



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 10:19 AM EDT

PDB ID : 7LAL  
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO) COMPLEX WITH COMPOUND-18 AKA 7-(3-(2,3-DIHYDRO-1H-INDEN-1-YLAMINO)-1-PHENYLPROPYL)-1H-[1,2,3]TRIAZOLO[4,5-B]PYRIDIN-5-AMINE  
Authors : Khan, J.A.  
Deposited on : 2021-01-06  
Resolution : 2.75 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	:	2.18
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)	:	2.18

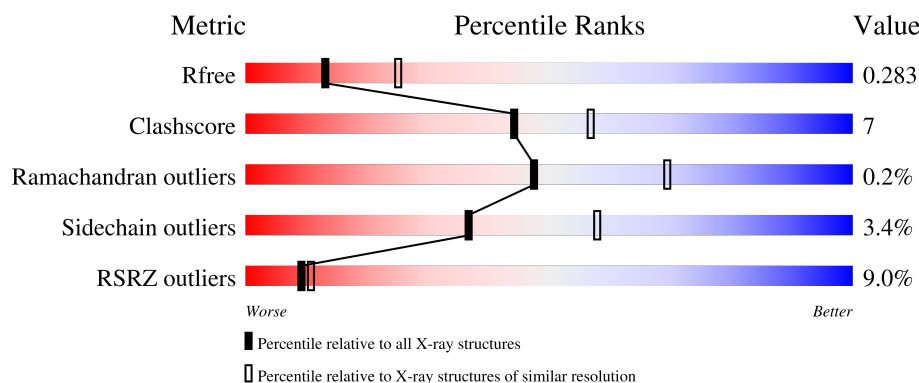
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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.



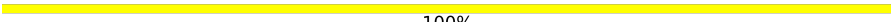
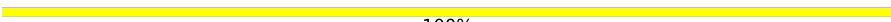
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	105	<div> <div>3%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	D	105	<div> <div>%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
2	B	466	<div> <div>15%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	E	466	<div> <div>6%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
3	C	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	4	 100%
4	G	4	 100%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 9008 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	103	Total	C	N	O	S	0	0	0
			796	506	137	148	5			
1	D	104	Total	C	N	O	S	0	0	0
			815	517	143	150	5			

- Molecule 2 is a protein called Isoform H14 of Myeloperoxidase.

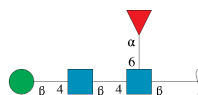
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	5	0	0
			3422	2147	621	630	24			
2	E	465	Total	C	N	O	S	33	0	0
			3642	2304	651	660	27			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called 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.

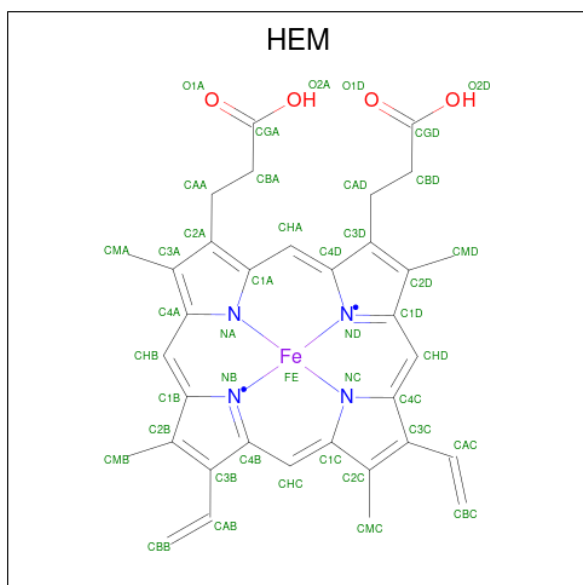


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total 49	C 28	N 2	O 19	0	0	0
4	G	4	Total 49	C 28	N 2	O 19	0	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).

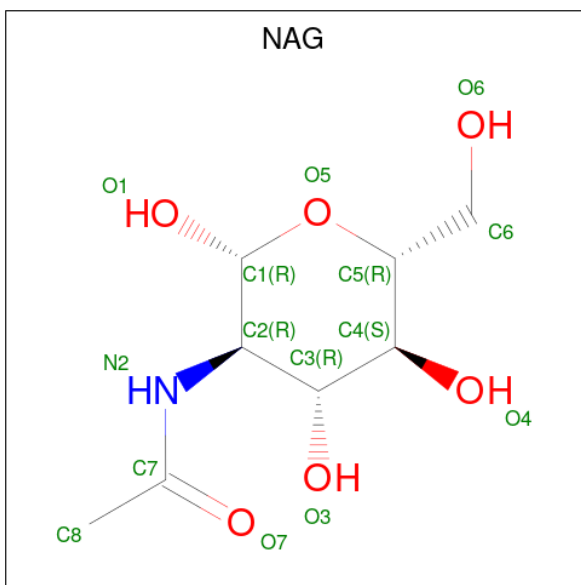


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		

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

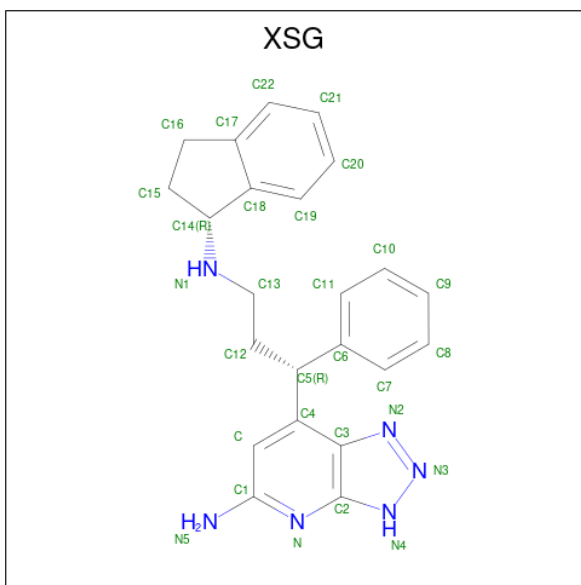
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	E	1	Total	Ca	0	0
			1	1		

- Molecule 9 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
9	E	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is 7-[(1R)-3-{[(1R)-2,3-dihydro-1H-inden-1-yl]amino}-1-phenylpropyl]-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (three-letter code: XSG) (formula:  $C_{23}H_{24}N_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	N	0	0
			29	23	6		

- Molecule 11 is water.

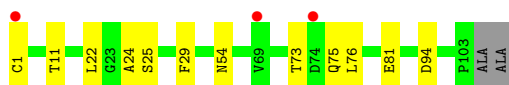
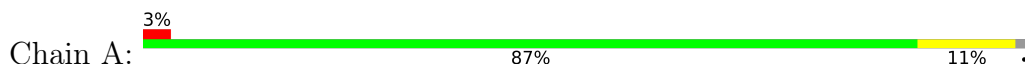
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	O	0	0
			2	2		
11	E	1	Total	O	0	0
			1	1		



### 3 Residue-property plots

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.

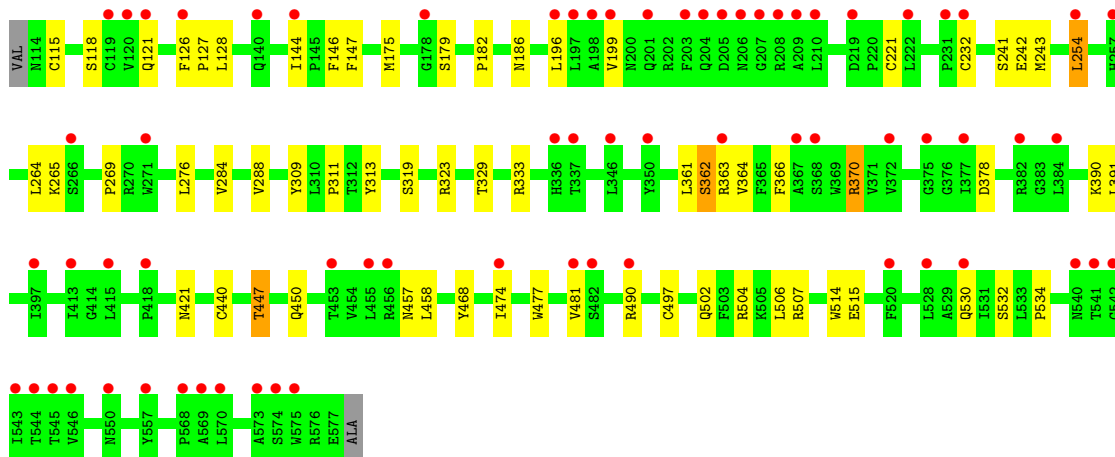
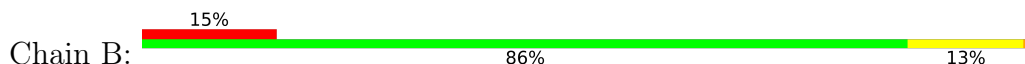
- Molecule 1: Myeloperoxidase light chain



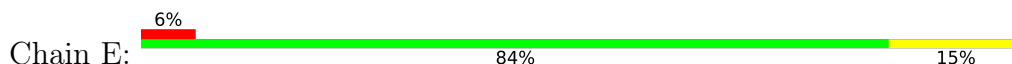
- Molecule 1: Myeloperoxidase light chain

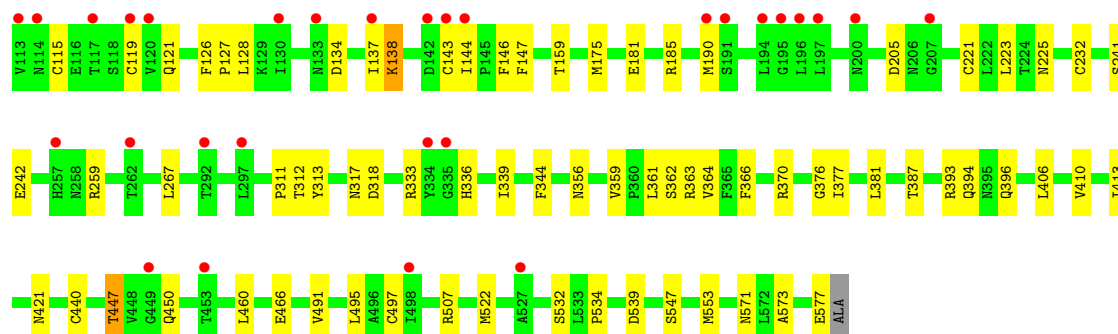


- Molecule 2: Isoform H14 of Myeloperoxidase



- Molecule 2: Isoform H14 of Myeloperoxidase





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

Chain C:  100%

NAG1  
NAG2

- Molecule 4: 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:  100%

NAG1  
NAG2  
BMA3  
FUC4

- Molecule 4: 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 G:  100%

NAG1  
NAG2  
BMA3  
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.72Å 107.72Å 239.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.93 – 2.75 47.10 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.93-2.75) 100.0 (47.10-2.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.227 , 0.270 0.244 , 0.283	Depositor DCC
$R_{free}$ test set	1873 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.9	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: HEM, FUC, BMA, CL, NAG, XSG, MAN, CA

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	0.51	0/821	0.74	0/1123
1	D	0.54	0/840	0.75	0/1148
2	B	0.51	0/3503	0.69	0/4782
2	E	0.52	0/3727	0.70	0/5070
All	All	0.52	0/8891	0.71	0/12123

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	796	0	725	11	0
1	D	815	0	761	6	0
2	B	3422	0	3108	42	0
2	E	3642	0	3556	41	0
3	C	28	0	25	0	0
4	F	49	0	43	4	0
4	G	49	0	42	4	0
5	A	1	0	0	0	0
6	B	43	0	30	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	43	0	30	9	0
7	B	22	0	20	2	0
7	E	22	0	20	4	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
9	E	42	0	38	2	0
10	E	29	0	0	0	0
11	D	2	0	0	0	0
11	E	1	0	0	0	0
All	All	9008	0	8398	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 7.

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)
2:E:317:ASN:HD21	4:G:1:NAG:C1	1.38	1.34
2:E:317:ASN:ND2	4:G:1:NAG:C1	2.14	1.11
7:E:601:MAN:C1	4:F:3:BMA:O3	2.10	0.99
2:E:242:GLU:OE2	6:E:603:HEM:HMB1	1.67	0.95
2:E:225:ASN:HD21	9:E:605:NAG:C1	1.79	0.94
2:E:225:ASN:ND2	9:E:605:NAG:C1	2.32	0.91
2:B:221:CYS:HG	2:B:232:CYS:HG	0.99	0.91
2:B:242:GLU:OE2	6:B:601:HEM:HMB1	1.71	0.90
1:D:94:ASP:OD2	6:E:603:HEM:CMD	2.23	0.86
1:D:94:ASP:OD2	6:E:603:HEM:HMD3	1.76	0.85
2:B:313:TYR:HD1	2:B:507:ARG:HD3	1.42	0.84
2:E:119:CYS:HG	2:E:143:CYS:HG	0.86	0.84
2:E:313:TYR:HD1	2:E:507:ARG:HD3	1.42	0.84
2:B:440:CYS:HG	2:B:497:CYS:HG	1.04	0.83
1:A:94:ASP:OD2	6:B:601:HEM:CMD	2.27	0.82
2:E:221:CYS:HG	2:E:232:CYS:HG	0.84	0.81
1:A:94:ASP:OD2	6:B:601:HEM:HMD3	1.80	0.79
2:B:530:GLN:NE2	2:B:530:GLN:HA	1.98	0.78
2:B:447:THR:HG22	2:B:450:GLN:HG3	1.67	0.76
2:E:447:THR:HG22	2:E:450:GLN:HG3	1.70	0.74
2:B:313:TYR:CD1	2:B:507:ARG:HD3	2.22	0.74
2:E:313:TYR:CD1	2:E:507:ARG:HD3	2.23	0.74
1:A:76:LEU:CD1	2:B:390:LYS:HG3	2.18	0.73
7:B:603:MAN:C1	4:G:3:BMA:H62	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:602:MAN:C1	4:F:3:BMA:H62	2.20	0.72
6:E:603:HEM:HBC2	6:E:603:HEM:HMC2	1.76	0.67
2:B:243:MET:SD	6:B:601:HEM:HAB	2.36	0.65
6:B:601:HEM:HMC1	6:B:601:HEM:HBC2	1.80	0.63
2:B:242:GLU:OE2	6:B:601:HEM:CMB	2.47	0.62
2:B:264:LEU:HD23	2:B:276:LEU:HD23	1.79	0.62
1:A:76:LEU:HD11	2:B:390:LYS:HG3	1.82	0.61
2:E:333:ARG:HH11	2:E:421:ASN:ND2	1.99	0.61
2:B:333:ARG:HH11	2:B:421:ASN:ND2	2.00	0.60
2:B:440:CYS:CB	2:B:497:CYS:HG	2.18	0.57
2:E:394:GLN:HB3	2:E:460:LEU:HD22	1.87	0.57
2:E:363:ARG:O	2:E:370:ARG:NH1	2.38	0.55
2:E:440:CYS:CB	2:E:497:CYS:HG	2.19	0.55
2:B:530:GLN:HA	2:B:530:GLN:HE21	1.72	0.55
2:E:333:ARG:HH11	2:E:421:ASN:HD22	1.54	0.53
2:E:242:GLU:OE2	6:E:603:HEM:CMB	2.48	0.53
2:B:221:CYS:CB	2:B:232:CYS:HG	2.21	0.53
7:E:601:MAN:C1	4:F:3:BMA:C3	2.86	0.53
1:A:11:THR:O	1:A:24:ALA:HA	2.10	0.52
2:E:361:LEU:HA	2:E:364:VAL:HG22	1.92	0.52
1:A:94:ASP:OD2	6:B:601:HEM:HMD2	2.10	0.52
1:D:11:THR:O	1:D:24:ALA:HA	2.10	0.52
2:B:333:ARG:HH11	2:B:421:ASN:HD22	1.56	0.51
1:D:94:ASP:OD2	6:E:603:HEM:HMD2	2.07	0.51
1:D:94:ASP:CG	6:E:603:HEM:HMD3	2.30	0.51
2:E:241:SER:O	2:E:366:PHE:HA	2.11	0.51
2:E:406:LEU:HD21	6:E:603:HEM:HMA1	1.92	0.51
1:A:81:GLU:HB3	2:B:490:ARG:NH2	2.25	0.50
2:E:336:HIS:HA	2:E:339:ILE:HD12	1.93	0.50
2:E:223:LEU:HB2	2:E:410:VAL:HG12	1.94	0.49
2:B:241:SER:O	2:B:366:PHE:HA	2.12	0.49
2:B:311:PRO:O	2:B:507:ARG:NH2	2.38	0.49
2:B:115:CYS:HB2	2:B:147:PHE:CZ	2.49	0.48
2:B:199:VAL:HG12	2:B:254:LEU:HD21	1.95	0.48
2:E:532:SER:HB2	2:E:534:PRO:HD2	1.95	0.48
1:D:81:GLU:O	2:E:553:MET:HG3	2.14	0.48
2:B:361:LEU:HA	2:B:364:VAL:HG22	1.95	0.47
2:E:311:PRO:O	2:E:507:ARG:NH2	2.36	0.47
1:A:22:LEU:HD22	2:B:323:ARG:NE	2.29	0.47
2:E:121:GLN:HG3	2:E:127:PRO:HD2	1.95	0.47
1:A:94:ASP:CG	6:B:601:HEM:HMD3	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:PHE:O	2:B:146:PHE:HB3	2.16	0.46
2:E:128:LEU:HB2	2:E:144:ILE:HB	1.96	0.46
2:E:447:THR:HG22	2:E:450:GLN:CG	2.44	0.46
2:E:126:PHE:O	2:E:146:PHE:HB3	2.16	0.46
2:B:128:LEU:HB2	2:B:144:ILE:HB	1.98	0.46
2:E:137:ILE:HG12	2:E:413:ILE:HD11	1.98	0.46
2:E:333:ARG:HD3	2:E:421:ASN:ND2	2.30	0.46
2:E:134:ASP:O	2:E:138:LYS:HE2	2.15	0.46
2:E:356:ASN:HB3	2:E:359:VAL:HG22	1.97	0.46
6:B:601:HEM:HBC2	6:B:601:HEM:CMC	2.44	0.46
7:B:603:MAN:C1	4:G:3:BMA:C6	2.93	0.45
2:B:121:GLN:HG3	2:B:127:PRO:HD2	1.97	0.45
1:A:29:PHE:CZ	2:B:329:THR:HG21	2.51	0.45
2:B:309:TYR:O	2:B:504:ARG:HD2	2.15	0.45
2:E:205:ASP:OD1	2:E:376:GLY:HA3	2.16	0.45
2:B:333:ARG:HD3	2:B:421:ASN:ND2	2.31	0.45
2:B:532:SER:HB2	2:B:534:PRO:HD2	1.97	0.45
2:E:344:PHE:CD1	2:E:387:THR:HG21	2.51	0.45
2:E:571:ASN:HD21	2:E:573:ALA:HB3	1.81	0.45
2:B:182:PRO:O	2:B:186:ASN:ND2	2.50	0.44
2:E:181:GLU:HG3	2:E:185:ARG:NH1	2.33	0.44
2:B:514:TRP:CE2	2:B:515:GLU:HG3	2.53	0.43
6:E:603:HEM:HBC2	6:E:603:HEM:CMC	2.47	0.43
2:E:115:CYS:HB2	2:E:147:PHE:CZ	2.53	0.43
2:B:447:THR:HG22	2:B:450:GLN:CG	2.43	0.43
2:E:259:ARG:HD2	2:E:539:ASP:HB3	2.00	0.43
2:E:393:ARG:HB2	2:E:396:GLN:HB2	2.02	0.42
2:B:468:TYR:CD2	2:B:474:ILE:HG12	2.56	0.41
2:B:362:SER:H	2:B:362:SER:HG	1.60	0.41
2:B:477:TRP:O	2:B:481:VAL:HG22	2.20	0.41
2:E:491:VAL:HB	2:E:495:LEU:HB2	2.01	0.41
7:E:602:MAN:C1	4:F:3:BMA:C6	2.93	0.41
2:B:502:GLN:O	2:B:506:LEU:HG	2.20	0.41
2:E:377:ILE:HD12	2:E:381:LEU:HD11	2.02	0.41
2:B:265:LYS:HD2	2:B:269:PRO:HA	2.03	0.41
1:A:25:SER:HB3	2:B:179:SER:HB3	2.03	0.41
2:B:363:ARG:O	2:B:370:ARG:NH1	2.54	0.40
2:B:284:VAL:O	2:B:288:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/105 (96%)	97 (96%)	3 (3%)	1 (1%)	15	27
1	D	102/105 (97%)	98 (96%)	4 (4%)	0	100	100
2	B	462/466 (99%)	440 (95%)	21 (4%)	1 (0%)	47	69
2	E	463/466 (99%)	442 (96%)	21 (4%)	0	100	100
All	All	1128/1142 (99%)	1077 (96%)	49 (4%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
2	B	457	ASN

### 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	80/90 (89%)	77 (96%)	3 (4%)	33	53
1	D	84/90 (93%)	81 (96%)	3 (4%)	35	55
2	B	327/411 (80%)	316 (97%)	11 (3%)	37	58
2	E	388/411 (94%)	375 (97%)	13 (3%)	37	58
All	All	879/1002 (88%)	849 (97%)	30 (3%)	37	58

All (30) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	1	CYS
1	A	54	ASN
1	A	73	THR
2	B	118	SER
2	B	175	MET
2	B	196	LEU
2	B	254	LEU
2	B	319	SER
2	B	362	SER
2	B	370	ARG
2	B	378	ASP
2	B	391	LEU
2	B	447	THR
2	B	458	LEU
1	D	1	CYS
1	D	54	ASN
1	D	73	THR
2	E	138	LYS
2	E	159	THR
2	E	175	MET
2	E	190	MET
2	E	267	LEU
2	E	312	THR
2	E	318	ASP
2	E	362	SER
2	E	447	THR
2	E	466	GLU
2	E	522	MET
2	E	547	SER
2	E	577	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	250	HIS
2	B	396	GLN
2	B	421	ASN
2	B	530	GLN
2	B	563	ASN
2	E	225	ASN
2	E	250	HIS
2	E	317	ASN
2	E	421	ASN

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Mol	Chain	Res	Type
2	E	563	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

10 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	C	1	2,3	14,14,15	0.26	0	17,19,21	0.90	1 (5%)
3	NAG	C	2	3	14,14,15	0.34	0	17,19,21	1.56	3 (17%)
4	NAG	F	1	4	14,14,15	0.31	0	17,19,21	0.93	1 (5%)
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	1.11	1 (5%)
4	BMA	F	3	4	11,11,12	0.23	0	15,15,17	0.48	0
4	FUC	F	4	4	10,10,11	0.57	0	14,14,16	1.02	2 (14%)
4	NAG	G	1	4	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	G	2	4	14,14,15	0.33	0	17,19,21	1.25	2 (11%)
4	BMA	G	3	4	11,11,12	0.34	0	15,15,17	0.65	0
4	FUC	G	4	4	10,10,11	0.51	0	14,14,16	0.86	1 (7%)

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	C	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
4	NAG	F	1	4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	FUC	F	4	4	-	-	0/1/1/1
4	NAG	G	1	4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	O5-C1-C2	-4.59	104.04	111.29
4	G	2	NAG	C1-O5-C5	3.73	117.24	112.19
4	F	2	NAG	C1-O5-C5	3.56	117.02	112.19
3	C	1	NAG	O5-C1-C2	3.12	116.22	111.29
3	C	2	NAG	C3-C4-C5	2.93	115.47	110.24
4	F	1	NAG	C1-O5-C5	2.51	115.59	112.19
4	F	4	FUC	C1-O5-C5	2.45	118.33	112.78
4	F	4	FUC	C1-C2-C3	2.40	112.62	109.67
4	G	4	FUC	C1-C2-C3	2.12	112.27	109.67
3	C	2	NAG	C1-C2-N2	2.10	114.08	110.49
4	G	2	NAG	O5-C5-C6	-2.08	103.94	107.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	BMA	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

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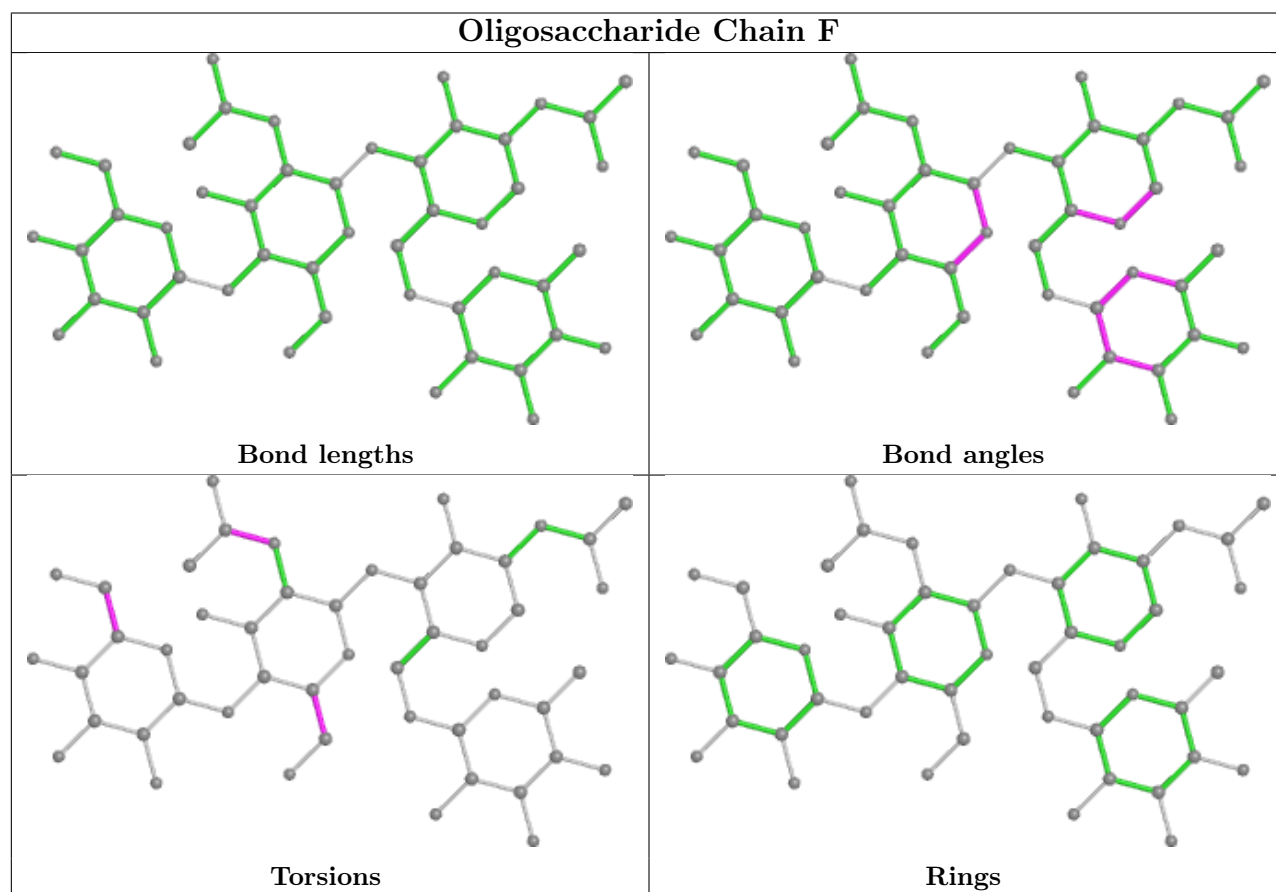
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2

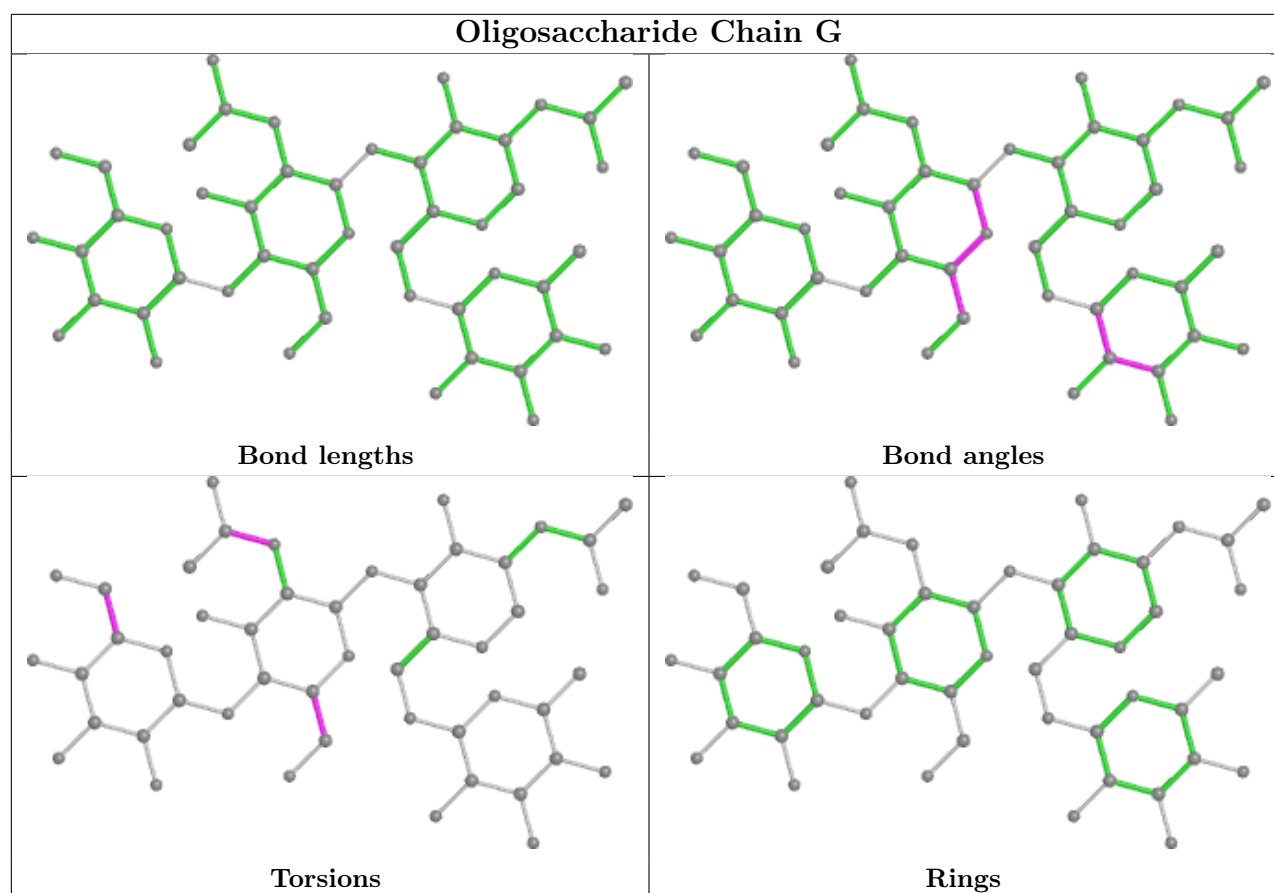
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3	BMA	2	0
4	G	1	NAG	2	0
4	F	3	BMA	4	0

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





## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z  > 2$
7	MAN	B	603	-	11,11,12	0.30	0	15,15,17	0.83	0
7	MAN	B	602	-	11,11,12	0.36	0	15,15,17	0.83	0
9	NAG	E	604	2	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
6	HEM	B	601	2	27,50,50	1.45	3 (11%)	17,82,82	2.19	8 (47%)
7	MAN	E	602	-	11,11,12	0.35	0	15,15,17	0.82	0
9	NAG	E	605	-	14,14,15	0.35	0	17,19,21	1.01	1 (5%)
9	NAG	E	606	-	14,14,15	0.25	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	XSG	E	608	-	31,33,33	1.54	3 (9%)	32,46,46	0.89	1 (3%)
6	HEM	E	603	2	27,50,50	1.67	4 (14%)	17,82,82	2.65	9 (52%)
7	MAN	E	601	-	11,11,12	0.31	0	15,15,17	0.96	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	B	603	-	-	0/2/19/22	0/1/1/1
7	MAN	B	602	-	-	2/2/19/22	0/1/1/1
9	NAG	E	604	2	-	2/6/23/26	0/1/1/1
6	HEM	B	601	2	-	0/6/54/54	-
7	MAN	E	602	-	-	0/2/19/22	0/1/1/1
9	NAG	E	605	-	-	0/6/23/26	0/1/1/1
9	NAG	E	606	-	-	0/6/23/26	0/1/1/1
10	XSG	E	608	-	-	2/14/23/23	0/5/5/5
6	HEM	E	603	2	-	0/6/54/54	-
7	MAN	E	601	-	-	1/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	608	XSG	C2-N4	6.88	1.45	1.34
6	E	603	HEM	C3B-C2B	-6.01	1.32	1.40
6	B	601	HEM	C3B-C2B	-5.46	1.32	1.40
6	E	603	HEM	C3D-C2D	-3.32	1.27	1.37
10	E	608	XSG	C3-N2	2.99	1.43	1.37
10	E	608	XSG	C15-C14	2.81	1.57	1.54
6	E	603	HEM	C1A-CHA	-2.75	1.33	1.41
6	B	601	HEM	C3D-C2D	-2.70	1.29	1.37
6	B	601	HEM	C1A-CHA	-2.47	1.34	1.41
6	E	603	HEM	CMB-C2B	-2.01	1.46	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	603	HEM	CAA-CBA-CGA	5.27	121.51	112.67
6	E	603	HEM	CBA-CAA-C2A	-4.55	104.10	112.49
6	B	601	HEM	CBD-CAD-C3D	-4.28	104.59	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	603	HEM	CBD-CAD-C3D	-4.27	104.62	112.48
6	B	601	HEM	CBA-CAA-C2A	-3.73	105.61	112.49
9	E	605	NAG	O5-C1-C2	3.37	116.61	111.29
7	E	601	MAN	C1-O5-C5	3.29	116.65	112.19
6	E	603	HEM	CMA-C3A-C2A	3.27	131.11	124.94
6	B	601	HEM	C4A-C3A-C2A	-3.10	104.84	107.00
6	E	603	HEM	C4A-C3A-C2A	-3.01	104.90	107.00
6	E	603	HEM	CMA-C3A-C4A	-2.94	123.94	128.46
6	B	601	HEM	CMD-C2D-C1D	2.80	132.76	128.46
10	E	608	XSG	C6-C5-C4	-2.78	106.04	111.73
6	E	603	HEM	CMD-C2D-C3D	-2.72	119.81	124.94
6	E	603	HEM	CMC-C2C-C3C	2.69	129.70	124.68
6	B	601	HEM	CMD-C2D-C3D	-2.60	120.05	124.94
6	B	601	HEM	CMA-C3A-C2A	2.48	129.62	124.94
6	B	601	HEM	CAA-CBA-CGA	2.47	116.81	112.67
9	E	604	NAG	C1-O5-C5	2.36	115.39	112.19
6	E	603	HEM	CMD-C2D-C1D	2.27	131.95	128.46
6	B	601	HEM	CMC-C2C-C3C	2.24	128.86	124.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

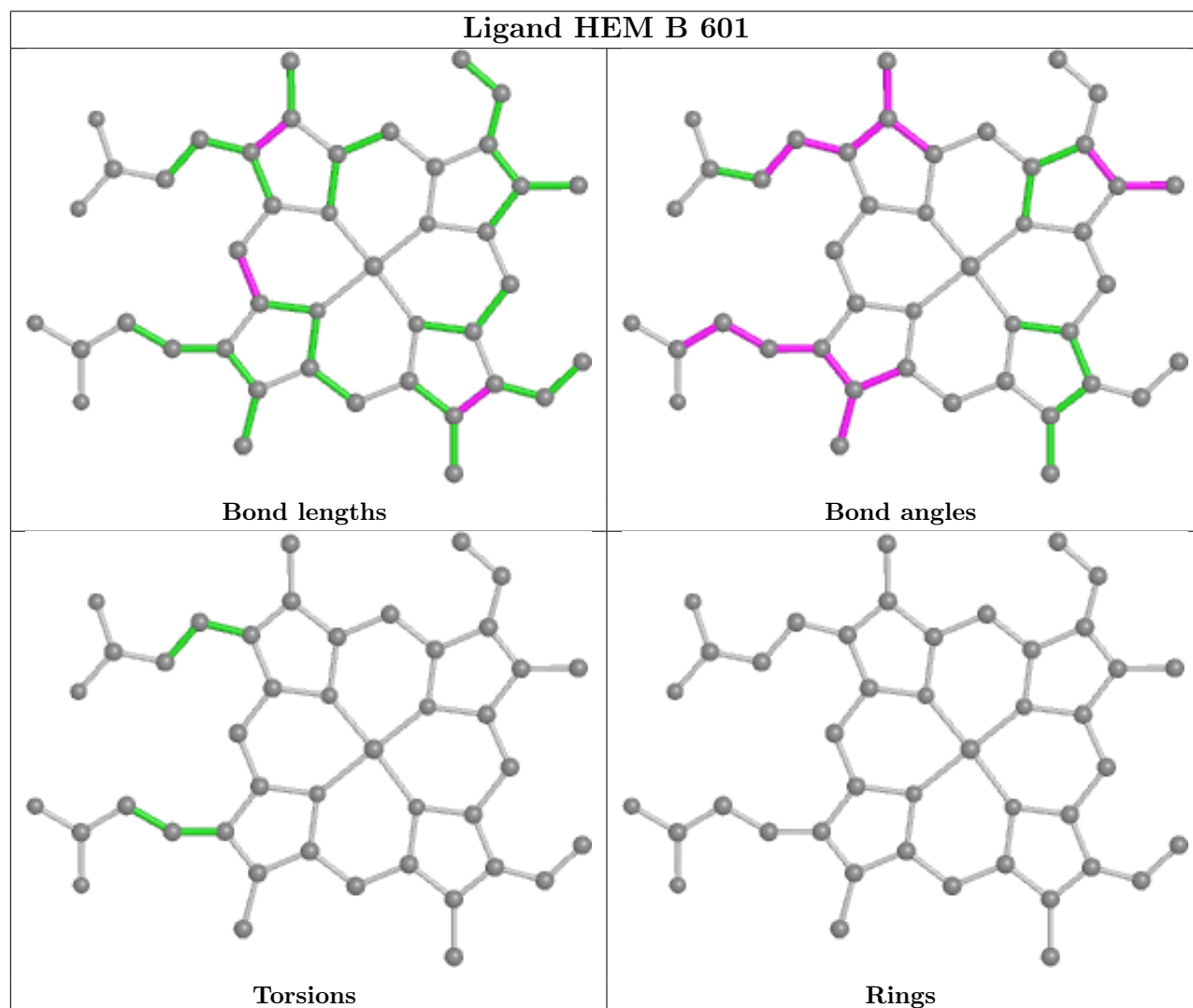
Mol	Chain	Res	Type	Atoms
10	E	608	XSG	C18-C14-N1-C13
7	B	602	MAN	O5-C5-C6-O6
7	B	602	MAN	C4-C5-C6-O6
9	E	604	NAG	C4-C5-C6-O6
10	E	608	XSG	C12-C13-N1-C14
9	E	604	NAG	O5-C5-C6-O6
7	E	601	MAN	O5-C5-C6-O6

There are no ring outliers.

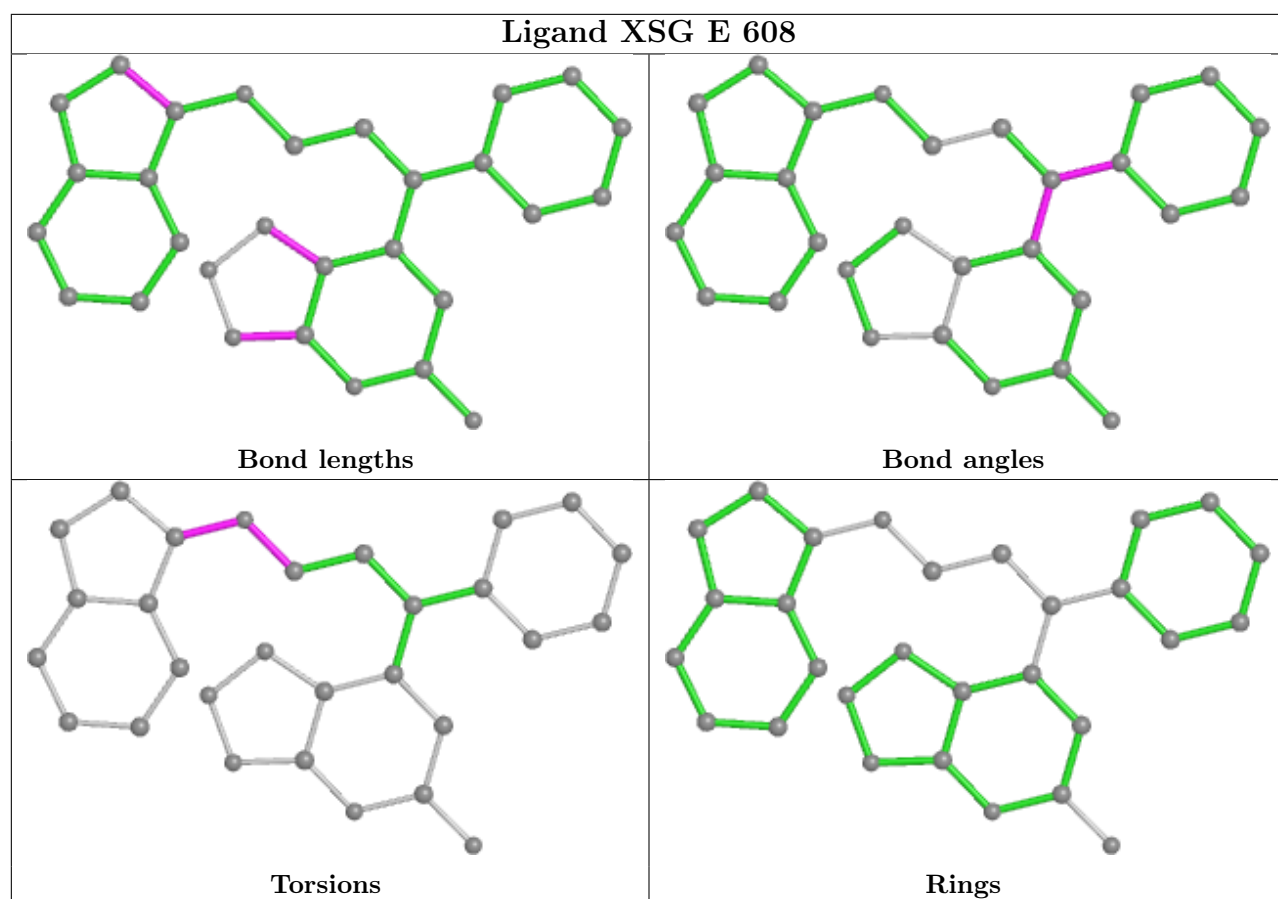
6 monomers are involved in 26 short contacts:

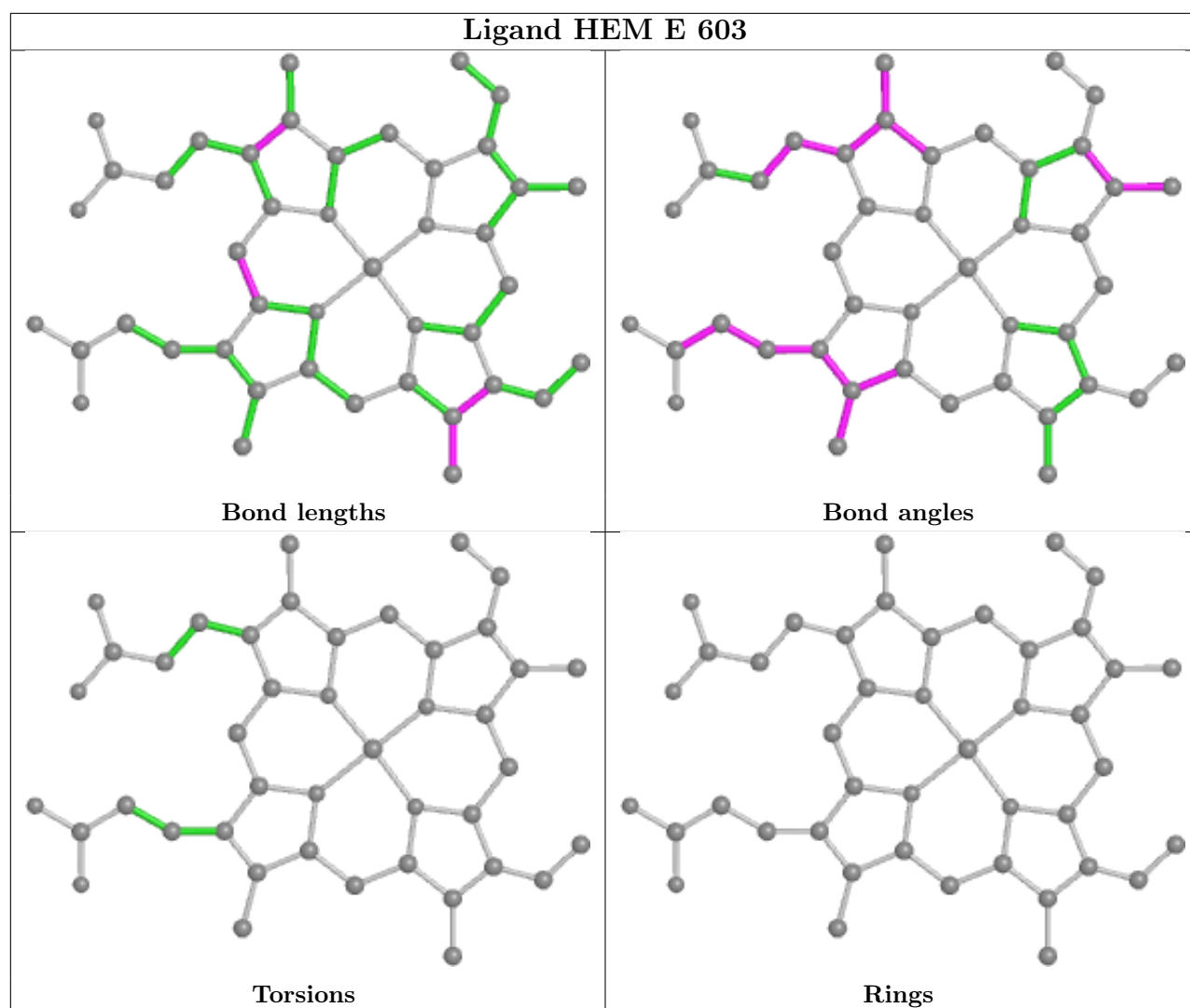
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	603	MAN	2	0
6	B	601	HEM	9	0
7	E	602	MAN	2	0
9	E	605	NAG	2	0
6	E	603	HEM	9	0
7	E	601	MAN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	103/105 (98%)	0.28	3 (2%) 51 61	49, 80, 134, 153	0
1	D	104/105 (99%)	-0.02	1 (0%) 82 87	45, 69, 95, 109	0
2	B	464/466 (99%)	0.76	69 (14%) 2 2	53, 104, 178, 216	2 (0%)
2	E	465/466 (99%)	0.28	29 (6%) 20 25	45, 79, 110, 139	11 (2%)
All	All	1136/1142 (99%)	0.45	102 (8%) 9 11	45, 86, 150, 216	13 (1%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	209	ALA	8.8
2	B	198	ALA	6.9
2	B	384	LEU	6.7
2	B	545	THR	6.1
2	B	210	LEU	5.5
2	B	377	ILE	4.8
2	B	231	PRO	4.6
2	B	542	GLY	4.5
2	B	257	HIS	4.5
2	E	130	ILE	4.5
2	B	543	ILE	4.4
2	B	197	LEU	4.3
2	E	120	VAL	4.3
2	B	254	LEU	4.2
1	A	74	ASP	4.2
2	E	133	ASN	4.1
2	B	119	CYS	4.0
2	B	568	PRO	4.0
2	B	120	VAL	4.0
2	B	196	LEU	3.9
2	B	530	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
2	E	113	VAL	3.8
2	E	207	GLY	3.8
2	B	546	VAL	3.7
2	B	455	LEU	3.7
2	B	456	ARG	3.6
2	B	204	GLN	3.6
2	B	222	LEU	3.5
2	B	413	ILE	3.5
2	B	415	LEU	3.5
2	E	196	LEU	3.4
2	E	117	THR	3.3
2	E	190	MET	3.3
2	B	232	CYS	3.3
2	B	382	ARG	3.3
2	B	490	ARG	3.3
2	B	199	VAL	3.2
2	B	206	ASN	3.1
2	E	453	THR	3.0
2	E	262	THR	3.0
2	B	207	GLY	2.9
2	B	575	TRP	2.9
2	B	203	PHE	2.9
2	B	569	ALA	2.8
2	B	350	TYR	2.8
2	E	143	CYS	2.8
2	B	540	ASN	2.8
2	B	375	GLY	2.8
2	E	191	SER	2.8
2	B	346	LEU	2.8
2	B	140	GLN	2.7
2	B	337	THR	2.7
2	E	114	ASN	2.7
2	B	205	ASP	2.7
2	B	178	GLY	2.7
2	E	449	GLY	2.6
2	B	372	VAL	2.6
2	B	541	THR	2.6
2	E	197	LEU	2.6
2	E	137	ILE	2.6
2	B	481	VAL	2.6
2	B	474	ILE	2.6
2	E	200	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	418	PRO	2.5
2	B	208	ARG	2.5
2	E	292	THR	2.5
2	E	144	ILE	2.5
2	E	194	LEU	2.5
2	E	142	ASP	2.5
2	B	336	HIS	2.5
2	B	482	SER	2.4
2	B	368	SER	2.4
2	B	520	PHE	2.4
2	B	453	THR	2.4
2	B	144	ILE	2.4
2	B	574	SER	2.3
2	B	219	ASP	2.3
1	A	1	CYS	2.3
2	B	121	GLN	2.3
2	E	498	ILE	2.3
2	B	266	SER	2.2
2	B	271	TRP	2.2
2	B	367	ALA	2.2
2	B	544	THR	2.2
2	E	195	GLY	2.2
2	B	573	ALA	2.2
2	E	119	CYS	2.2
2	B	397	ILE	2.2
2	B	570	LEU	2.2
2	B	363	ARG	2.1
1	A	69	VAL	2.1
1	D	68	ILE	2.1
2	B	201	GLN	2.1
2	E	257	HIS	2.1
2	E	527	ALA	2.1
2	E	297	LEU	2.1
2	B	126	PHE	2.1
2	E	334	TYR	2.1
2	E	335	GLY	2.1
2	B	528	LEU	2.1
2	B	550	ASN	2.1
2	B	557	TYR	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](#)

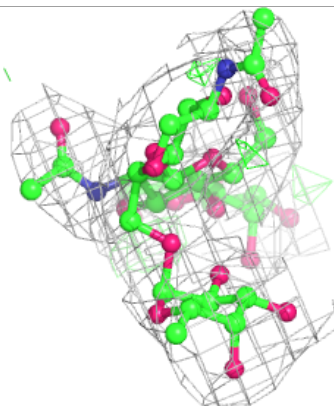
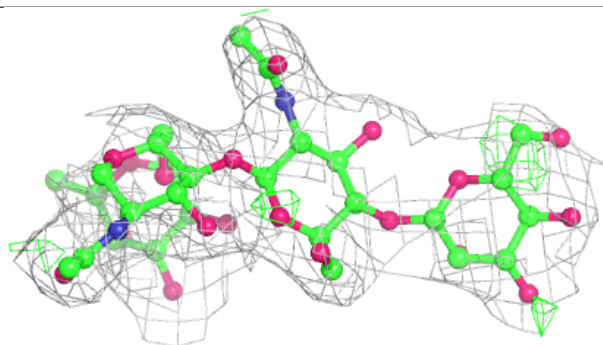
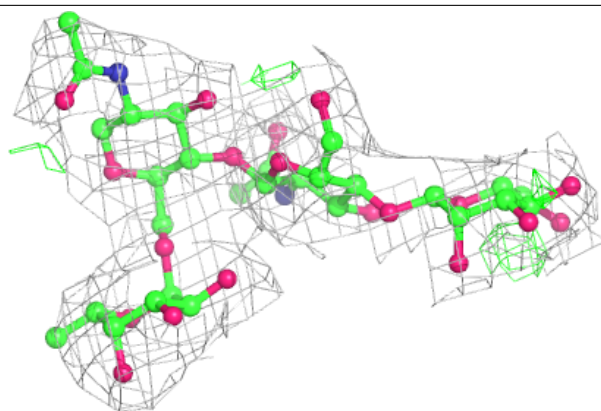
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	C	2	14/15	0.79	0.21	136,147,157,159	0
3	NAG	C	1	14/15	0.81	0.19	124,126,131,138	0
4	BMA	F	3	11/12	0.87	0.25	87,89,93,97	0
4	BMA	G	3	11/12	0.93	0.22	89,100,104,109	0
4	NAG	F	1	14/15	0.94	0.19	72,79,86,88	0
4	FUC	F	4	10/11	0.95	0.23	82,86,91,96	0
4	NAG	F	2	14/15	0.95	0.20	61,68,77,79	0
4	NAG	G	2	14/15	0.97	0.17	51,65,73,76	0
4	NAG	G	1	14/15	0.97	0.17	58,65,75,77	0
4	FUC	G	4	10/11	0.97	0.18	57,69,72,72	0

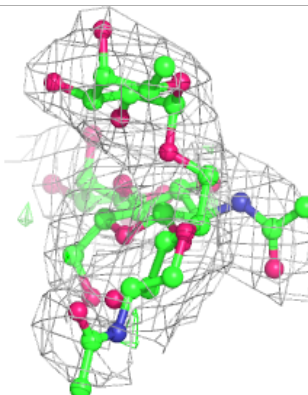
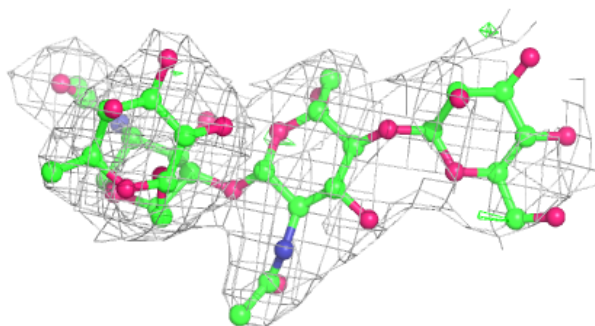
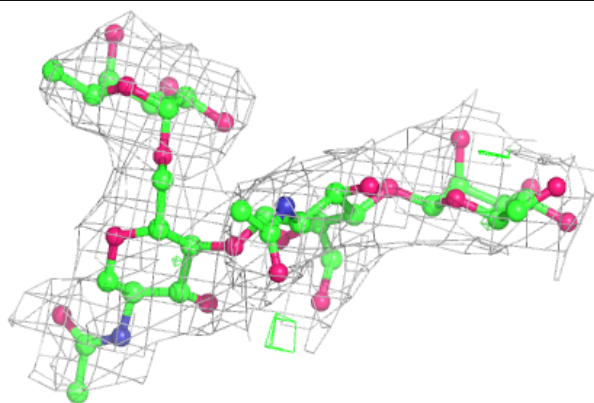
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain F:**

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

**Electron density around Chain G:**

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



## 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.

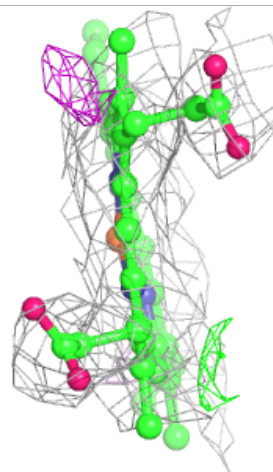
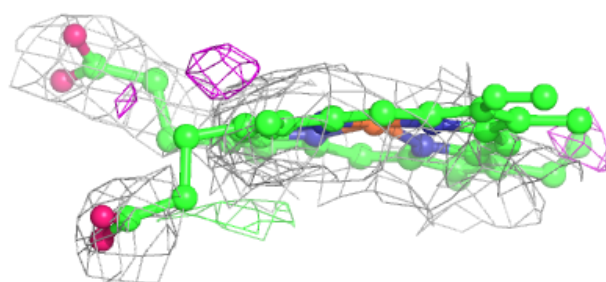
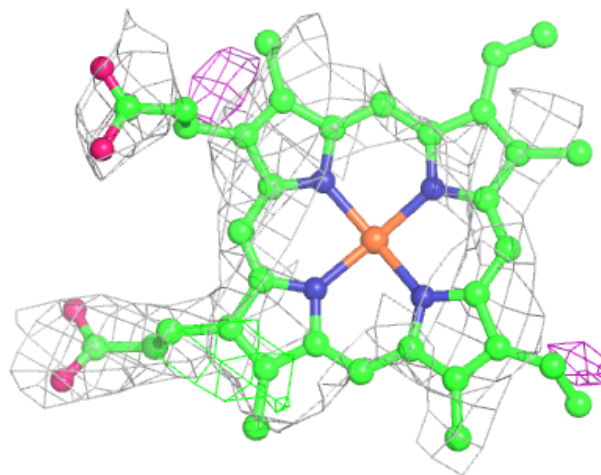
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	NAG	E	606	14/15	0.67	0.20	131,147,161,162	0
7	MAN	E	601	11/12	0.83	0.21	119,123,127,127	0
7	MAN	B	602	11/12	0.85	0.12	106,111,115,122	0
9	NAG	E	605	14/15	0.87	0.15	112,117,126,132	0
9	NAG	E	604	14/15	0.91	0.32	86,97,108,112	0
7	MAN	B	603	11/12	0.93	0.28	76,85,90,92	0
6	HEM	B	601	43/43	0.93	0.26	84,88,97,106	0
7	MAN	E	602	11/12	0.93	0.29	56,73,79,84	0
10	XSG	E	608	29/29	0.93	0.20	56,64,87,87	0
5	CL	A	201	1/1	0.97	0.21	62,62,62,62	0
8	CA	B	604	1/1	0.98	0.20	94,94,94,94	0
8	CA	E	607	1/1	0.98	0.13	58,58,58,58	0
6	HEM	E	603	43/43	0.98	0.19	56,58,64,76	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.



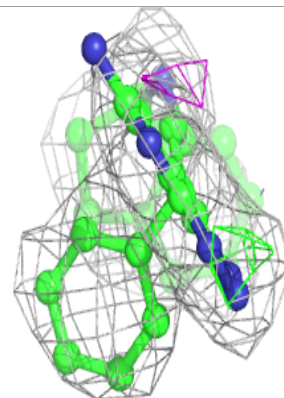
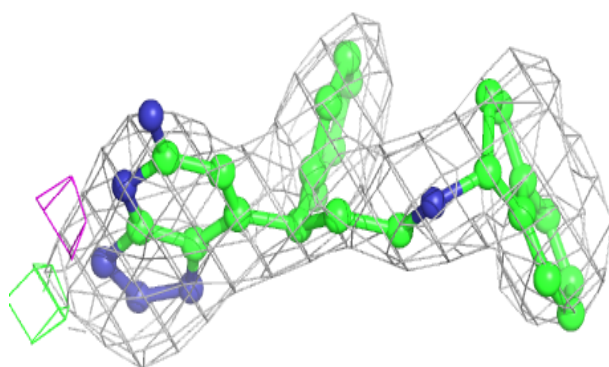
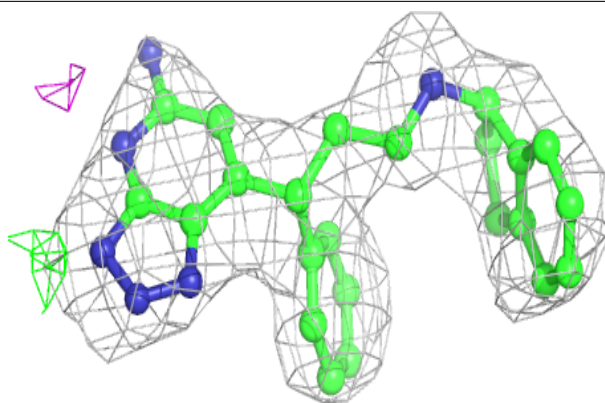
**Electron density around HEM B 601:**

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

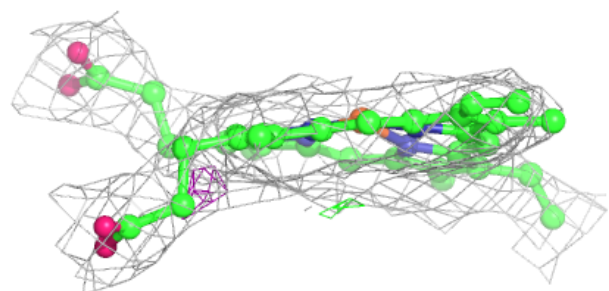
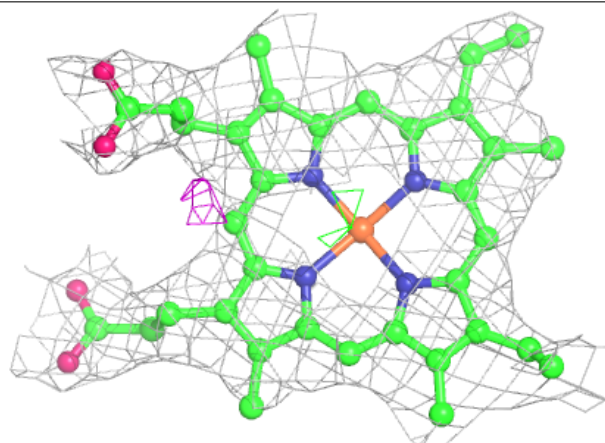


**Electron density around XSG E 608:**

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

**Electron density around HEM E 603:**

$2mF_o-DF_c$  (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.