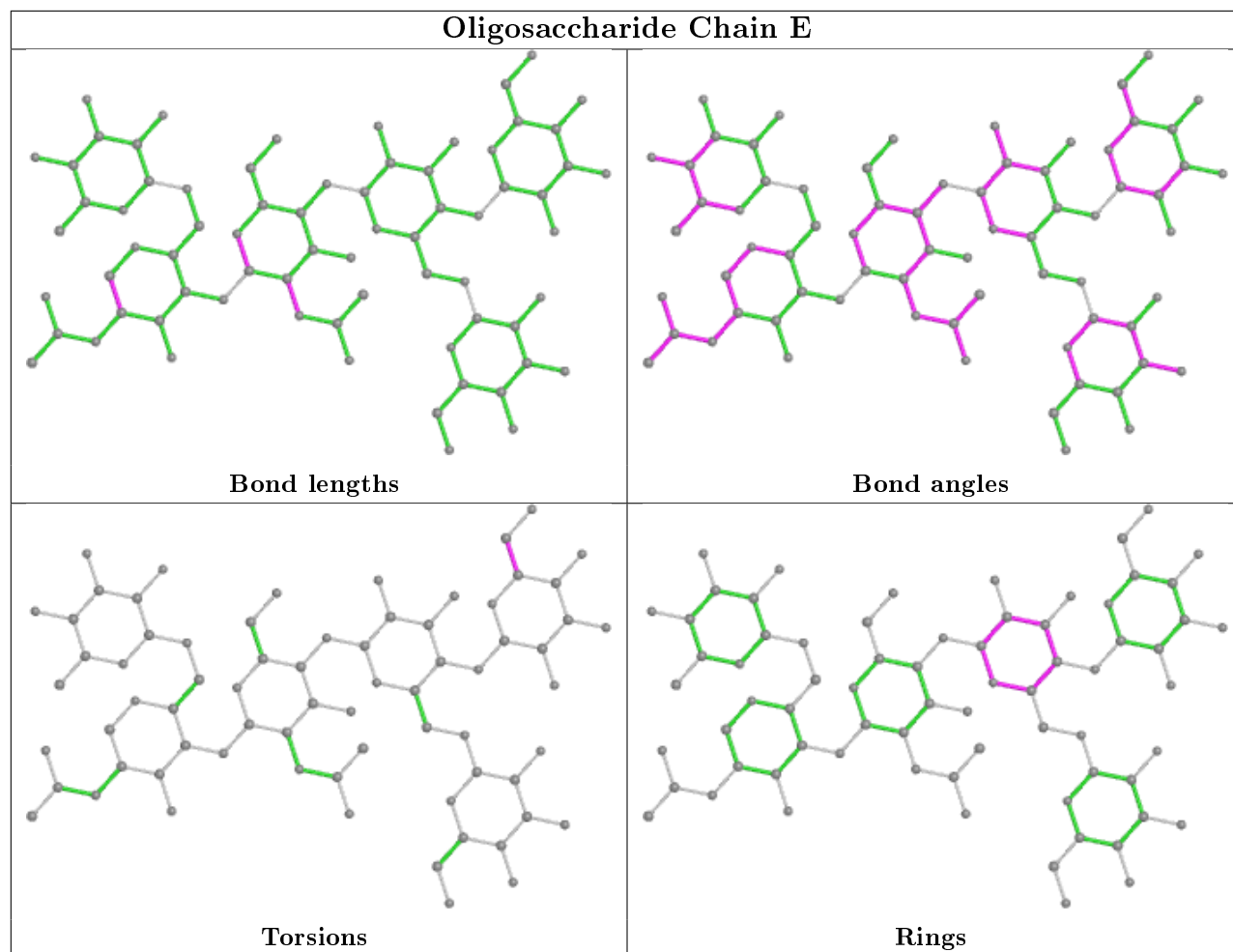
All (1) ring outliers are listed below:

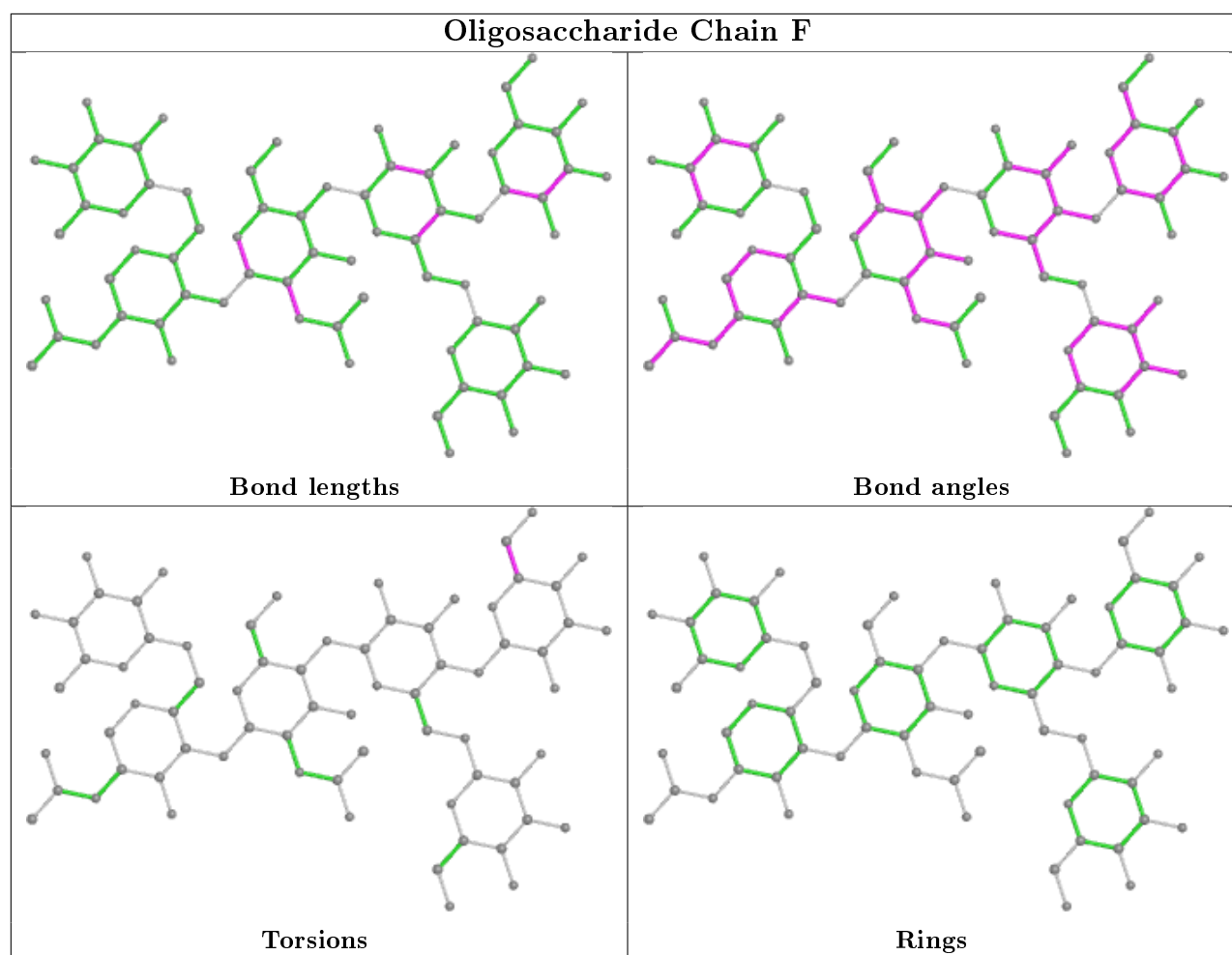
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	C1-C2-C3-C4-C5-O5

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	MAN	3	0
3	E	4	MAN	3	0
3	F	5	MAN	1	0
3	F	3	BMA	3	0
3	E	3	BMA	4	0
3	E	6	FUC	1	0
3	E	5	MAN	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.





## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\# Z  > 2$
5	NIH	B	606	-	28,28,28	1.25	4 (14%)	36,42,42	2.48	10 (27%)
6	SO4	B	1003	-	4,4,4	0.37	0	6,6,6	0.37	0
5	NIH	A	606	-	28,28,28	1.40	3 (10%)	36,42,42	2.55	8 (22%)
10	ACT	C	1582	-	1,3,3	1.94	0	0,3,3	0.00	-
4	HEM	B	605	2	27,50,50	1.61	10 (37%)	17,82,82	1.88	6 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	ACT	D	1583	-	1,3,3	1.62	0	0,3,3	0.00	-
10	ACT	C	1583	-	1,3,3	1.60	0	0,3,3	0.00	-
11	NAG	D	2630	2	14,14,15	0.61	0	17,19,21	1.49	3 (17%)
7	GOL	C	631	-	5,5,5	0.30	0	5,5,5	0.47	0
4	HEM	A	605	2	27,50,50	1.29	4 (14%)	17,82,82	2.19	7 (41%)
10	ACT	D	1582	-	1,3,3	1.17	0	0,3,3	0.00	-
11	NAG	C	1630	2	14,14,15	0.73	0	17,19,21	2.13	7 (41%)
7	GOL	D	631	-	5,5,5	0.39	0	5,5,5	0.59	0
11	NAG	D	2620	2	14,14,15	0.52	0	17,19,21	1.44	2 (11%)
11	NAG	C	1620	2	14,14,15	0.66	0	17,19,21	1.71	6 (35%)
10	ACT	D	1581	-	1,3,3	1.99	0	0,3,3	0.00	-
6	SO4	C	1581	-	4,4,4	0.33	0	6,6,6	0.46	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
5	NIH	B	606	-	-	2/23/23/23	0/2/2/2
7	GOL	C	631	-	-	4/4/4/4	-
5	NIH	A	606	-	-	3/23/23/23	0/2/2/2
4	HEM	B	605	2	-	0/6/54/54	-
11	NAG	D	2630	2	-	0/6/23/26	0/1/1/1
4	HEM	A	605	2	-	0/6/54/54	-
11	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
7	GOL	D	631	-	-	2/4/4/4	-
11	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
11	NAG	C	1620	2	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	NIH	C2-N12	3.66	1.40	1.34
4	B	605	HEM	C1B-C2B	2.97	1.49	1.42
4	B	605	HEM	CBC-CAC	2.82	1.47	1.29
5	B	606	NIH	C5-C7	-2.79	1.45	1.50
4	B	605	HEM	CBB-CAB	2.76	1.47	1.29
5	A	606	NIH	C5-C7	-2.72	1.45	1.50
4	A	605	HEM	C4D-C3D	2.58	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	HEM	C4A-CHB	2.51	1.48	1.41
4	B	605	HEM	C1D-CHD	2.39	1.47	1.41
4	A	605	HEM	CBB-CAB	2.37	1.45	1.29
4	B	605	HEM	C4B-NB	-2.35	1.31	1.36
4	A	605	HEM	CBC-CAC	2.25	1.44	1.29
4	B	605	HEM	C1D-ND	-2.23	1.31	1.36
4	B	605	HEM	C1C-C2C	2.19	1.47	1.42
5	B	606	NIH	F23-C20	2.18	1.40	1.32
4	B	605	HEM	C4D-C3D	2.13	1.47	1.42
4	B	605	HEM	C1A-NA	-2.11	1.31	1.36
5	A	606	NIH	C7-N8	2.04	1.35	1.32
4	A	605	HEM	C4B-NB	-2.02	1.32	1.36
5	B	606	NIH	F22-C20	2.02	1.40	1.32
5	B	606	NIH	F25-C24	2.01	1.40	1.32

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	NIH	C5-C6-N1	-10.76	116.90	124.40
5	B	606	NIH	C5-C6-N1	-10.41	117.14	124.40
5	A	606	NIH	N3-C2-N1	-7.05	119.87	126.55
11	C	1630	NAG	C1-O5-C5	5.20	119.24	112.19
5	B	606	NIH	N3-C2-N1	-4.79	122.01	126.55
4	A	605	HEM	CMB-C2B-C3B	4.43	132.97	124.68
5	A	606	NIH	C4-N3-C2	3.92	121.79	115.88
4	A	605	HEM	CBD-CAD-C3D	-3.79	105.49	112.48
4	B	605	HEM	CBD-CAD-C3D	-3.67	105.71	112.48
4	A	605	HEM	CMC-C2C-C3C	3.67	131.54	124.68
5	A	606	NIH	C6-N1-C2	3.52	121.49	115.18
5	B	606	NIH	C4-N3-C2	3.50	121.16	115.88
11	C	1630	NAG	O4-C4-C3	3.49	118.42	110.35
4	B	605	HEM	CMC-C2C-C3C	3.41	131.06	124.68
11	C	1620	NAG	C1-O5-C5	3.29	116.65	112.19
5	B	606	NIH	F27-C24-C16	-3.19	105.93	112.93
5	B	606	NIH	C5-C4-N3	-3.14	119.55	124.49
4	A	605	HEM	C4A-C3A-C2A	-3.14	104.81	107.00
5	B	606	NIH	C6-N1-C2	3.08	120.69	115.18
5	A	606	NIH	O11-N8-C7	3.02	127.11	119.64
11	C	1630	NAG	C3-C4-C5	-2.96	104.96	110.24
11	D	2630	NAG	O3-C3-C2	-2.92	103.43	109.47
11	D	2620	NAG	C1-O5-C5	2.87	116.09	112.19
11	D	2620	NAG	O5-C5-C6	-2.78	102.85	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1620	NAG	C1-C2-N2	-2.63	105.99	110.49
11	D	2630	NAG	C3-C4-C5	-2.60	105.59	110.24
11	C	1630	NAG	O5-C1-C2	-2.60	107.18	111.29
4	A	605	HEM	C1D-C2D-C3D	-2.57	105.21	107.00
4	B	605	HEM	C4A-C3A-C2A	-2.55	105.22	107.00
11	C	1620	NAG	C4-C3-C2	-2.49	107.37	111.02
4	B	605	HEM	CMB-C2B-C3B	2.46	129.28	124.68
5	A	606	NIH	C5-C4-N3	-2.46	120.63	124.49
11	D	2630	NAG	O4-C4-C5	2.42	115.31	109.30
4	B	605	HEM	CBA-CAA-C2A	-2.42	108.03	112.49
5	A	606	NIH	N12-C2-N3	2.35	120.75	117.22
5	A	606	NIH	F26-C24-C16	-2.35	107.76	112.93
11	C	1620	NAG	O5-C1-C2	-2.33	107.61	111.29
4	A	605	HEM	CAA-CBA-CGA	-2.27	108.86	112.67
5	B	606	NIH	C13-N12-C2	-2.27	120.10	123.28
5	B	606	NIH	C19-C18-C20	-2.27	116.52	119.58
11	C	1630	NAG	O7-C7-N2	2.22	126.03	121.95
11	C	1630	NAG	O7-C7-C8	-2.21	117.95	122.06
11	C	1620	NAG	O4-C4-C3	-2.15	105.38	110.35
4	A	605	HEM	CMA-C3A-C2A	2.13	128.96	124.94
5	B	606	NIH	C17-C18-C20	2.13	122.45	119.58
11	C	1620	NAG	C2-N2-C7	-2.12	119.89	122.90
4	B	605	HEM	C1D-C2D-C3D	-2.10	105.53	107.00
11	C	1630	NAG	O5-C5-C6	2.08	110.46	107.20
5	B	606	NIH	F23-C20-C18	-2.03	108.47	112.93

There are no chirality outliers.

All (11) torsion outliers are listed below:

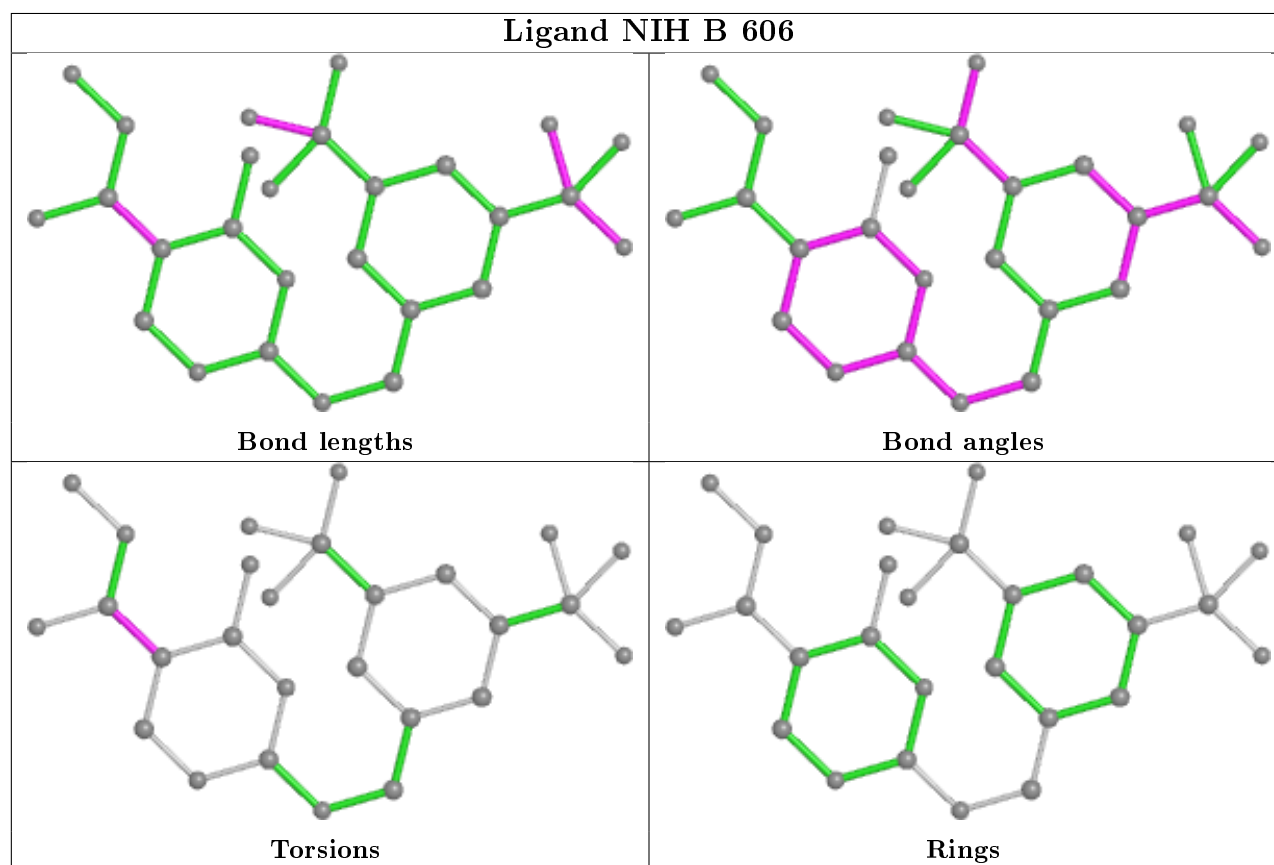
Mol	Chain	Res	Type	Atoms
7	C	631	GOL	O1-C1-C2-C3
7	C	631	GOL	C1-C2-C3-O3
7	D	631	GOL	C1-C2-C3-O3
7	C	631	GOL	O2-C2-C3-O3
7	D	631	GOL	O2-C2-C3-O3
7	C	631	GOL	O1-C1-C2-O2
5	B	606	NIH	C4-C5-C7-O9
5	A	606	NIH	C4-C5-C7-O9
5	A	606	NIH	C6-C5-C7-O9
5	B	606	NIH	C6-C5-C7-N8
5	A	606	NIH	C6-C5-C7-N8

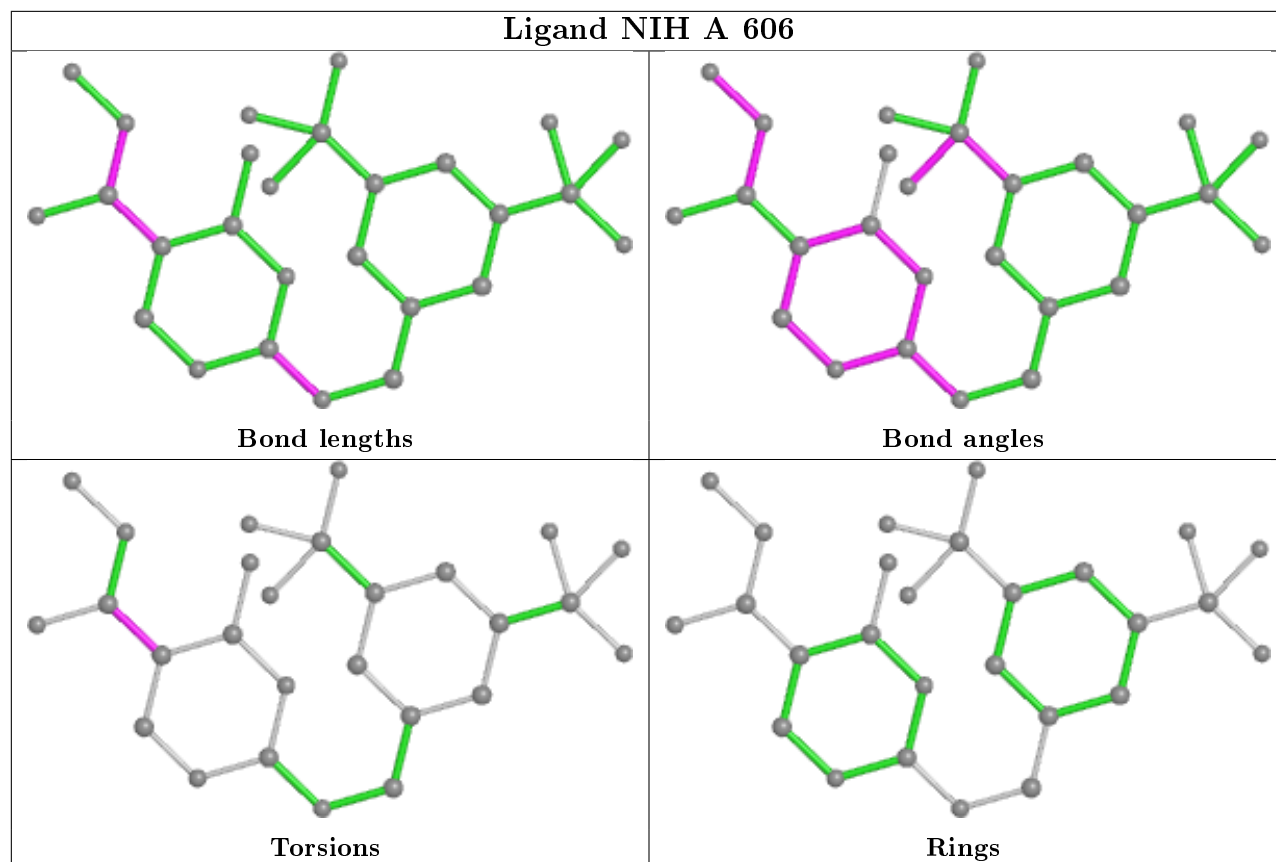
There are no ring outliers.

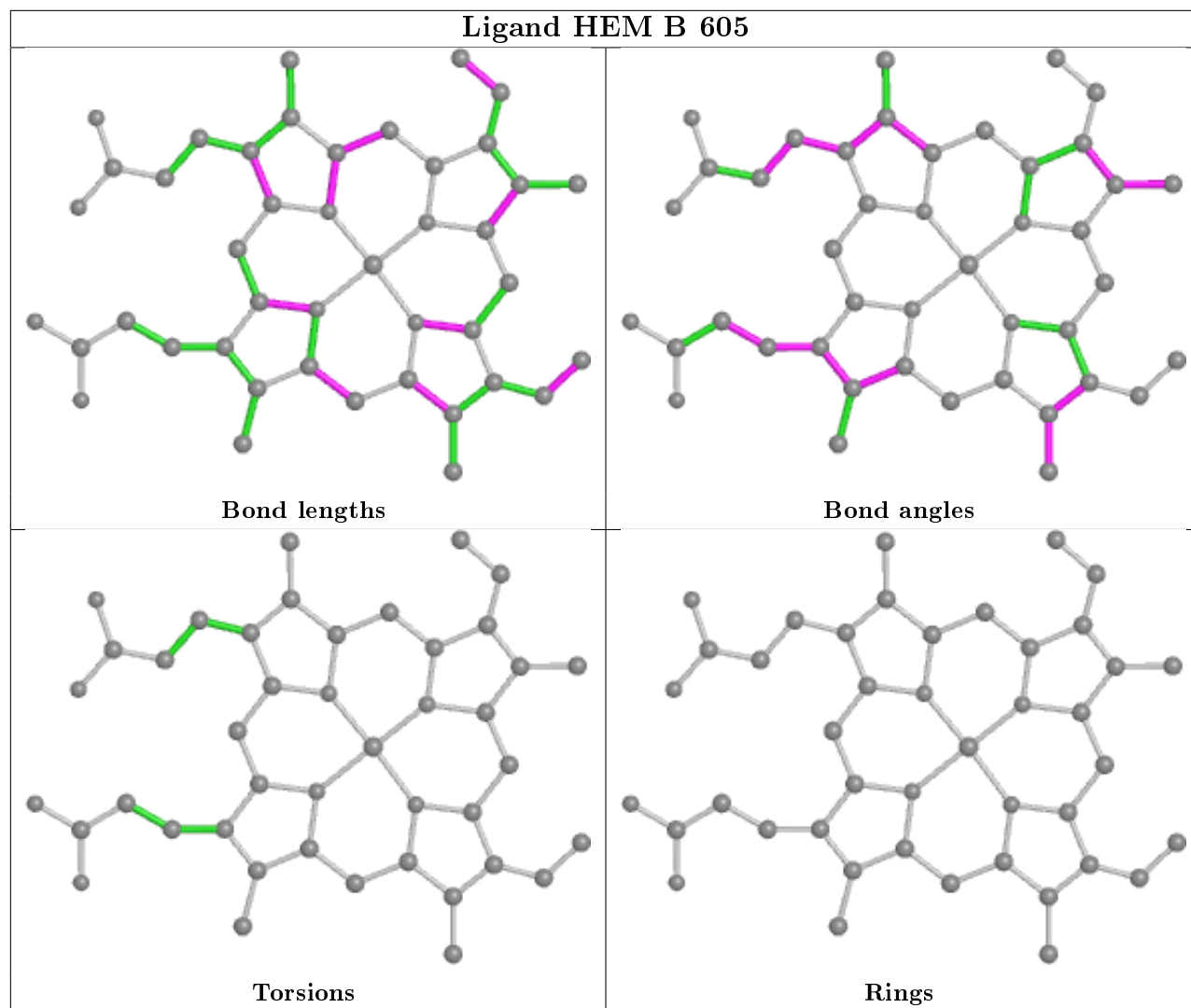
4 monomers are involved in 29 short contacts:

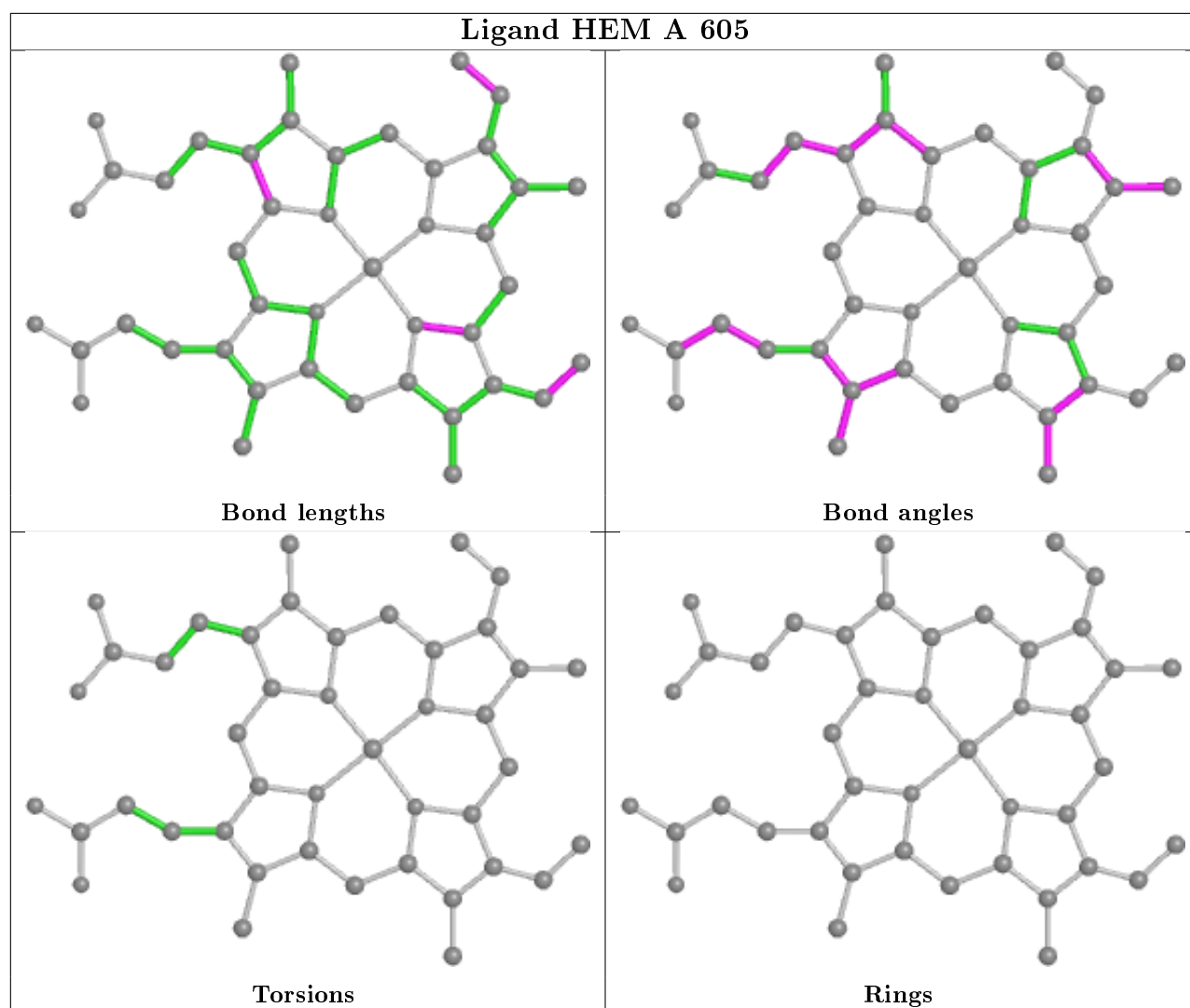
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	NIH	1	0
5	A	606	NIH	1	0
4	B	605	HEM	17	0
4	A	605	HEM	10	0

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	102/108 (94%)	0.36	3 (2%) 51 50	4, 8, 21, 44	0
1	B	105/108 (97%)	0.34	2 (1%) 66 65	6, 11, 26, 35	0
2	C	466/467 (99%)	0.32	7 (1%) 73 72	3, 10, 24, 37	0
2	D	466/467 (99%)	0.52	26 (5%) 24 23	4, 15, 32, 42	0
All	All	1139/1150 (99%)	0.41	38 (3%) 46 45	3, 12, 29, 44	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	11.3
2	D	578	ALA	6.0
2	C	355	PRO	4.7
2	D	217	HIS	4.2
2	D	269	PRO	4.1
2	D	267	LEU	4.0
2	D	113	VAL	3.8
2	C	113	VAL	3.7
2	D	569	ALA	3.6
2	D	270	ARG	3.5
1	B	105	ALA	3.3
2	D	565	SER	3.3
2	D	579	SER	3.3
1	A	4	GLN	3.1
2	D	218	ASP	3.1
2	C	569	ALA	3.0
2	D	355	PRO	2.9
2	C	578	ALA	2.9
2	D	541	THR	2.8
2	C	216	LEU	2.8
2	D	568	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	190	MET	2.7
2	C	217	HIS	2.6
1	B	2	PRO	2.5
2	D	119	CYS	2.5
2	D	350	TYR	2.4
2	D	410	VAL	2.3
2	D	567	LEU	2.3
2	D	141	ALA	2.3
2	D	356	ASN	2.2
2	D	271	TRP	2.2
2	D	193	GLN	2.2
2	D	543	ILE	2.2
2	D	227	SER	2.2
2	D	185	ARG	2.1
2	C	549	ASN	2.1
1	A	5	ASP	2.1
2	D	262	THR	2.0

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

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	D	150	7/8	0.94	0.12	8,10,16,19	0
2	CSO	C	150	7/8	0.96	0.11	5,6,10,12	0

## 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<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.

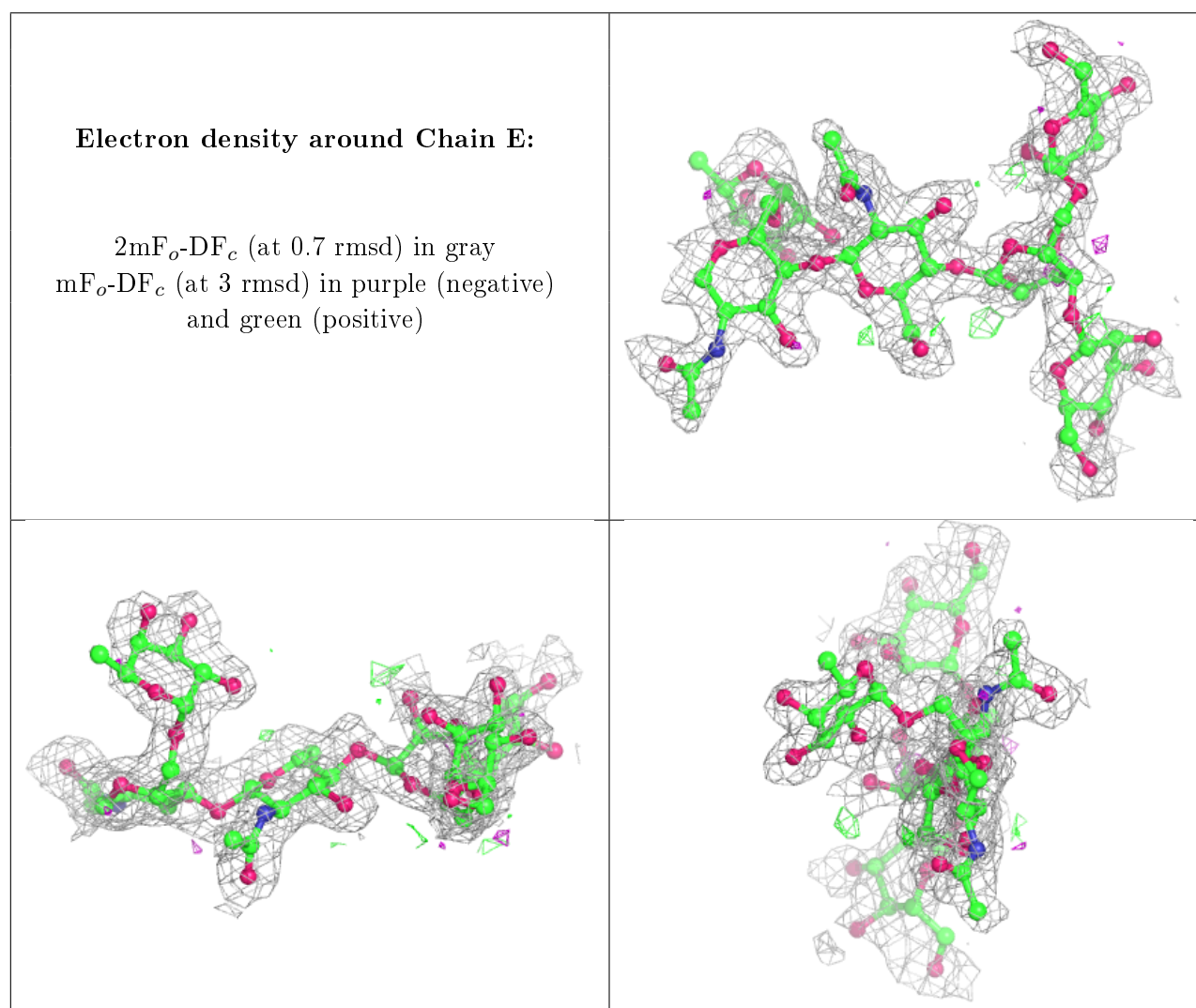
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	F	4	11/12	0.42	0.33	36,43,46,46	0
3	MAN	F	5	11/12	0.61	0.24	21,24,25,29	0
3	MAN	E	4	11/12	0.70	0.26	36,42,46,48	0
3	BMA	F	3	11/12	0.70	0.22	24,27,36,41	0

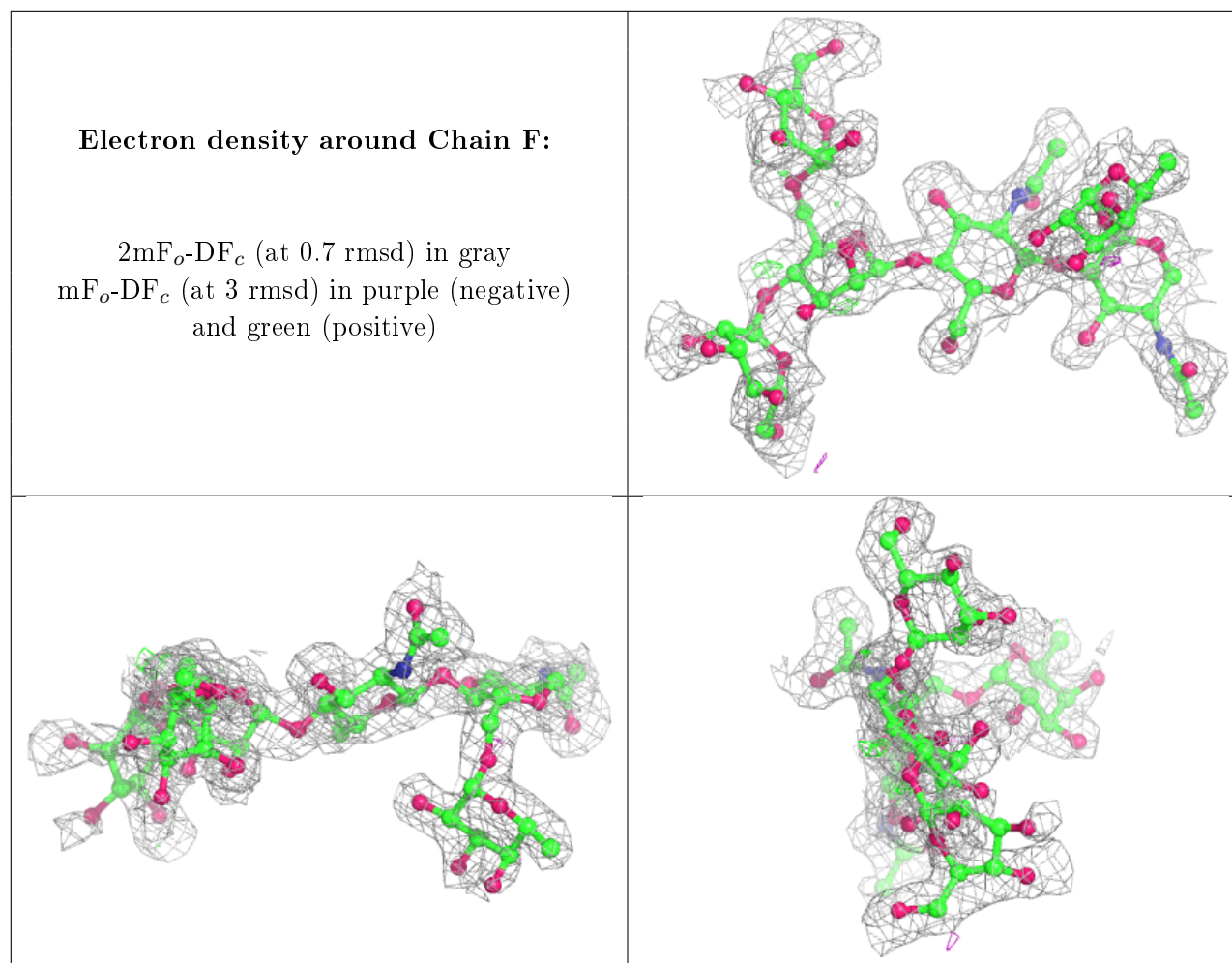
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	E	3	11/12	0.76	0.28	19,23,28,32	0
3	FUC	F	6	10/11	0.83	0.22	23,25,28,30	0
3	MAN	E	5	11/12	0.87	0.13	24,25,27,28	0
3	FUC	E	6	10/11	0.88	0.23	17,20,21,22	0
3	NAG	F	2	14/15	0.89	0.14	9,11,13,17	0
3	NAG	E	2	14/15	0.92	0.14	8,10,12,15	0
3	NAG	F	1	14/15	0.92	0.14	10,12,13,17	0
3	NAG	E	1	14/15	0.92	0.14	10,11,14,15	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 ⓘ

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
10	ACT	D	1582	4/4	0.52	0.27	39,39,40,40	0
6	SO4	B	1003	5/5	0.60	0.40	29,29,31,31	5
7	GOL	D	631	6/6	0.63	0.24	32,34,36,37	0
11	NAG	D	2630	14/15	0.71	0.20	31,34,36,37	0
5	NIH	B	606	27/27	0.78	0.31	10,12,13,14	27
10	ACT	D	1581	4/4	0.78	0.22	22,27,27,28	0
11	NAG	D	2620	14/15	0.83	0.19	22,23,25,27	0
11	NAG	C	1630	14/15	0.83	0.16	19,21,24,25	0
5	NIH	A	606	27/27	0.84	0.30	4,6,7,8	27
10	ACT	D	1583	4/4	0.85	0.14	34,34,34,36	0

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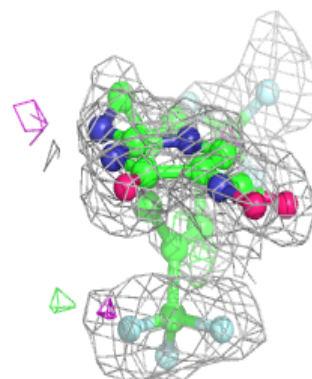
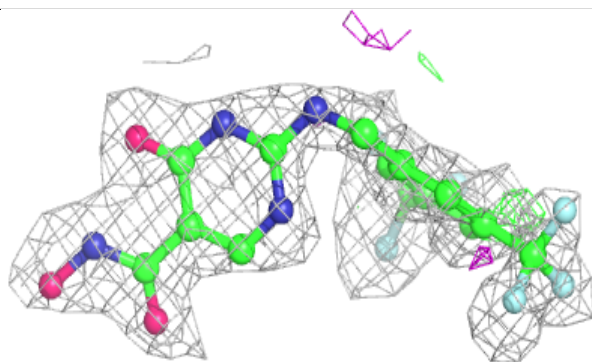
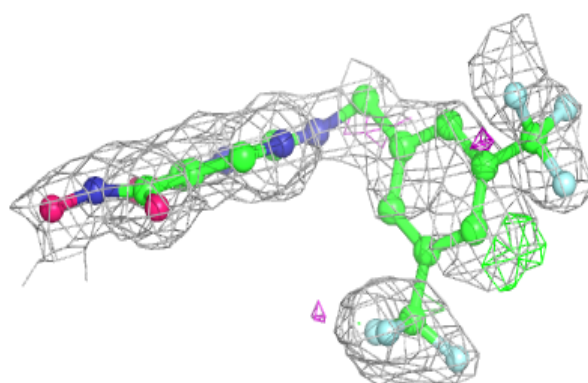
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	C	631	6/6	0.86	0.19	35,39,41,46	0
10	ACT	C	1582	4/4	0.86	0.16	35,37,38,38	0
10	ACT	C	1583	4/4	0.91	0.12	25,26,27,27	0
11	NAG	C	1620	14/15	0.92	0.14	15,17,19,20	0
4	HEM	A	605	43/43	0.93	0.15	4,5,7,10	0
4	HEM	B	605	43/43	0.94	0.14	5,7,9,12	0
6	SO4	C	1581	5/5	0.95	0.16	34,34,36,37	0
8	CA	D	1579	1/1	0.99	0.07	7,7,7,7	0
8	CA	C	1579	1/1	0.99	0.06	4,4,4,4	0
9	CL	D	1580	1/1	0.99	0.13	6,6,6,6	0
9	CL	C	1580	1/1	1.00	0.13	4,4,4,4	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.

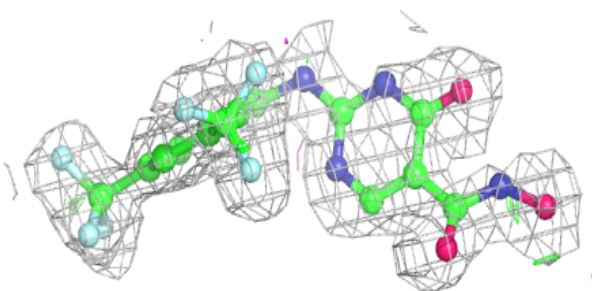
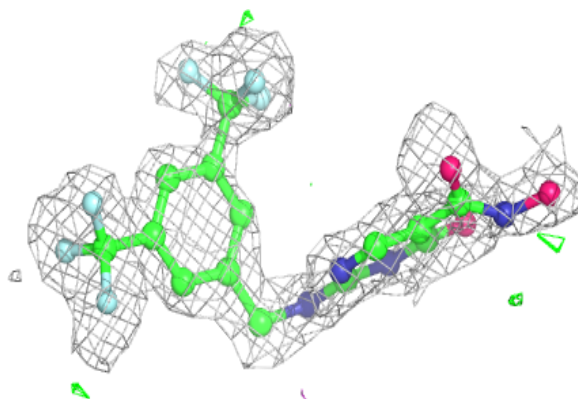
#### Electron density around NIH B 606:

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)



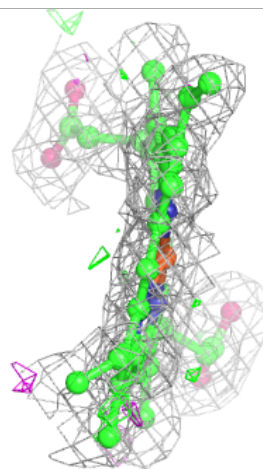
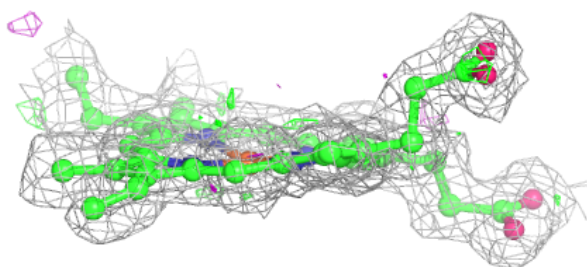
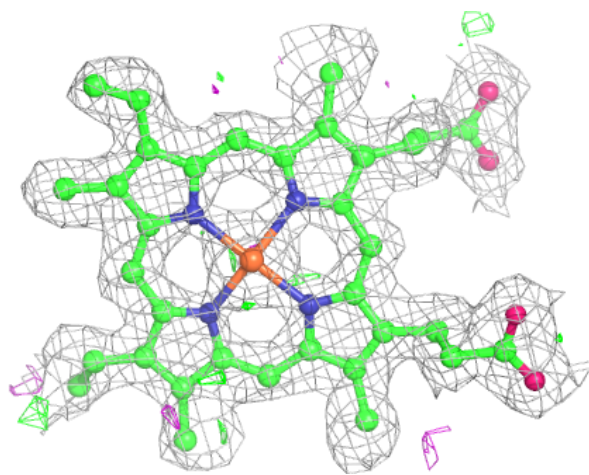
**Electron density around NIH A 606:**

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



**Electron density around HEM A 605:**

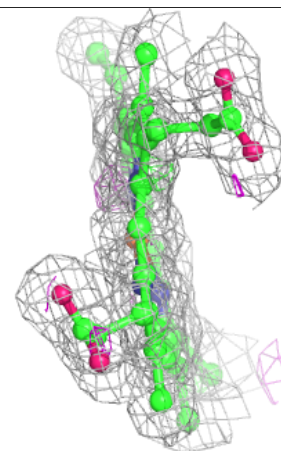
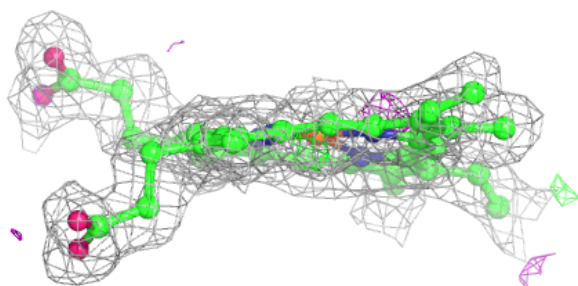
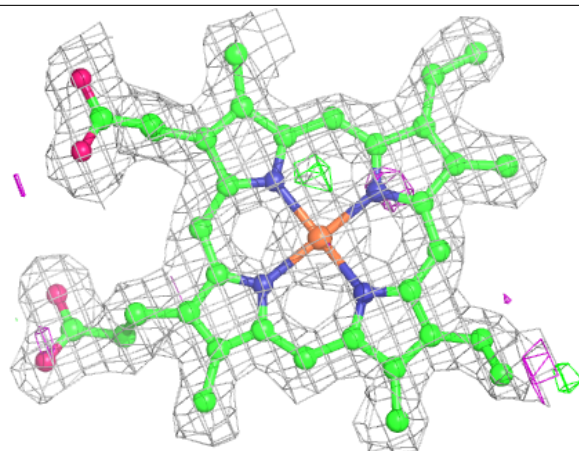
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM B 605:**

$2mF_o-DF_c$  (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.