



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 11:34 pm GMT

PDB ID : 5FIW
Title : CRYSTAL STRUCTURE OF HUMAN MYELOPEROXIDASE AT 1.7
ANGSTROMS RESOLUTION
Authors : Bonnefond, L.; Cavarelli, J.
Deposited on : 2015-10-02
Resolution : 1.70 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (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

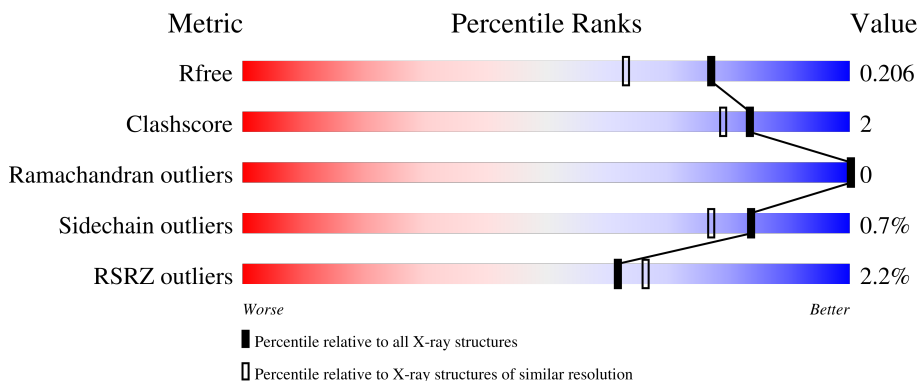
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 4% 97%
1	B	105	 5% 94%
2	C	466	 2% 94% 5%
2	D	466	 2% 94% 5%
3	E	5	 60% 40%

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Mol	Chain	Length	Quality of chain
3	F	5	 20% 80%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10331 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

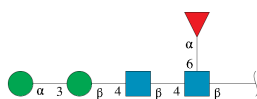
- Molecule 1 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	105	Total 842	C 532	N 149	O 156	S 5	0	0	0
1	B	103	Total 832	C 526	N 147	O 154	S 5	0	0	0

- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	464	Total 3720	C 2343	N 685	O 665	S 27	0	0	0
2	D	464	Total 3720	C 2343	N 685	O 665	S 27	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O			
3	E	5	Total 60	C 34	N 2	O 24	0	0	0
3	F	5	Total 60	C 34	N 2	O 24	0	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

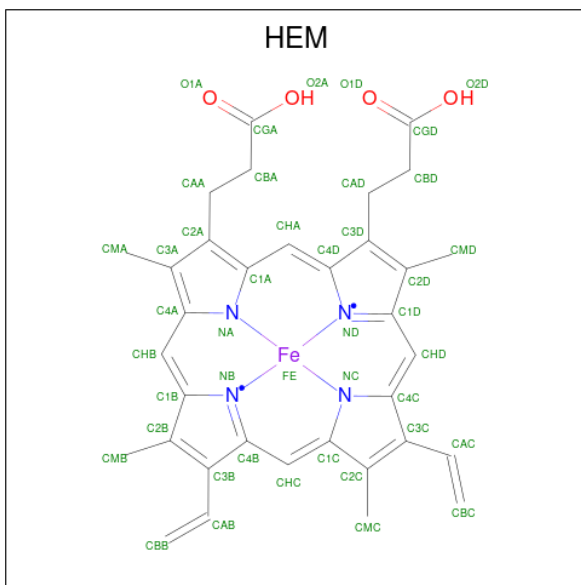
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total 1 Cl 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0
4	D	1	Total Cl 1 1	0	0

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



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

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

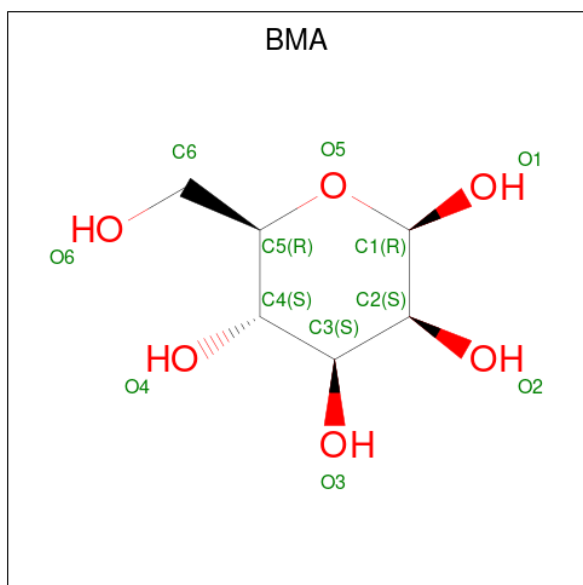
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		

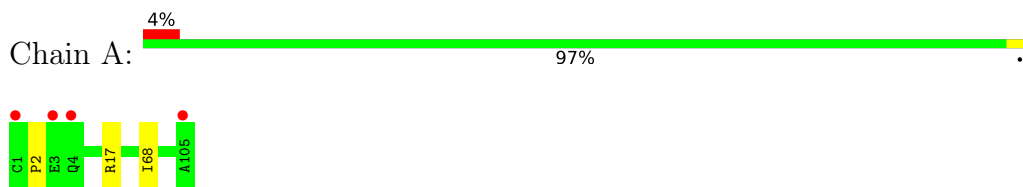
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	129	Total	O	0	0
			129	129		
9	B	118	Total	O	0	0
			118	118		
9	C	334	Total	O	0	0
			334	334		
9	D	345	Total	O	0	0
			345	345		

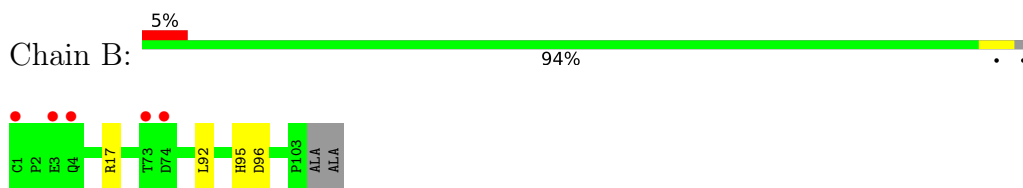
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

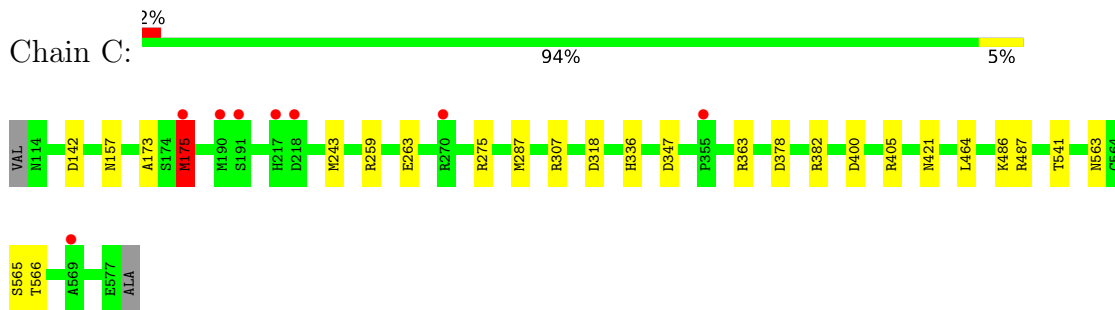
- Molecule 1: MYELOPEROXIDASE



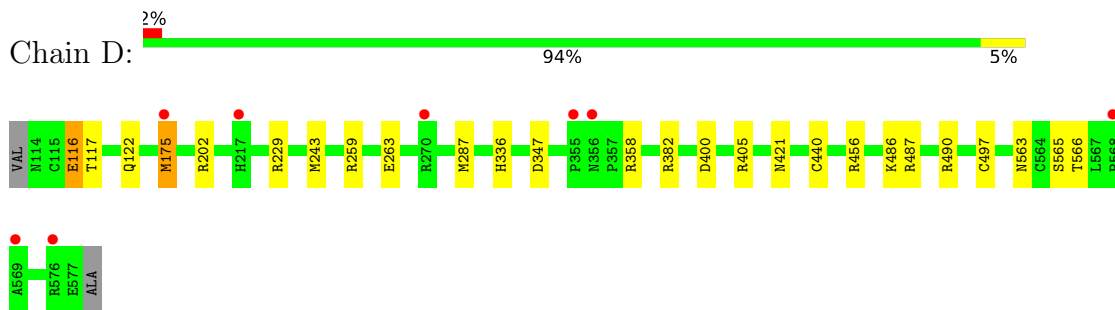
- Molecule 1: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 3: alpha-D-mannopyranose-(1-3)-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-glucopyranos

e

Chain E:  60% 40%

• Molecule 3: alpha-D-mannopyranose-(1-3)-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-glucopyranos
e

Chain F:  20% 80%

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.16Å 105.16Å 225.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.31 – 1.70 52.87 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.31-1.70) 99.8 (52.87-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.163 , 0.193 0.178 , 0.206	Depositor DCC
R_{free} test set	6869 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10331	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, BMA, CA, HEM, CL, MAN, CSO, FUC

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	0.76	0/867	0.91	0/1181
1	B	0.75	0/857	0.94	1/1167 (0.1%)
2	C	0.74	0/3798	0.88	12/5151 (0.2%)
2	D	0.78	4/3798 (0.1%)	0.89	14/5151 (0.3%)
All	All	0.76	4/9320 (0.0%)	0.89	27/12650 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	116	GLU	CD-OE2	9.72	1.36	1.25
2	D	116	GLU	CG-CD	6.16	1.61	1.51
2	D	116	GLU	CB-CG	5.60	1.62	1.52
2	D	175	MET	CA-CB	5.04	1.65	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	243	MET	CG-SD-CE	8.77	114.23	100.20
2	C	243	MET	CG-SD-CE	8.11	113.17	100.20
2	C	175	MET	CG-SD-CE	-6.92	89.14	100.20
2	C	382	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	D	358	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	C	347	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	17	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	D	382	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	D	490	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	D	287	MET	CG-SD-CE	-5.90	90.77	100.20
2	D	382	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	D	229	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	D	175	MET	CB-CG-SD	5.56	129.08	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	287	MET	CG-SD-CE	-5.51	91.39	100.20
2	C	405	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	C	487	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	D	400	ASP	CB-CG-OD1	5.40	123.16	118.30
2	D	456	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	D	487	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	C	142	ASP	CB-CG-OD1	5.36	123.13	118.30
2	D	347	ASP	CB-CG-OD1	5.35	123.12	118.30
2	D	486	LYS	CB-CG-CD	5.31	125.40	111.60
2	C	363	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	D	405	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	C	275	ARG	NE-CZ-NH1	5.05	122.82	120.30
2	C	382	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	C	400	ASP	CB-CG-OD1	5.02	122.82	118.30

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	842	0	803	3	0
1	B	832	0	793	8	0
2	C	3720	0	3713	9	0
2	D	3720	0	3713	13	0
3	E	60	0	53	5	0
3	F	60	0	53	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	43	0	30	0	0
5	B	43	0	30	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	C	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	28	0	26	0	0
8	C	11	0	10	3	0
8	D	11	0	10	3	0
9	A	129	0	0	0	0
9	B	118	0	0	1	0
9	C	334	0	0	2	0
9	D	345	0	0	5	0
All	All	10331	0	9260	39	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 2.

All (39) 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)
8:C:644:BMA:C1	3:E:3:BMA:O6	2.00	1.09
8:D:644:BMA:C1	3:F:3:BMA:O6	2.02	1.08
8:C:644:BMA:C1	3:E:3:BMA:C6	2.36	1.03
8:C:644:BMA:C1	3:E:3:BMA:H61	2.00	0.89
8:D:644:BMA:C1	3:F:3:BMA:C6	2.51	0.88
2:D:202:ARG:NH2	9:D:2099:HOH:O	2.07	0.86
2:D:440:CYS:HG	2:D:497:CYS:HG	1.11	0.82
3:E:3:BMA:C3	3:E:4:MAN:C1	2.60	0.80
2:C:157:ASN:ND2	9:C:2060:HOH:O	2.16	0.77
1:B:96:ASP:HB2	2:D:175:MET:HE3	1.66	0.76
3:F:3:BMA:C3	3:F:4:MAN:C1	2.63	0.76
3:F:1:NAG:C6	3:F:5:FUC:C1	2.64	0.75
2:C:336:HIS:HD1	2:C:421:ASN:HD21	1.38	0.71
2:D:336:HIS:HD1	2:D:421:ASN:HD21	1.38	0.71
3:E:3:BMA:O3	3:E:4:MAN:C2	2.44	0.66
3:F:3:BMA:O3	3:F:4:MAN:C2	2.43	0.65
8:D:644:BMA:C1	3:F:3:BMA:H61	2.27	0.64
1:B:92:LEU:HG	2:D:175:MET:HE2	1.80	0.64
1:B:95:HIS:HD2	9:D:2134:HOH:O	1.85	0.59
1:B:92:LEU:O	2:D:175:MET:CE	2.51	0.58
2:C:259:ARG:NH1	2:C:263:GLU:OE2	2.38	0.56
3:F:1:NAG:O6	3:F:5:FUC:C2	2.49	0.55
2:D:259:ARG:NH1	2:D:263:GLU:OE2	2.40	0.54
2:C:563:ASN:OD1	2:C:566:THR:HG23	2.10	0.52
2:D:563:ASN:OD1	2:D:566:THR:HG23	2.10	0.51
2:D:116:GLU:HG3	2:D:117:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:563:ASN:ND2	9:D:2327:HOH:O	2.24	0.50
5:B:605:HEM:HBC2	5:B:605:HEM:HMC1	1.94	0.49
2:C:173:ALA:HA	2:C:175:MET:HE1	1.94	0.49
1:B:92:LEU:HG	2:D:175:MET:CE	2.43	0.48
2:C:563:ASN:ND2	9:C:2313:HOH:O	2.41	0.47
1:B:95:HIS:CD2	9:D:2134:HOH:O	2.65	0.47
1:A:2:PRO:O	1:A:17:ARG:NH1	2.50	0.45
2:D:563:ASN:ND2	9:D:2328:HOH:O	2.48	0.45
1:B:92:LEU:O	2:D:175:MET:HE2	2.16	0.43
1:A:68:ILE:CD1	2:C:464:LEU:HD23	2.49	0.42
1:A:68:ILE:HD13	2:C:464:LEU:HD23	2.00	0.42
1:B:95:HIS:HE1	9:B:2107:HOH:O	2.02	0.41
2:C:378:ASP:OD1	2:C:541:THR:HB	2.21	0.41

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	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
1	B	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
2	C	461/466 (99%)	452 (98%)	9 (2%)	0	100	100
2	D	461/466 (99%)	454 (98%)	7 (2%)	0	100	100
All	All	1126/1142 (99%)	1107 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	90/90 (100%)	90 (100%)	0	100	100
1	B	90/90 (100%)	90 (100%)	0	100	100
2	C	409/410 (100%)	404 (99%)	5 (1%)	71	59
2	D	409/410 (100%)	407 (100%)	2 (0%)	88	83
All	All	998/1000 (100%)	991 (99%)	7 (1%)	84	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	175	MET
2	C	307	ARG
2	C	318	ASP
2	C	486	LYS
2	C	565	SER
2	D	122	GLN
2	D	565	SER

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

Mol	Chain	Res	Type
1	B	95	HIS
2	C	250	HIS
2	C	396	GLN
2	C	523	GLN
2	D	250	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](#)

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	0.85	0	0,6,8	-	-
2	CSO	D	150	2	3,6,7	0.84	0	0,6,8	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	C	150	2	-	0/1/5/7	-
2	CSO	D	150	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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	E	1	3,2	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
3	NAG	E	2	3	14,14,15	1.12	1 (7%)	17,19,21	1.48	4 (23%)
3	BMA	E	3	3	11,11,12	0.96	0	15,15,17	2.69	5 (33%)
3	MAN	E	4	3	11,11,12	0.43	0	15,15,17	1.85	3 (20%)
3	FUC	E	5	3	10,10,11	0.59	0	14,14,16	1.27	3 (21%)
3	NAG	F	1	3,2	14,14,15	0.46	0	17,19,21	2.12	8 (47%)
3	NAG	F	2	3	14,14,15	0.96	1 (7%)	17,19,21	1.33	2 (11%)
3	BMA	F	3	3	11,11,12	1.07	1 (9%)	15,15,17	2.86	6 (40%)
3	MAN	F	4	3	11,11,12	0.61	0	15,15,17	1.93	5 (33%)
3	FUC	F	5	3	10,10,11	0.87	0	14,14,16	0.92	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	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	FUC	E	5	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	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	FUC	F	5	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	-2.33	1.40	1.43
3	E	2	NAG	O5-C1	-2.30	1.40	1.43
3	F	3	BMA	O5-C1	2.02	1.46	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	C1-C2-C3	-7.82	100.06	109.67
3	E	3	BMA	O5-C5-C6	6.17	116.87	107.20
3	E	4	MAN	O5-C1-C2	5.50	119.26	110.77
3	E	3	BMA	C6-C5-C4	-4.78	101.81	113.00
3	E	3	BMA	C1-C2-C3	-4.56	104.06	109.67
3	F	4	MAN	O5-C1-C2	4.27	117.37	110.77
3	F	3	BMA	O5-C5-C6	4.09	113.61	107.20
3	F	2	NAG	C4-C3-C2	-3.74	105.54	111.02
3	F	1	NAG	O4-C4-C5	-3.73	100.04	109.30
3	F	3	BMA	O3-C3-C2	-3.71	102.90	109.99
3	E	3	BMA	O3-C3-C4	-3.60	102.02	110.35
3	E	2	NAG	O3-C3-C4	3.57	118.60	110.35
3	F	4	MAN	C1-O5-C5	3.42	116.83	112.19
3	E	2	NAG	C1-O5-C5	-3.09	108.00	112.19
3	F	1	NAG	O5-C5-C4	-3.05	103.40	110.83
3	F	3	BMA	C1-O5-C5	-3.04	108.07	112.19
3	F	4	MAN	C1-C2-C3	3.01	113.36	109.67
3	F	1	NAG	C3-C4-C5	2.92	115.46	110.24
3	F	1	NAG	O5-C1-C2	-2.90	106.70	111.29
3	F	3	BMA	C2-C3-C4	2.88	115.87	110.89
3	F	1	NAG	O4-C4-C3	-2.76	103.96	110.35
3	F	4	MAN	O2-C2-C1	-2.70	103.62	109.15
3	E	3	BMA	O3-C3-C2	-2.69	104.84	109.99
3	E	5	FUC	O3-C3-C2	-2.59	105.04	109.99
3	E	4	MAN	C1-O5-C5	2.54	115.63	112.19
3	E	2	NAG	C4-C3-C2	-2.50	107.35	111.02
3	F	2	NAG	O5-C1-C2	2.43	115.12	111.29
3	F	3	BMA	C6-C5-C4	-2.41	107.37	113.00
3	F	5	FUC	O5-C1-C2	2.26	114.26	110.77
3	E	5	FUC	O5-C1-C2	2.24	114.24	110.77
3	E	2	NAG	C1-C2-N2	-2.24	106.67	110.49
3	F	1	NAG	C1-O5-C5	2.23	115.22	112.19
3	E	4	MAN	O2-C2-C1	-2.17	104.71	109.15
3	F	1	NAG	C4-C3-C2	-2.14	107.89	111.02
3	F	4	MAN	O4-C4-C3	-2.11	105.47	110.35
3	E	5	FUC	O4-C4-C3	-2.07	105.56	110.35
3	E	1	NAG	O4-C4-C3	-2.04	105.63	110.35
3	F	1	NAG	O7-C7-N2	-2.02	118.23	121.95
3	E	1	NAG	C3-C4-C5	2.02	113.84	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

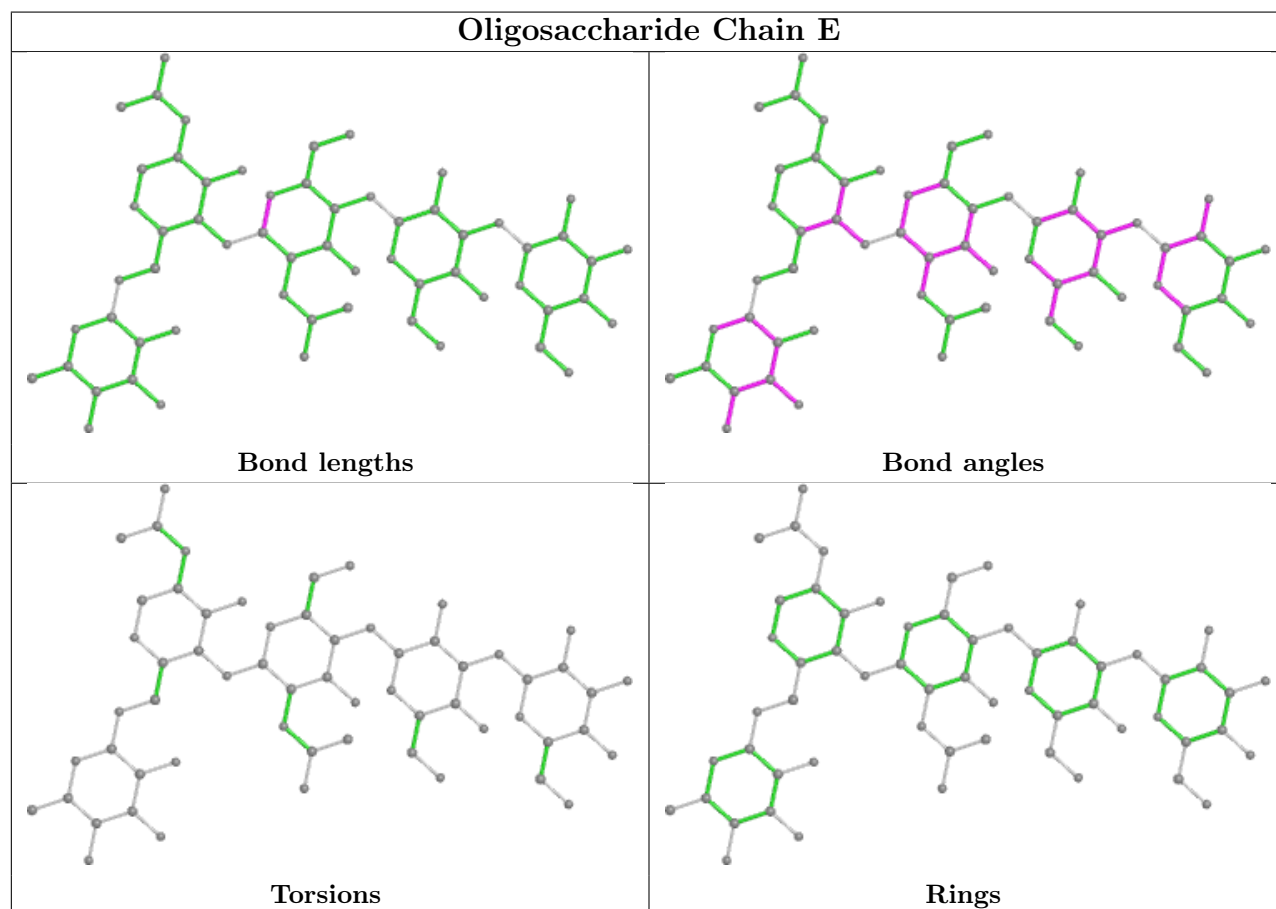
Mol	Chain	Res	Type	Atoms
3	F	3	BMA	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6

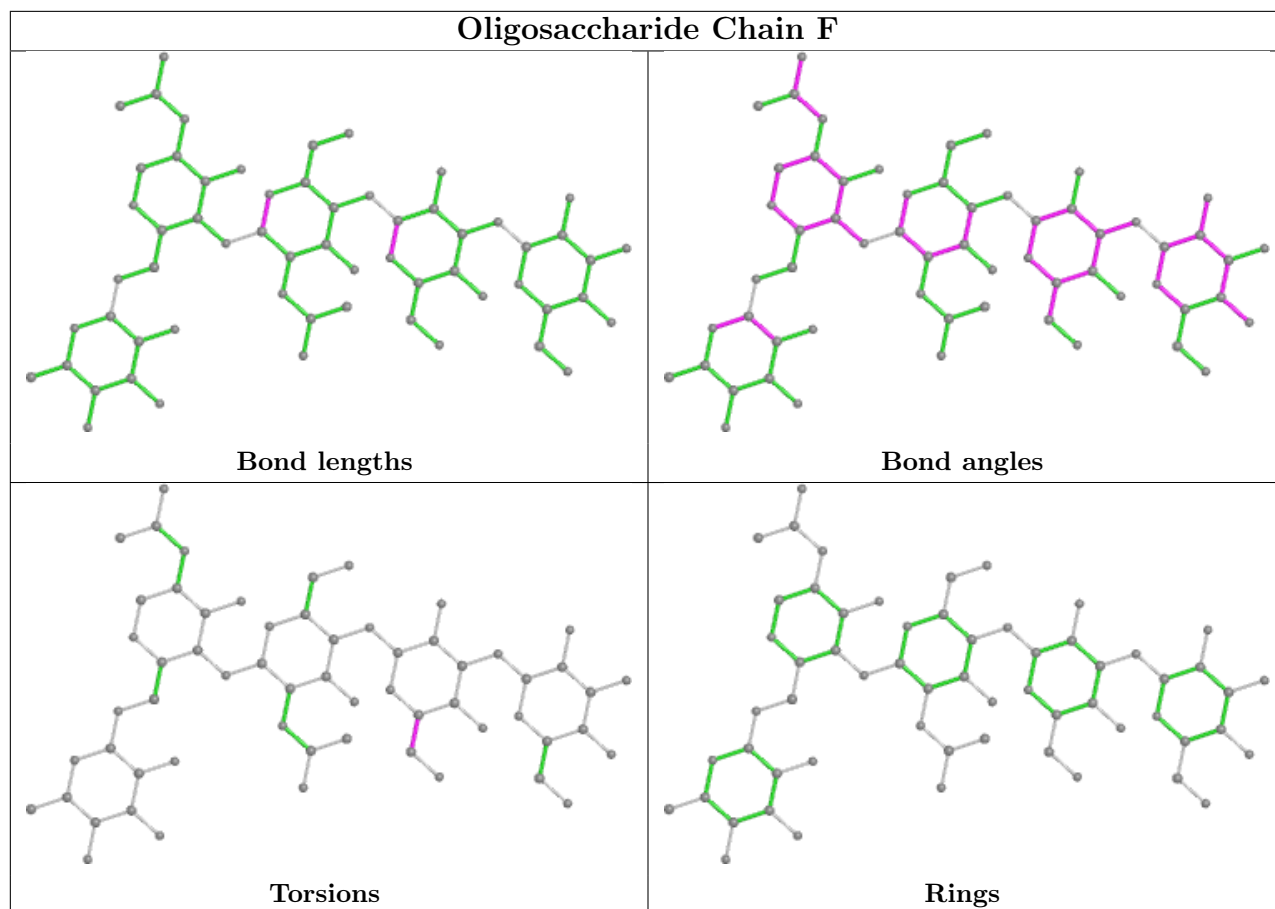
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	BMA	5	0
3	F	1	NAG	2	0
3	F	5	FUC	2	0
3	E	4	MAN	2	0
3	E	3	BMA	5	0
3	F	4	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 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\# Z > 2$
8	BMA	D	644	-	11,11,12	0.71	0	15,15,17	1.17	2 (13%)
8	BMA	C	644	-	11,11,12	0.48	0	15,15,17	1.06	1 (6%)
7	NAG	D	620	2	14,14,15	0.87	0	17,19,21	0.96	1 (5%)
5	HEM	B	605	1,2	41,50,50	1.98	10 (24%)	45,82,82	2.06	17 (37%)
7	NAG	D	630	2	14,14,15	0.48	0	17,19,21	1.52	1 (5%)
5	HEM	A	605	1,2	41,50,50	1.91	11 (26%)	45,82,82	2.26	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	630	2	14,14,15	0.57	0	17,19,21	1.33	2 (11%)
7	NAG	C	620	2	14,14,15	0.83	0	17,19,21	0.96	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	D	644	-	-	0/2/19/22	0/1/1/1
8	BMA	C	644	-	-	0/2/19/22	0/1/1/1
7	NAG	D	620	2	-	0/6/23/26	0/1/1/1
5	HEM	B	605	1,2	-	4/12/54/54	-
7	NAG	D	630	2	-	0/6/23/26	0/1/1/1
5	HEM	A	605	1,2	-	4/12/54/54	-
7	NAG	C	630	2	-	0/6/23/26	0/1/1/1
7	NAG	C	620	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	B	605	HEM	C1B-NB	-5.36	1.31	1.40
5	B	605	HEM	C4D-ND	-4.87	1.31	1.40
5	B	605	HEM	C4D-C3D	4.47	1.52	1.45
5	A	605	HEM	C3B-C4B	4.22	1.53	1.44
5	B	605	HEM	C1A-NA	4.20	1.44	1.36
5	A	605	HEM	C1D-C2D	4.15	1.52	1.44
5	A	605	HEM	C4B-NB	-3.45	1.31	1.38
5	A	605	HEM	FE-NB	3.27	2.13	1.96
5	A	605	HEM	C1A-NA	3.04	1.42	1.36
5	A	605	HEM	C1D-ND	-3.04	1.32	1.38
5	A	605	HEM	CHB-C1B	2.98	1.42	1.35
5	B	605	HEM	FE-NB	2.95	2.11	1.96
5	A	605	HEM	CHA-C4D	2.87	1.42	1.35
5	A	605	HEM	C4D-C3D	2.67	1.49	1.45
5	B	605	HEM	CHB-C1B	2.50	1.41	1.35
5	B	605	HEM	CHA-C4D	2.36	1.41	1.35
5	A	605	HEM	CAB-C3B	2.35	1.53	1.47
5	A	605	HEM	C1B-C2B	2.31	1.49	1.44
5	B	605	HEM	C3B-C4B	2.18	1.49	1.44
5	B	605	HEM	CBD-CGD	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	HEM	CBA-CGA	2.06	1.55	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	HEM	C4B-C3B-C2B	-6.27	102.14	107.11
7	D	630	NAG	C1-C2-N2	-5.36	101.34	110.49
5	A	605	HEM	C4D-ND-C1D	-4.93	99.98	105.07
5	A	605	HEM	C2D-C1D-ND	4.38	115.13	109.88
5	B	605	HEM	C3D-C4D-ND	4.27	114.92	110.17
5	B	605	HEM	CHA-C4D-C3D	-4.00	117.82	125.33
5	B	605	HEM	CBA-CAA-C2A	-3.75	106.22	112.62
5	B	605	HEM	C4B-CHC-C1C	3.74	127.49	122.56
5	B	605	HEM	C4D-ND-C1D	-3.41	101.55	105.07
5	A	605	HEM	CBA-CAA-C2A	-3.32	106.95	112.62
5	A	605	HEM	C3D-C4D-ND	3.26	113.80	110.17
5	A	605	HEM	CHA-C4D-C3D	-3.25	119.23	125.33
7	C	630	NAG	C1-O5-C5	3.23	116.57	112.19
5	A	605	HEM	C3C-C4C-NC	-3.22	104.87	110.94
5	B	605	HEM	CHC-C4B-NB	2.98	127.66	124.43
5	B	605	HEM	CHD-C1D-C2D	-2.97	120.34	124.98
5	A	605	HEM	CHC-C4B-C3B	-2.96	120.03	124.57
5	B	605	HEM	O2D-CGD-CBD	2.86	123.23	114.03
5	B	605	HEM	C4B-C3B-C2B	-2.82	104.88	107.11
5	A	605	HEM	CAB-C3B-C4B	2.76	137.31	124.47
5	B	605	HEM	C2C-C3C-C4C	-2.76	104.97	106.90
5	B	605	HEM	C3C-C4C-NC	-2.73	105.80	110.94
5	A	605	HEM	CHD-C1D-C2D	-2.69	120.77	124.98
5	A	605	HEM	CAB-C3B-C2B	-2.60	120.03	128.60
5	A	605	HEM	C4B-CHC-C1C	2.48	125.83	122.56
5	B	605	HEM	C4D-C3D-C2D	-2.46	103.31	106.90
8	C	644	BMA	O2-C2-C1	-2.41	104.22	109.15
7	C	630	NAG	O6-C6-C5	-2.40	103.04	111.29
5	A	605	HEM	C4D-C3D-C2D	-2.39	103.41	106.90
8	D	644	BMA	C2-C3-C4	-2.38	106.77	110.89
5	B	605	HEM	O2A-CGA-O1A	-2.35	117.44	123.30
5	B	605	HEM	CMC-C2C-C3C	2.34	129.06	124.68
5	A	605	HEM	CBD-CAD-C3D	-2.34	106.13	112.63
5	A	605	HEM	C1D-C2D-C3D	-2.31	104.52	106.96
7	D	620	NAG	O3-C3-C2	-2.24	104.84	109.47
8	D	644	BMA	O2-C2-C1	-2.24	104.58	109.15
5	A	605	HEM	O2A-CGA-O1A	-2.17	117.88	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	HEM	C2D-C1D-ND	2.16	112.47	109.88
5	A	605	HEM	O2A-CGA-CBA	2.15	120.94	114.03
5	A	605	HEM	CAD-C3D-C4D	2.12	128.36	124.66
5	B	605	HEM	CHB-C1B-C2B	-2.10	120.92	126.72
7	C	620	NAG	O4-C4-C3	2.07	115.14	110.35
5	B	605	HEM	CBD-CAD-C3D	-2.07	106.89	112.63
5	A	605	HEM	CMC-C2C-C3C	2.01	128.44	124.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

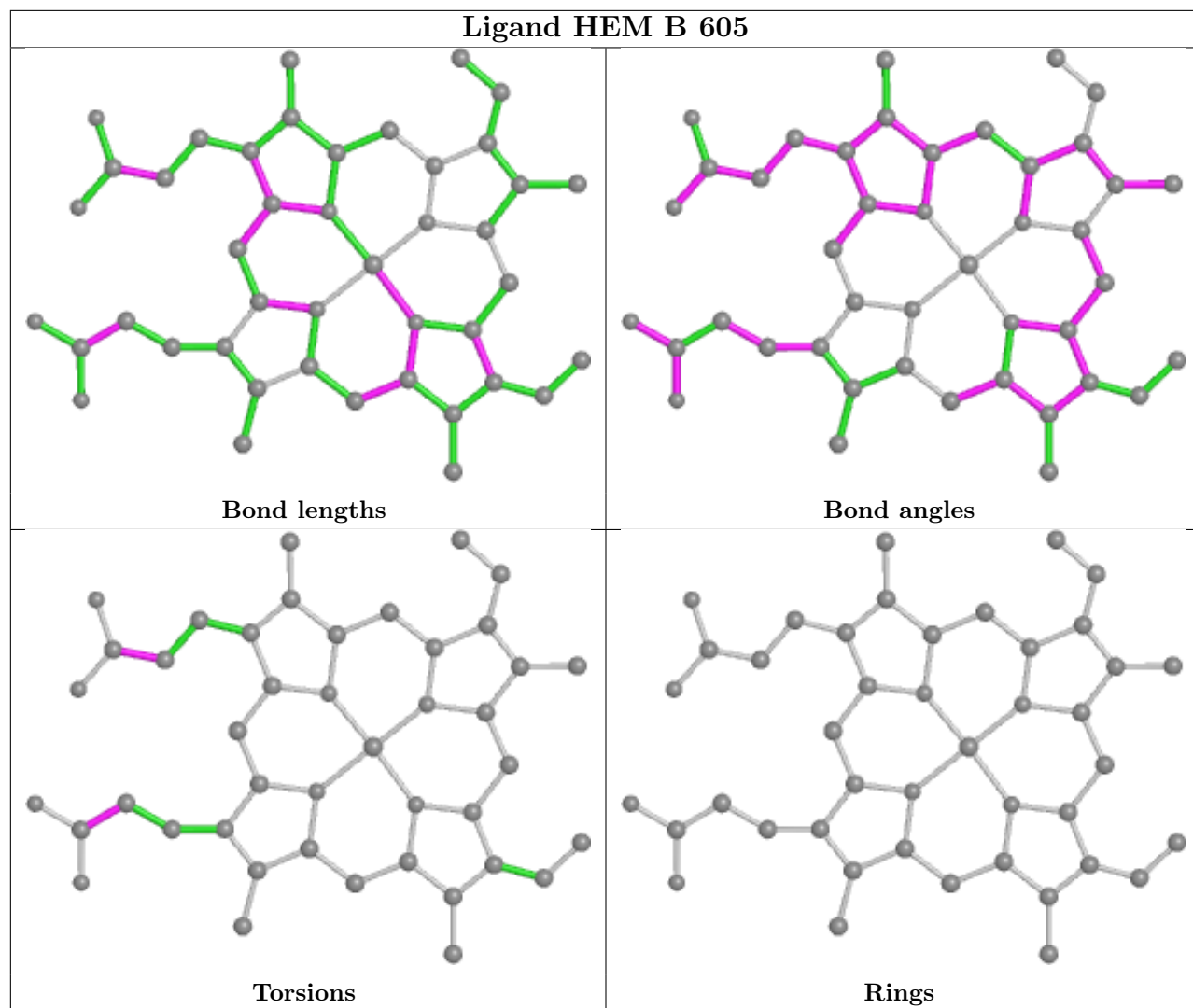
Mol	Chain	Res	Type	Atoms
5	A	605	HEM	CAD-CBD-CGD-O1D
5	B	605	HEM	CAA-CBA-CGA-O2A
5	B	605	HEM	CAD-CBD-CGD-O2D
5	B	605	HEM	CAD-CBD-CGD-O1D
5	A	605	HEM	CAD-CBD-CGD-O2D
5	B	605	HEM	CAA-CBA-CGA-O1A
5	A	605	HEM	CAA-CBA-CGA-O1A
5	A	605	HEM	CAA-CBA-CGA-O2A

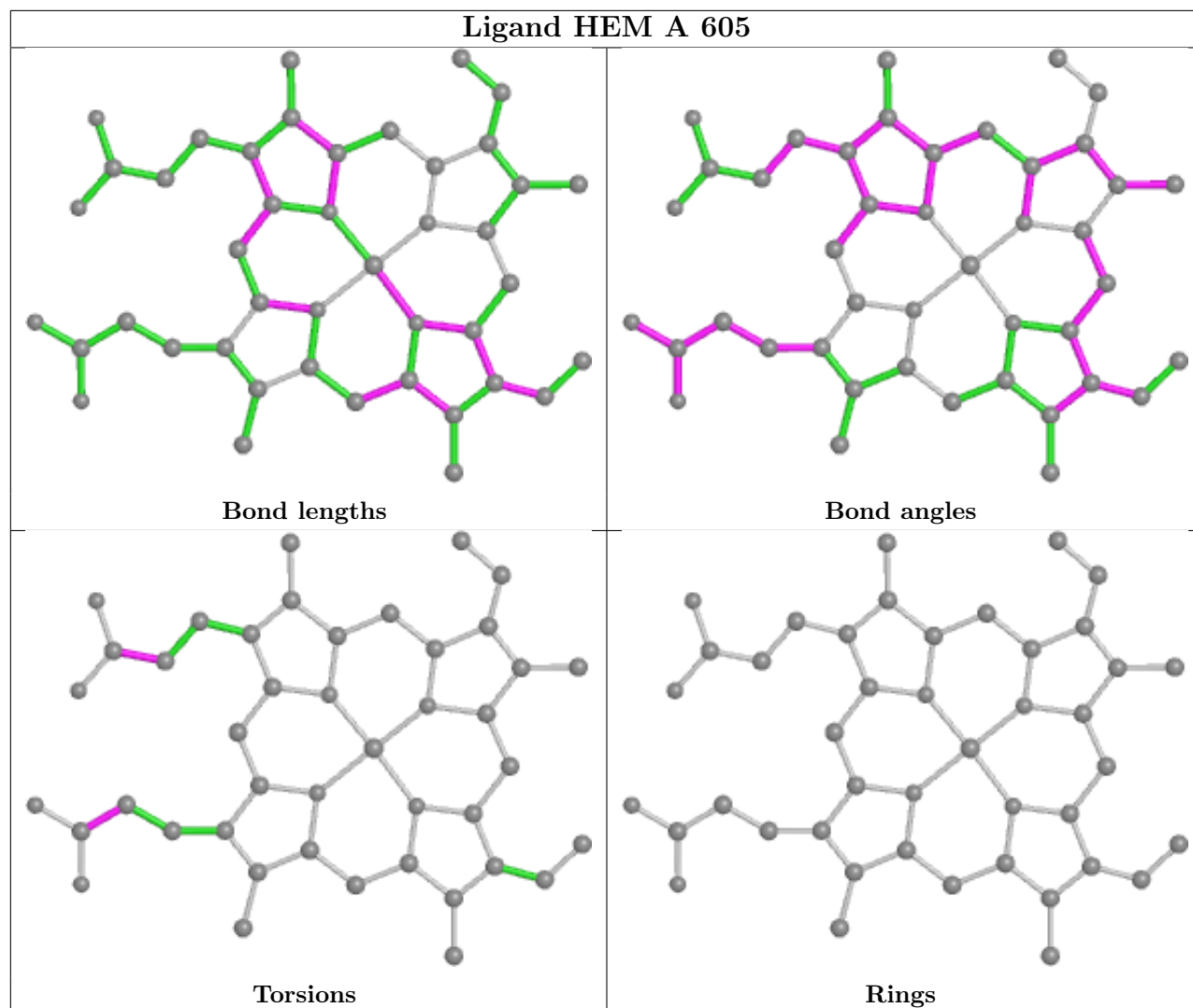
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	644	BMA	3	0
8	C	644	BMA	3	0
5	B	605	HEM	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/105 (100%)	0.26	4 (3%) 40 45	14, 19, 40, 81	0
1	B	103/105 (98%)	0.24	5 (4%) 29 33	14, 19, 41, 74	0
2	C	463/466 (99%)	0.18	8 (1%) 70 74	13, 20, 40, 80	0
2	D	463/466 (99%)	0.18	8 (1%) 70 74	13, 20, 41, 65	0
All	All	1134/1142 (99%)	0.19	25 (2%) 62 66	13, 20, 41, 81	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	355	PRO	4.2
1	A	1	CYS	3.9
1	A	3	GLU	3.8
2	D	569	ALA	3.5
2	C	217	HIS	3.5
2	C	190	MET	3.4
2	C	218	ASP	3.3
2	D	568	PRO	2.9
2	D	217	HIS	2.9
1	B	74	ASP	2.8
1	B	4	GLN	2.8
2	D	576	ARG	2.8
2	C	270	ARG	2.8
2	C	569	ALA	2.6
1	B	1	CYS	2.6
1	A	105	ALA	2.5
1	A	4	GLN	2.5
2	D	356	ASN	2.3
2	D	270	ARG	2.3
2	C	191	SER	2.2
2	D	175	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3	GLU	2.1
2	D	355	PRO	2.1
1	B	73	THR	2.1
2	C	175	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSO	C	150	7/8	0.96	0.09	12,17,26,36	0
2	CSO	D	150	7/8	0.96	0.12	14,16,27,40	0

6.3 Carbohydrates [i](#)

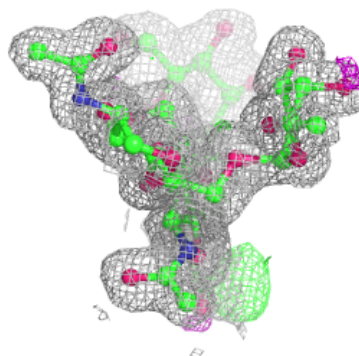
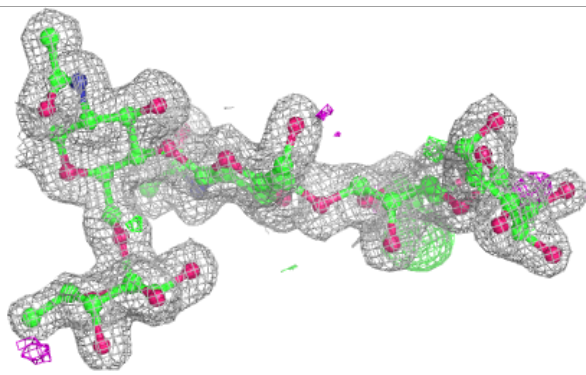
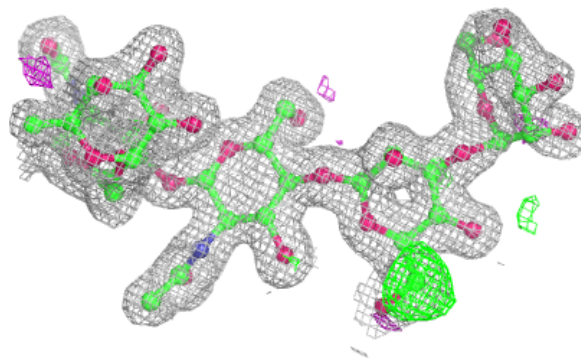
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	4	11/12	0.74	0.21	38,44,51,63	0
3	MAN	E	4	11/12	0.83	0.16	34,39,44,57	0
3	BMA	E	3	11/12	0.85	0.12	17,20,24,71	0
3	FUC	F	5	10/11	0.91	0.10	23,25,27,27	0
3	NAG	F	1	14/15	0.94	0.09	14,17,24,26	0
3	BMA	F	3	11/12	0.94	0.11	16,21,24,63	0
3	NAG	E	1	14/15	0.94	0.09	13,17,27,30	0
3	FUC	E	5	10/11	0.94	0.10	21,24,26,28	0
3	NAG	F	2	14/15	0.96	0.10	12,16,19,19	0
3	NAG	E	2	14/15	0.96	0.09	14,16,18,19	0

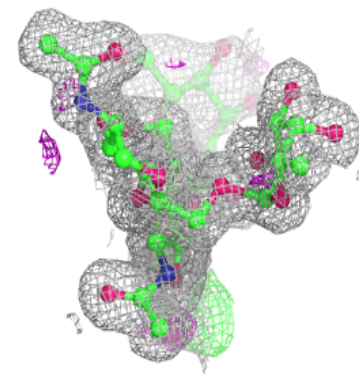
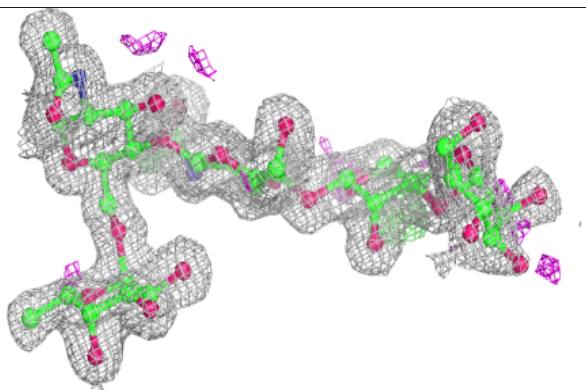
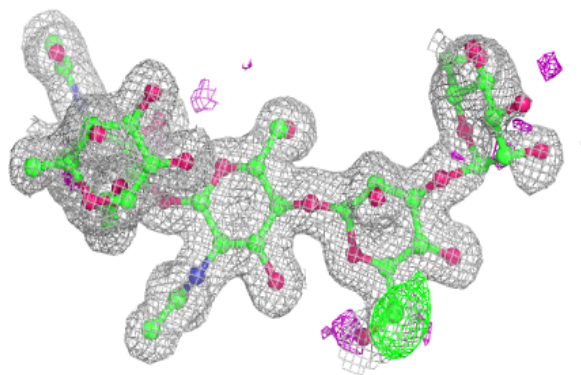
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands

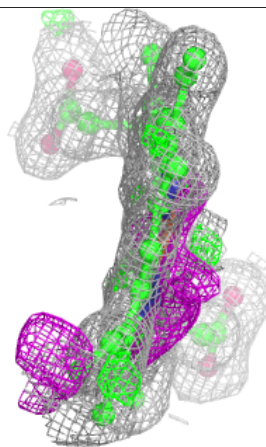
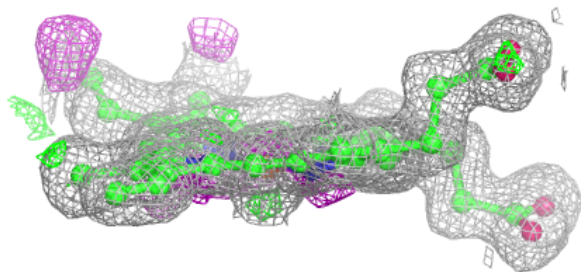
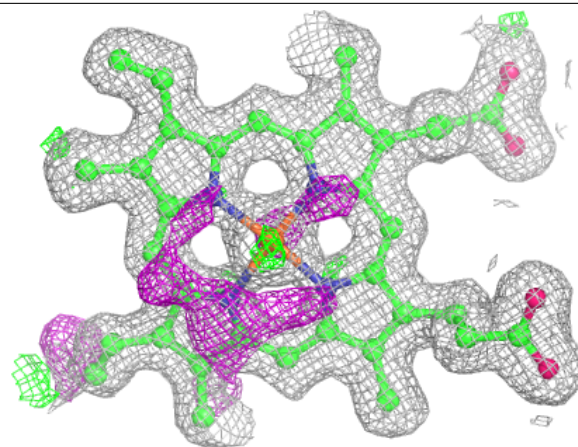
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

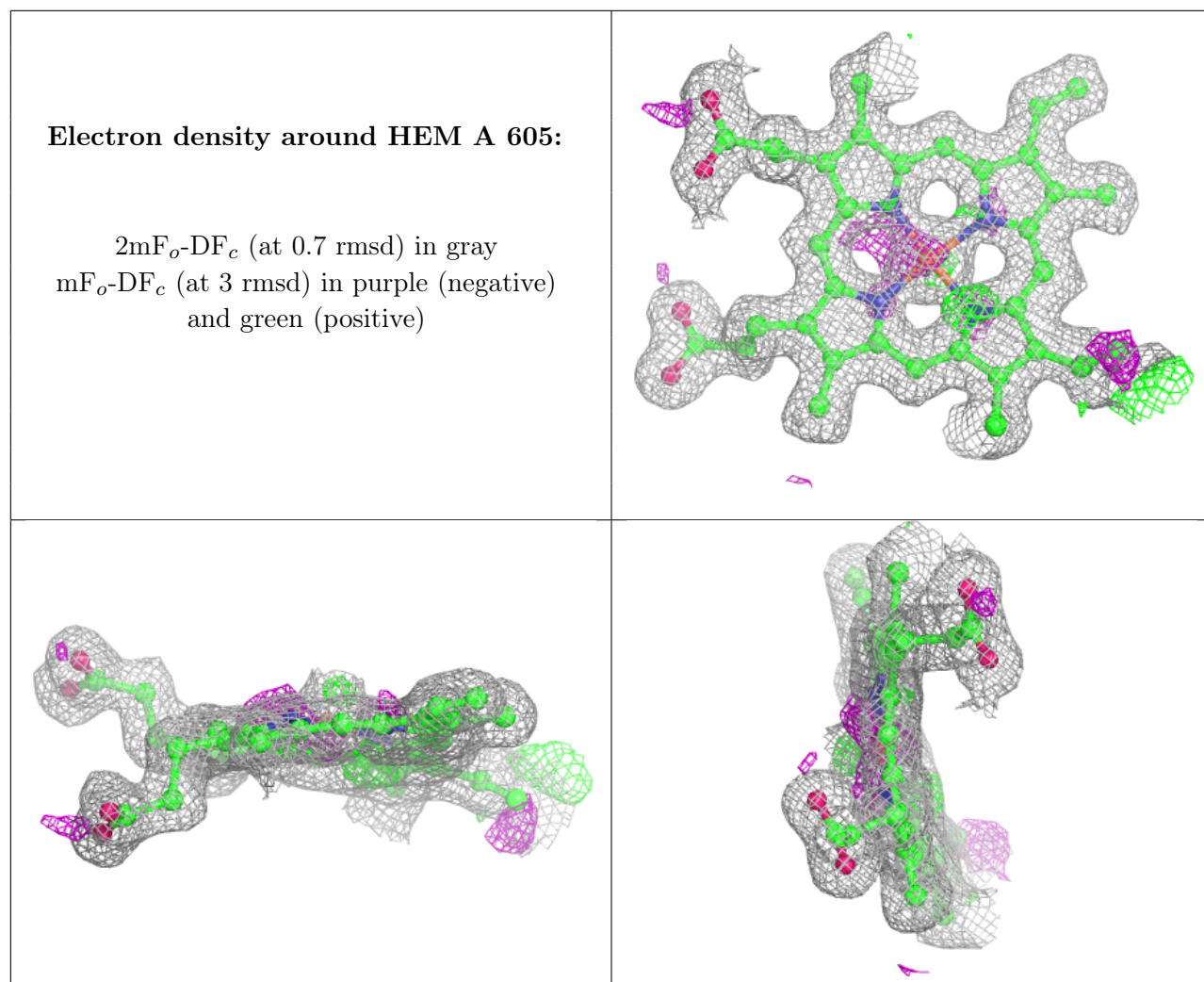
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	C	620	14/15	0.78	0.23	23,29,41,43	0
8	BMA	C	644	11/12	0.81	0.12	24,27,29,29	0
7	NAG	C	630	14/15	0.85	0.28	29,41,53,78	0
7	NAG	D	630	14/15	0.86	0.29	38,56,77,78	0
7	NAG	D	620	14/15	0.86	0.12	23,29,40,43	0
8	BMA	D	644	11/12	0.88	0.10	22,24,29,33	0
5	HEM	B	605	43/43	0.94	0.12	11,15,20,37	0
5	HEM	A	605	43/43	0.95	0.11	12,15,19,60	0
4	CL	C	612	1/1	0.98	0.09	29,29,29,29	0
4	CL	D	612	1/1	0.98	0.11	27,27,27,27	0
4	CL	A	602	1/1	0.99	0.13	14,14,14,14	0
4	CL	C	611	1/1	0.99	0.09	22,22,22,22	0
4	CL	B	201	1/1	1.00	0.13	14,14,14,14	0
6	CA	C	601	1/1	1.00	0.10	14,14,14,14	0
6	CA	D	701	1/1	1.00	0.12	10,10,10,10	1

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 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.