W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 01:17 PM BST

PDB ID	:	3WCU
Title	:	The structure of a deoxygenated 400 kda hemoglobin provides a more accurate description of the cooperative mechanism of giant hemoglobins: Deoxygenated form
Authors	:	Numoto, N.; Nakagawa, T.; Ohara, R.; Hasegawa, T.; Kita, A.; Yoshida, T.; Maruyama, T.; Imai, K.; Fukumori, Y.; Miki, K.
Deposited on	:	2013-06-01
Resolution	:	2.90 Å(reported)

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

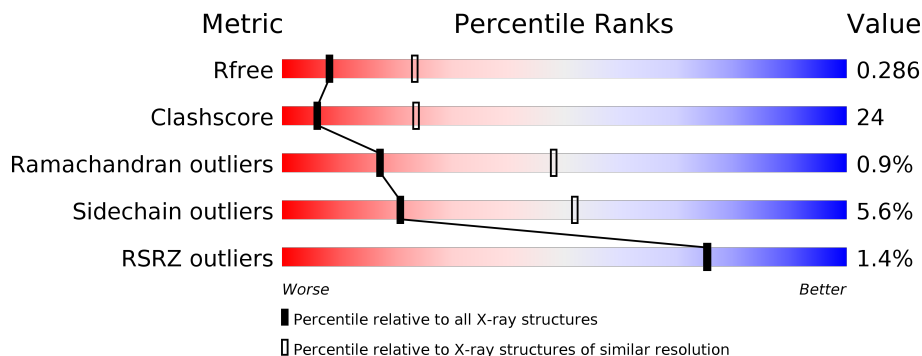|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.90 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		24
Ramachandran outliers		0.9%
Sidechain outliers		5.6%
RSRZ outliers		1.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 >=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 <=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	146	62% / 35% / ·
1	E	146	62% / 36% / ·
2	B	144	3% 50% / 49% / ·
2	F	144	% 48% / 51% / ·
3	C	150	3% 51% / 44% / 5%
3	G	150	2% 52% / 43% / 5%

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Mol	Chain	Length	Quality of chain
4	D	149	58% 39%
4	H	149	57% 40%
5	I	6	17% 83%
5	J	6	17% 83%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	I	3	-	-	-	X
5	MAN	I	4	-	-	-	X
5	MAN	I	5	-	-	-	X
5	NAG	J	2	-	-	-	X
5	MAN	J	3	-	-	-	X
5	MAN	J	4	-	-	-	X
5	MAN	J	5	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9626 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 A1 globin chain of giant V2 hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total 1151	C 736	N 198	O 209	S 8	0	0	0
1	E	146	Total 1151	C 736	N 198	O 209	S 8	0	0	0

- Molecule 2 is a protein called A2 globin chain of giant V2 hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total 1120	C 697	N 206	O 210	S 7	0	0	0
2	F	144	Total 1120	C 697	N 206	O 210	S 7	0	0	0

- Molecule 3 is a protein called B2 globin chain of giant V2 hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	150	Total 1158	C 718	N 211	O 221	S 8	0	0	0
3	G	150	Total 1158	C 718	N 211	O 221	S 8	0	0	0

- Molecule 4 is a protein called B1 globin chain of giant V2 hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	149	Total 1140	C 727	N 196	O 210	S 7	0	0	0
4	H	149	Total 1140	C 727	N 196	O 210	S 7	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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.
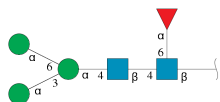
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	6	Total	C	N	O	0	0	0
			71	40	2	29			
5	J	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
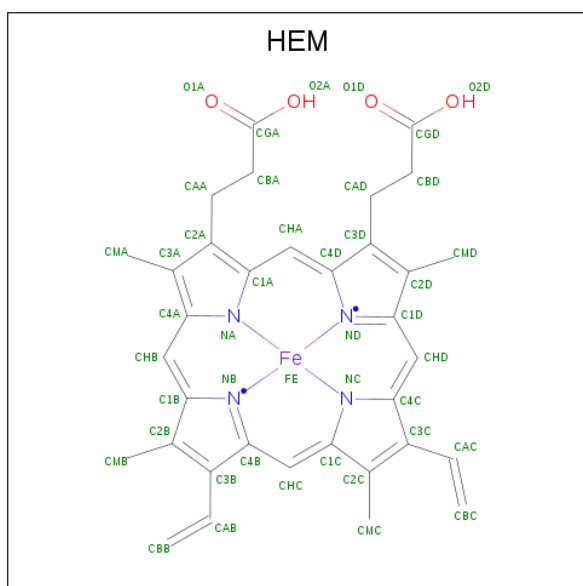
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Ca 1	0	0
7	F	1	Total 1	Ca 1	0	0

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.
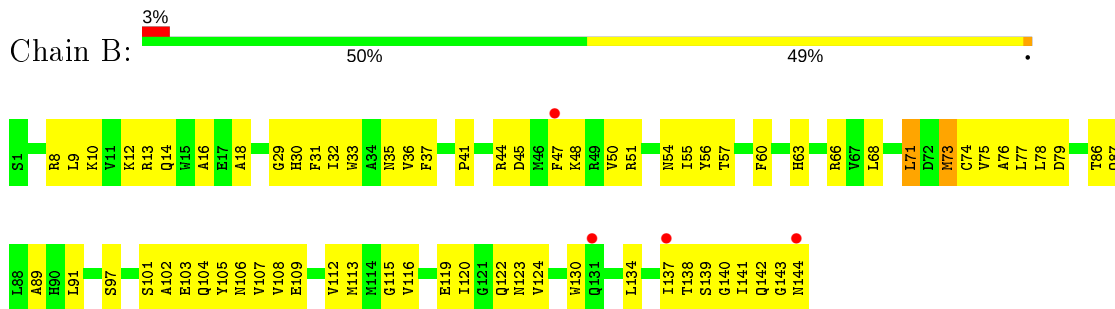
- Molecule 1: A1 globin chain of giant V2 hemoglobin
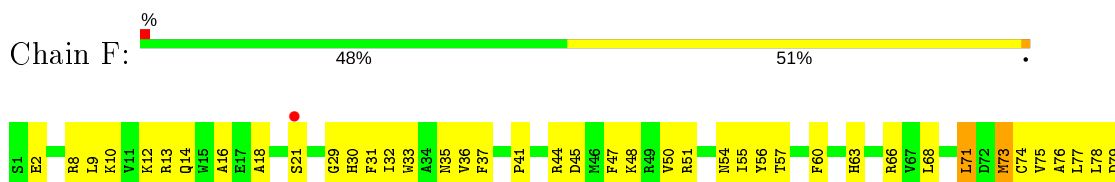

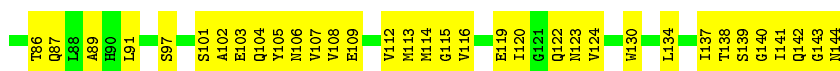- Molecule 1: A1 globin chain of giant V2 hemoglobin

- Molecule 2: A2 globin chain of giant V2 hemoglobin

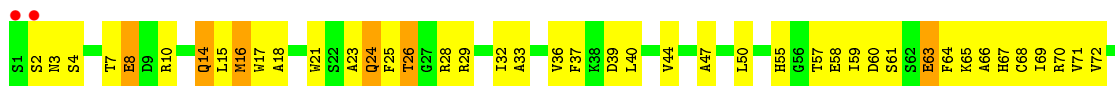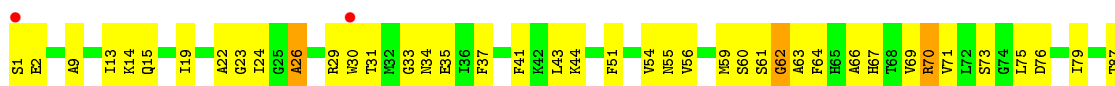- Molecule 2: A2 globin chain of giant V2 hemoglobin

T86 Q87 L88 A89 H90 L91 S97 S101 A102 E103 Q104 Y105 N106 V107 V108 E109 V112 M113 M114 G115 V116 E119 I120 G121 Q122 N123 V124 W130 L134 I137 T138 S139 G140 I141 Q142 G143 N144

- Molecule 3: B2 globin chain of giant V2 hemoglobin

Chain C:

3%
51% 44% 5%

S1 S2 N3 T7 E8 D9 R10 Q14 L15 M16 W17 A18 N19 V20 W21 S22 A23 Q24 F25 T26 G27 R28 R29 I32 A33 V36 F37 K38 D39 L40 V44 P45 D46 A47 V48 G49 L50 H55 G56 T57 E58 I59 D60 S61 S62 E63 F64 K65 A66 H67 C68 I69 R70 V71

V72 D76 S77 A78 L81 L88 Q91 L92 L95 A96 Q100 A103 T106 K107 I113 A114 Q115 S116 M121 P122 Q123 S126 C127 R135 C136 R139 I140 M144 T145 E146 G147 L148 A149 E150

- Molecule 3: B2 globin chain of giant V2 hemoglobin

Chain G:

2%
52% 43% 5%

S1 S2 N3 S4 T7 E8 D9 R10 Q14 L15 M16 W17 A18 W21 S22 A23 Q24 F25 T26 G27 R28 R29 I32 A33 V36 F37 K38 D39 L40 V44 A47 L50 H55 G56 T57 E58 I59 D60 S61 S62 E63 F64 K65 A66 H67 C68 I69 R70 V71 V72

D76 S77 A78 L81 L88 Q91 L92 L95 A96 Q100 A103 T106 K107 I113 A114 Q115 S116 M121 P122 Q123 S126 C127 D131 C136 R139 I140 M144 T145 E146 G147 E150

- Molecule 4: B1 globin chain of giant V2 hemoglobin

Chain D:

%
58% 39%

S1 E2 D8 A9 I13 K14 Q15 I19 A22 G23 I24 G25 A26 R29 W30 T31 M32 G33 N34 E35 I36 F37 F41 K42 L43 K44 F51 V54 N55 V56 M59 S60 S61 G62 A63 F64 H65 A66 H67 R70 V71 L72 S73 G74 L75 D76 I79 T87

H99 V100 A101 R102 L105 K106 Y109 F110 D111 A112 V116 L117 M118 T119 V120 L121 P122 S123 L124 I125 D126 M127 L137 L138 N142 K146 G147 L148 P149

- Molecule 4: B1 globin chain of giant V2 hemoglobin

Chain H:

%
57% 40%

S1 E2 A9 I13 K14 Q15 I19 A22 G23 I24 G25 A26 R29 W30 T31 M32 G33 N34 E35 I36 F37 F41 K42 L43 K44 F51 V54 N55 V56 M59 S60 S61 G62 A63 F64 H65 A66 H67 T68 V69 R70 V71 L72 S73 G74 L75 D76 I79 T87

H99 V100 A101 R102 K106 Y109 F110 D111 A112 V116 L117 M118 T119 V120 L121 P122 S123 L124 I125 D126 M127 L137 L138 N142 K146 G147 L148 P149

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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 I: 17%   83%

NAG1 NAG2 MAN3 MAN4 MAN5 FUC6

• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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 J: 17%   83%

NAG1 NAG2 MAN3 MAN4 MAN5 FUC6

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	108.87Å 108.87Å 195.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.45 – 2.90 42.45 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.45-2.90) 96.4 (42.45-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.292 0.237 , 0.286	Depositor DCC
R_{free} test set	1437 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.7	EDS
L-test for twinning [2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.065 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9626	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FUC, HEM, CA, NAG, 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	0.44	0/1178	0.60	0/1585
1	E	0.44	0/1178	0.60	0/1585
2	B	0.40	0/1143	0.59	0/1543
2	F	0.40	0/1143	0.59	0/1543
3	C	0.41	0/1181	0.63	0/1597
3	G	0.41	0/1181	0.63	0/1597
4	D	0.39	0/1164	0.60	0/1579
4	H	0.40	0/1164	0.60	0/1579
All	All	0.41	0/9332	0.60	0/12608

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	1151	0	1123	50	0
1	E	1151	0	1123	50	0
2	B	1120	0	1077	75	0
2	F	1120	0	1077	76	0
3	C	1158	0	1115	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1158	0	1115	83	0
4	D	1140	0	1140	59	0
4	H	1140	0	1140	61	0
5	I	71	0	61	0	0
5	J	71	0	61	0	0
6	A	43	0	30	1	0
6	B	43	0	30	1	0
6	C	43	0	30	1	0
6	D	43	0	30	3	0
6	E	43	0	30	1	0
6	F	43	0	30	1	0
6	G	43	0	30	1	0
6	H	43	0	30	3	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
All	All	9626	0	9272	461	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 24.

The worst 5 of 461 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:B:45:ASP:HA	2:B:48:LYS:HE2	1.47	0.95
2:F:45:ASP:HA	2:F:48:LYS:HE2	1.47	0.93
1:E:86:ASP:HB2	4:H:66:ALA:HB1	1.59	0.84
3:C:77:SER:O	3:C:81:LEU:HD23	1.78	0.83
1:A:86:ASP:HB2	4:D:66:ALA:HB1	1.59	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/146 (99%)	126 (88%)	17 (12%)	1 (1%)	22	54
1	E	144/146 (99%)	126 (88%)	17 (12%)	1 (1%)	22	54
2	B	142/144 (99%)	113 (80%)	29 (20%)	0	100	100
2	F	142/144 (99%)	113 (80%)	29 (20%)	0	100	100
3	C	148/150 (99%)	125 (84%)	22 (15%)	1 (1%)	22	54
3	G	148/150 (99%)	125 (84%)	22 (15%)	1 (1%)	22	54
4	D	147/149 (99%)	130 (88%)	14 (10%)	3 (2%)	7	27
4	H	147/149 (99%)	130 (88%)	14 (10%)	3 (2%)	7	27
All	All	1162/1178 (99%)	988 (85%)	164 (14%)	10 (1%)	17	48

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	77	PHE
1	A	77	PHE
4	D	26	ALA
4	D	101	ALA
4	H	26	ALA

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	120/120 (100%)	115 (96%)	5 (4%)	30	63
1	E	120/120 (100%)	115 (96%)	5 (4%)	30	63
2	B	116/116 (100%)	110 (95%)	6 (5%)	23	55
2	F	116/116 (100%)	110 (95%)	6 (5%)	23	55
3	C	124/124 (100%)	114 (92%)	10 (8%)	11	33
3	G	124/124 (100%)	114 (92%)	10 (8%)	11	33
4	D	122/122 (100%)	116 (95%)	6 (5%)	25	57
4	H	122/122 (100%)	116 (95%)	6 (5%)	25	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	964/964 (100%)	910 (94%)	54 (6%)	21 52

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	111	ASP
1	E	70	LEU
4	H	70	ARG
4	D	137	LEU
1	E	4	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	18	GLN
2	F	23	ASN
3	G	34	GLN
3	C	100	GLN
3	C	115	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

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
5	NAG	I	1	5,4	14,14,15	0.96	1 (7%)	17,19,21	1.11	1 (5%)
5	NAG	I	2	5	14,14,15	0.68	0	17,19,21	1.27	2 (11%)
5	MAN	I	3	5	11,11,12	1.06	1 (9%)	15,15,17	1.43	2 (13%)
5	MAN	I	4	5	11,11,12	0.94	0	15,15,17	0.82	1 (6%)
5	MAN	I	5	5	11,11,12	0.79	0	15,15,17	0.79	1 (6%)
5	FUC	I	6	5	10,10,11	0.66	0	14,14,16	0.85	0
5	NAG	J	1	5,4	14,14,15	0.95	1 (7%)	17,19,21	1.11	1 (5%)
5	NAG	J	2	5	14,14,15	0.68	0	17,19,21	1.26	2 (11%)
5	MAN	J	3	5	11,11,12	1.06	1 (9%)	15,15,17	1.43	2 (13%)
5	MAN	J	4	5	11,11,12	0.94	0	15,15,17	0.81	1 (6%)
5	MAN	J	5	5	11,11,12	0.79	0	15,15,17	0.79	1 (6%)
5	FUC	J	6	5	10,10,11	0.66	0	14,14,16	0.85	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	NAG	I	1	5,4	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	MAN	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	1/2/19/22	0/1/1/1
5	FUC	I	6	5	-	-	0/1/1/1
5	NAG	J	1	5,4	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1
5	MAN	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	1/2/19/22	0/1/1/1
5	FUC	J	6	5	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	3	MAN	C2-C3	2.89	1.56	1.52
5	I	3	MAN	C2-C3	2.89	1.56	1.52
5	I	1	NAG	O5-C1	-2.13	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	NAG	O5-C1	-2.09	1.40	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	MAN	C1-C2-C3	3.83	114.38	109.67
5	I	3	MAN	C1-C2-C3	3.82	114.36	109.67
5	I	2	NAG	C2-N2-C7	-3.23	118.30	122.90
5	J	2	NAG	C2-N2-C7	-3.19	118.36	122.90
5	I	2	NAG	C4-C3-C2	-2.93	106.72	111.02

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	I	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
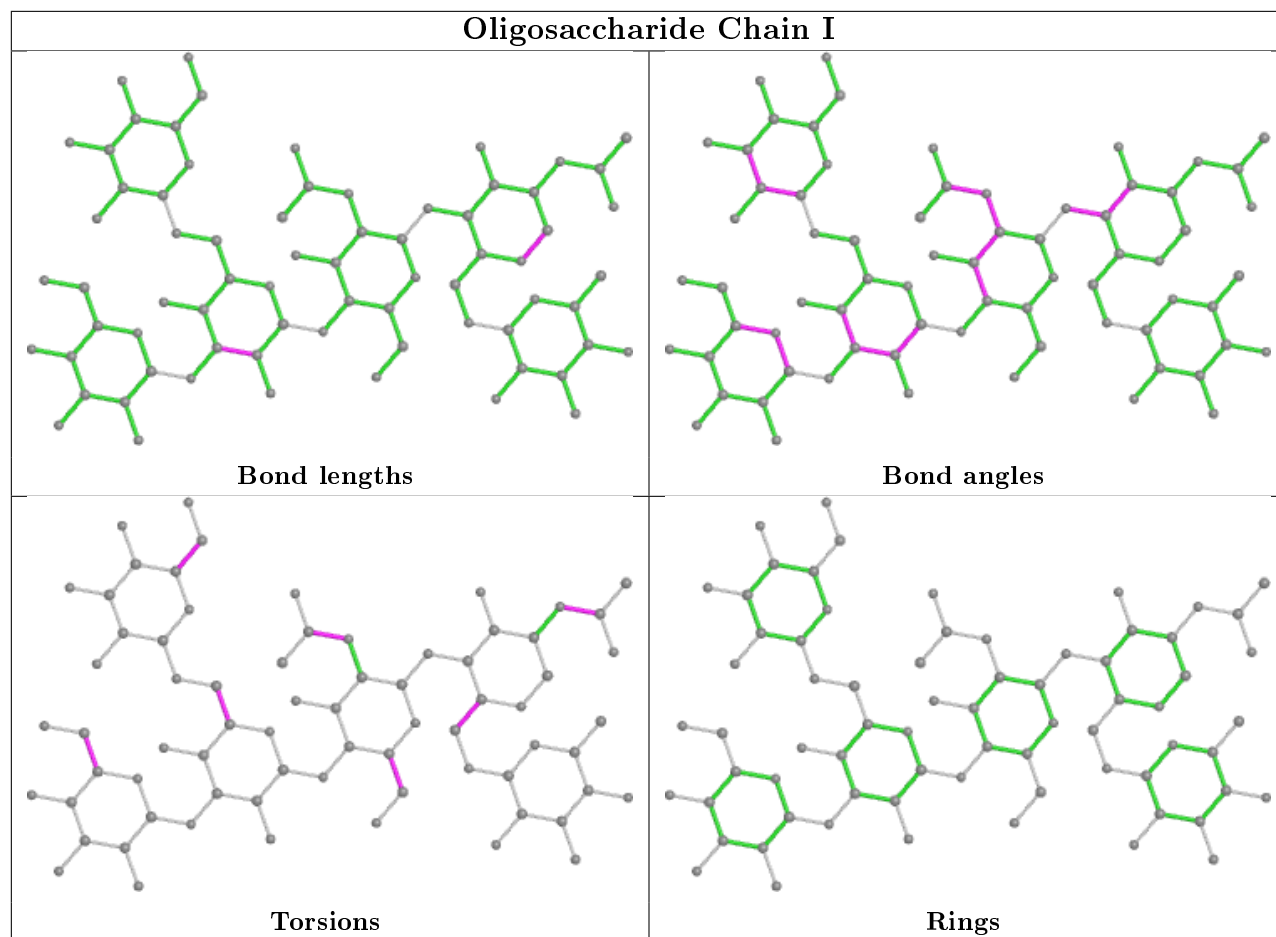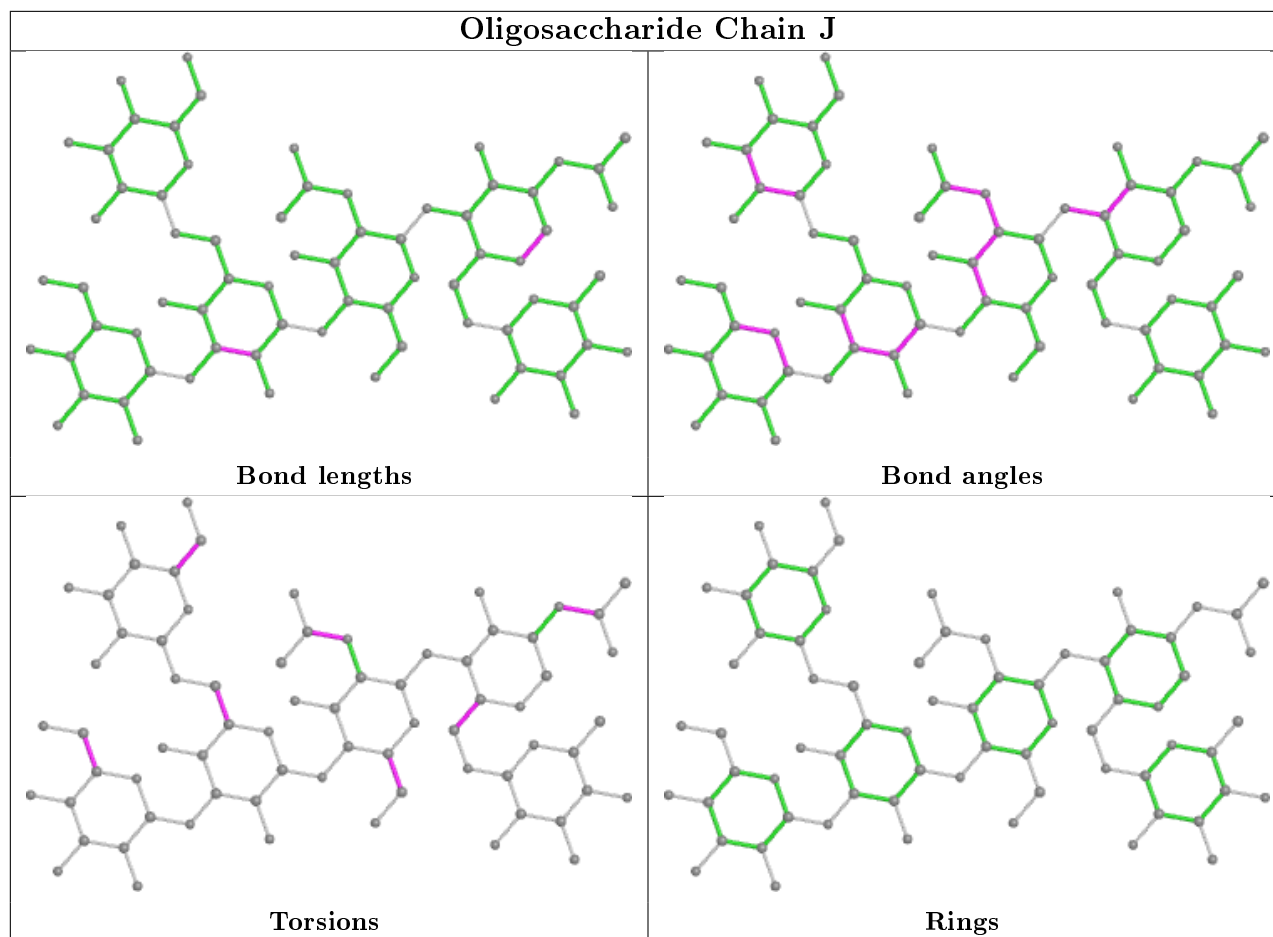
5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 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	#$|Z| > 2$
6	HEM	A	200	1	27,50,50	1.87	7 (25%)	17,82,82	2.49	9 (52%)
6	HEM	H	201	4	27,50,50	1.87	6 (22%)	17,82,82	2.44	9 (52%)
6	HEM	G	200	3	27,50,50	1.88	6 (22%)	17,82,82	2.43	9 (52%)
6	HEM	E	200	1	27,50,50	1.87	7 (25%)	17,82,82	2.49	9 (52%)
6	HEM	B	201	2	27,50,50	1.91	7 (25%)	17,82,82	2.31	8 (47%)
6	HEM	F	201	2	27,50,50	1.91	7 (25%)	17,82,82	2.31	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HEM	D	201	4	27,50,50	1.87	6 (22%)	17,82,82	2.44	9 (52%)
6	HEM	C	200	3	27,50,50	1.88	6 (22%)	17,82,82	2.43	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	A	200	1	-	2/6/54/54	-
6	HEM	H	201	4	-	0/6/54/54	-
6	HEM	G	200	3	-	0/6/54/54	-
6	HEM	E	200	1	-	2/6/54/54	-
6	HEM	B	201	2	-	2/6/54/54	-
6	HEM	F	201	2	-	2/6/54/54	-
6	HEM	D	201	4	-	0/6/54/54	-
6	HEM	C	200	3	-	0/6/54/54	-

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	201	HEM	C3C-CAC	-6.20	1.35	1.47
6	F	201	HEM	C3C-CAC	-6.19	1.35	1.47
6	E	200	HEM	C3C-CAC	-5.85	1.35	1.47
6	A	200	HEM	C3C-CAC	-5.85	1.35	1.47
6	G	200	HEM	C3C-CAC	-5.78	1.36	1.47

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	201	HEM	C4C-C3C-C2C	-5.02	103.39	106.90
6	D	201	HEM	C4C-C3C-C2C	-4.98	103.42	106.90
6	C	200	HEM	C4C-C3C-C2C	-4.93	103.45	106.90
6	G	200	HEM	C4C-C3C-C2C	-4.93	103.45	106.90
6	A	200	HEM	C4C-C3C-C2C	-4.77	103.57	106.90

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	200	HEM	C1A-C2A-CAA-CBA
6	A	200	HEM	C3A-C2A-CAA-CBA
6	E	200	HEM	C1A-C2A-CAA-CBA
6	E	200	HEM	C3A-C2A-CAA-CBA
6	B	201	HEM	C1A-C2A-CAA-CBA

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	200	HEM	1	0
6	H	201	HEM	3	0
6	G	200	HEM	1	0
6	E	200	HEM	1	0
6	B	201	HEM	1	0
6	F	201	HEM	1	0
6	D	201	HEM	3	0
6	C	200	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 then 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.

Ligand HEM A 200

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM H 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM G 200

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 200

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM F 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 200

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	146/146 (100%)	-0.24	0 100	100	34, 55, 83, 136	0
1	E	146/146 (100%)	-0.34	0 100	100	34, 55, 83, 136	0
2	B	144/144 (100%)	0.06	4 (2%) 53	49	40, 71, 107, 164	0
2	F	144/144 (100%)	-0.08	1 (0%) 87	87	40, 71, 107, 164	0
3	C	150/150 (100%)	0.12	4 (2%) 54	50	39, 69, 113, 170	0
3	G	150/150 (100%)	0.00	3 (2%) 65	63	39, 69, 113, 170	0
4	D	149/149 (100%)	-0.09	2 (1%) 77	77	40, 66, 104, 140	0
4	H	149/149 (100%)	-0.17	2 (1%) 77	77	40, 66, 104, 140	0
All	All	1178/1178 (100%)	-0.09	16 (1%) 75	75	34, 65, 107, 170	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	SER	9.0
3	G	1	SER	9.0
4	D	1	SER	4.6
4	H	1	SER	4.2
2	B	144	ASN	3.2

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, 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
5	MAN	J	4	11/12	0.03	1.12	236,237,238,239	0
5	MAN	I	4	11/12	0.33	0.88	236,237,238,239	0
5	MAN	J	5	11/12	0.38	0.60	218,220,221,222	0
5	MAN	I	5	11/12	0.54	0.81	218,220,221,222	0
5	MAN	J	3	11/12	0.61	0.66	230,233,236,237	0
5	NAG	I	1	14/15	0.63	0.30	156,156,156,156	0
5	NAG	J	2	14/15	0.72	0.43	153,153,153,153	0
5	NAG	J	1	14/15	0.73	0.40	156,156,156,156	0
5	MAN	I	3	11/12	0.74	0.45	230,233,236,237	0
5	FUC	J	6	10/11	0.83	0.29	106,106,106,106	0
5	NAG	I	2	14/15	0.84	0.38	153,153,153,153	0
5	FUC	I	6	10/11	0.89	0.28	106,106,106,106	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.
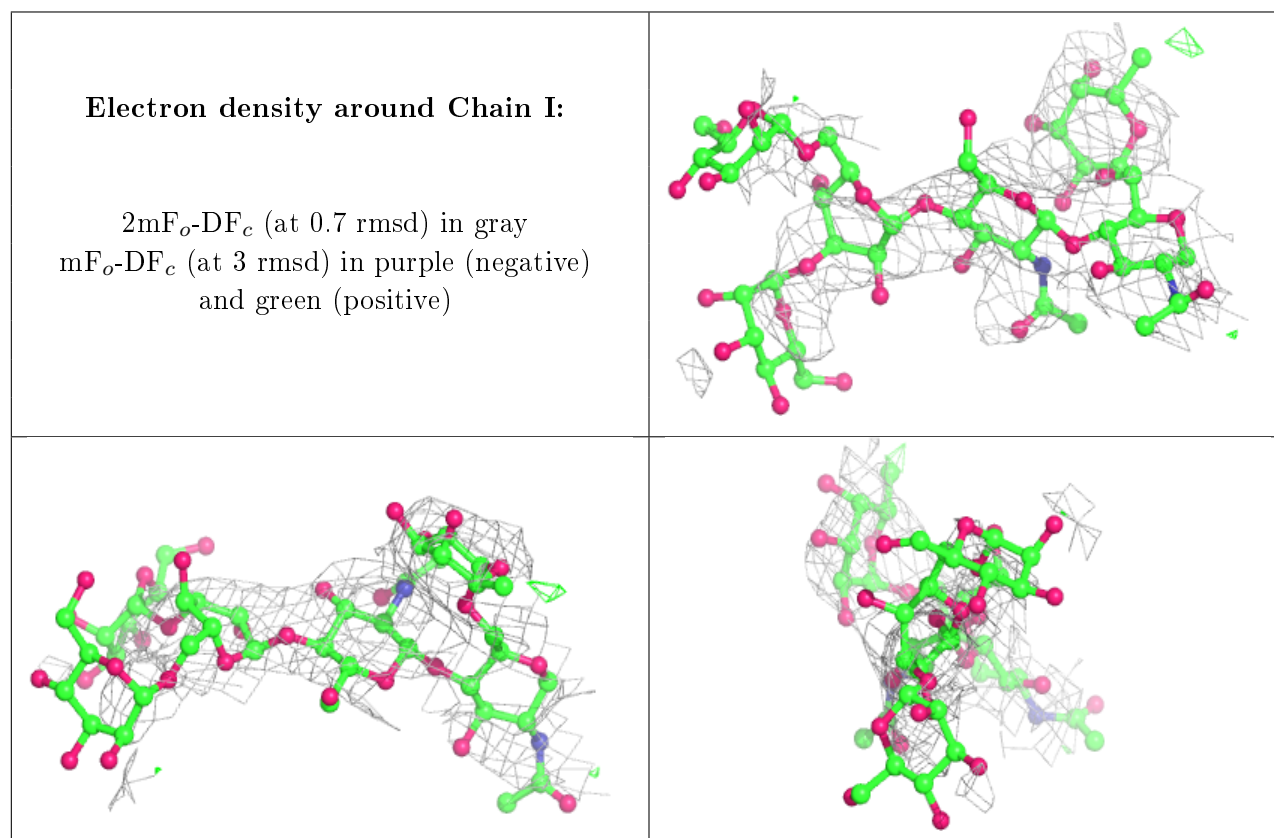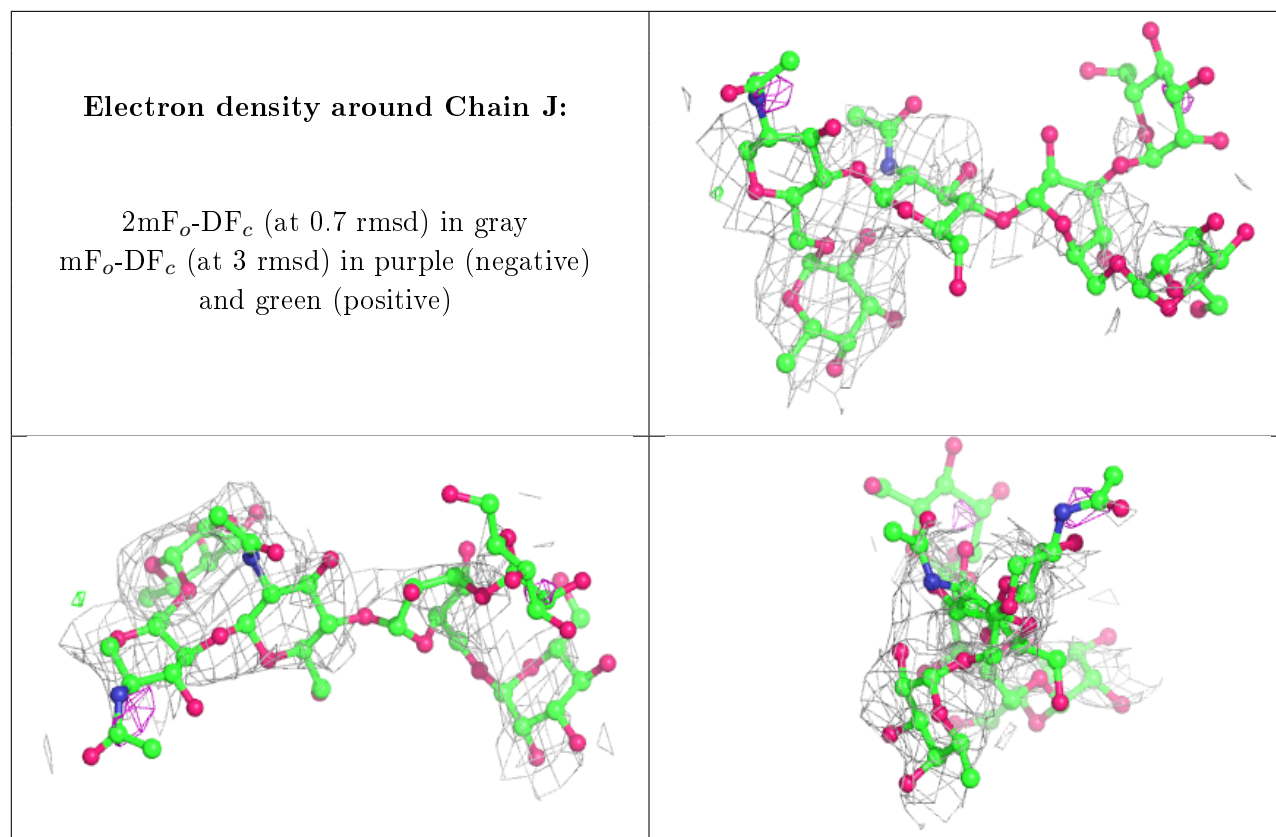
Electron density around Chain I:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
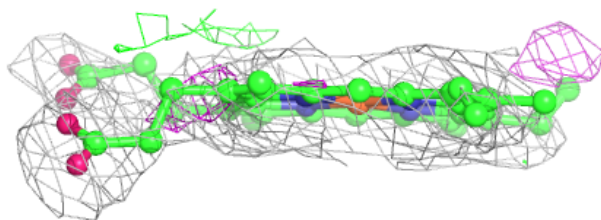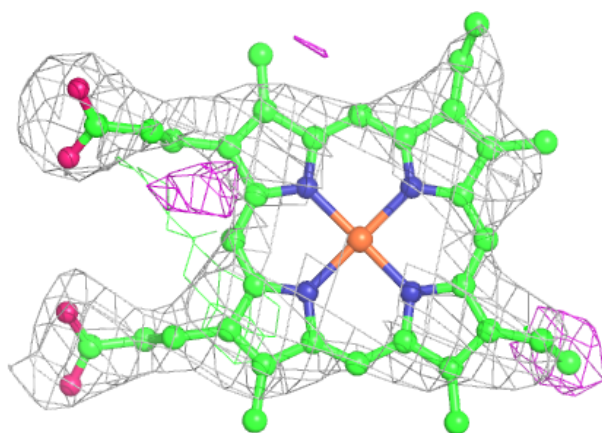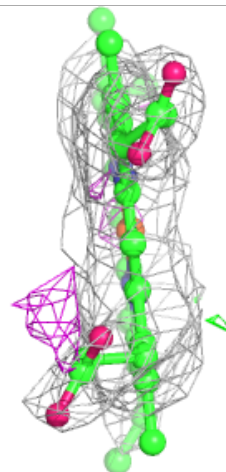mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain J:

$2mF_o$-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	CA	B	202	1/1	0.80	0.27	67,67,67,67	0
6	HEM	C	200	43/43	0.92	0.23	67,67,67,67	0
6	HEM	H	201	43/43	0.93	0.23	67,67,67,67	0
6	HEM	G	200	43/43	0.93	0.24	67,67,67,67	0
6	HEM	B	201	43/43	0.94	0.22	67,67,67,67	0
6	HEM	D	201	43/43	0.94	0.22	67,67,67,67	0
6	HEM	E	200	43/43	0.94	0.19	67,67,67,67	0
6	HEM	F	201	43/43	0.95	0.22	67,67,67,67	0
7	CA	F	202	1/1	0.95	0.04	67,67,67,67	0
6	HEM	A	200	43/43	0.95	0.21	67,67,67,67	0

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

Electron density around HEM C 200:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
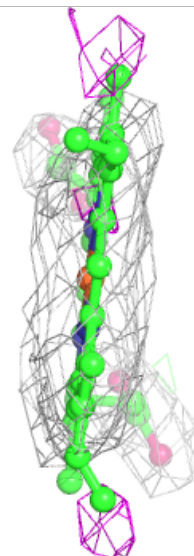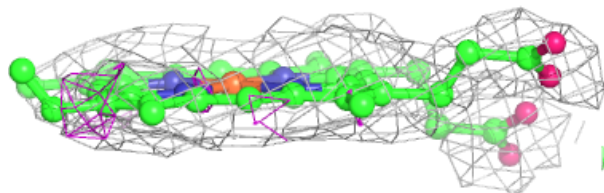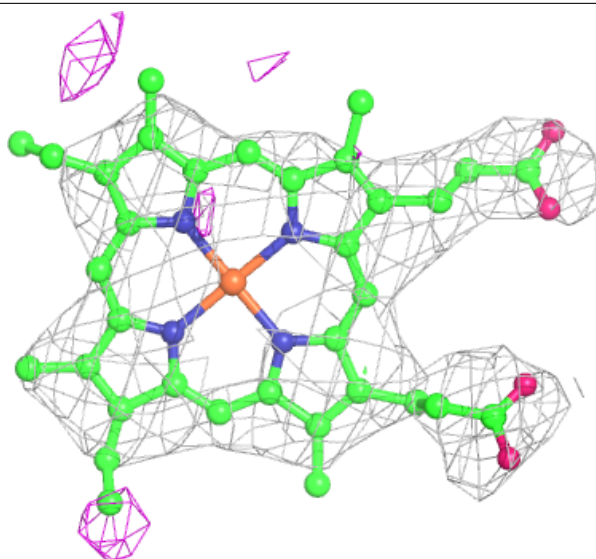
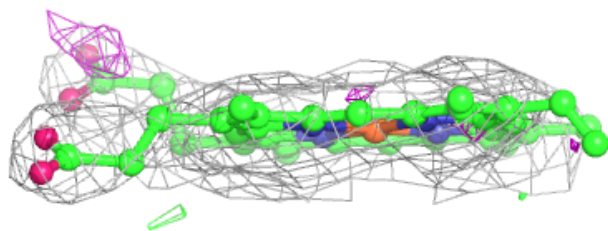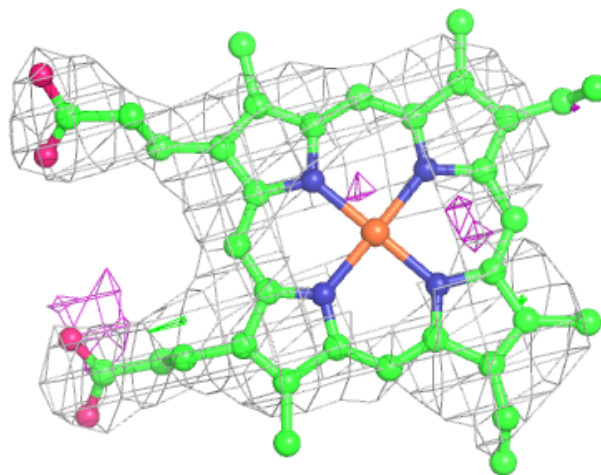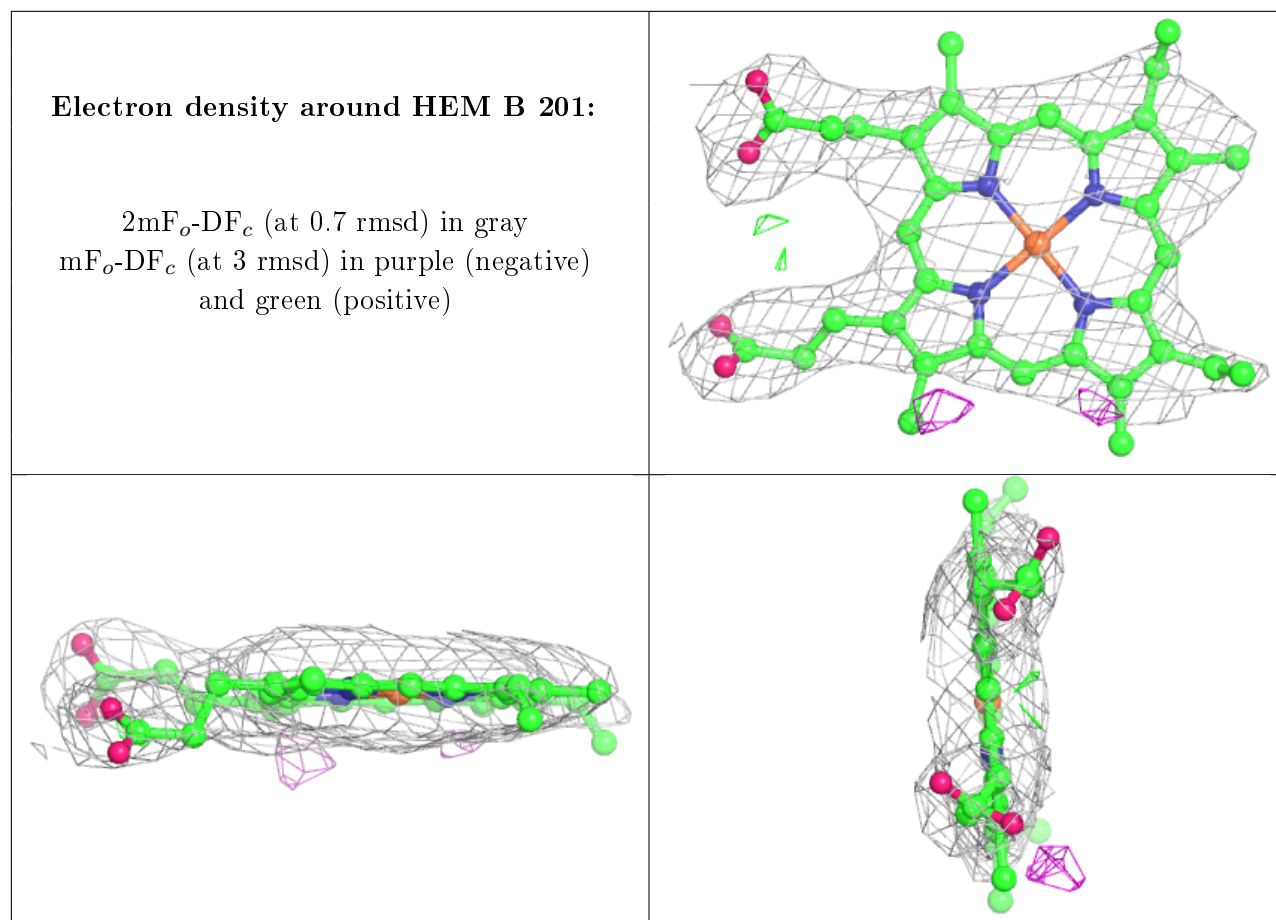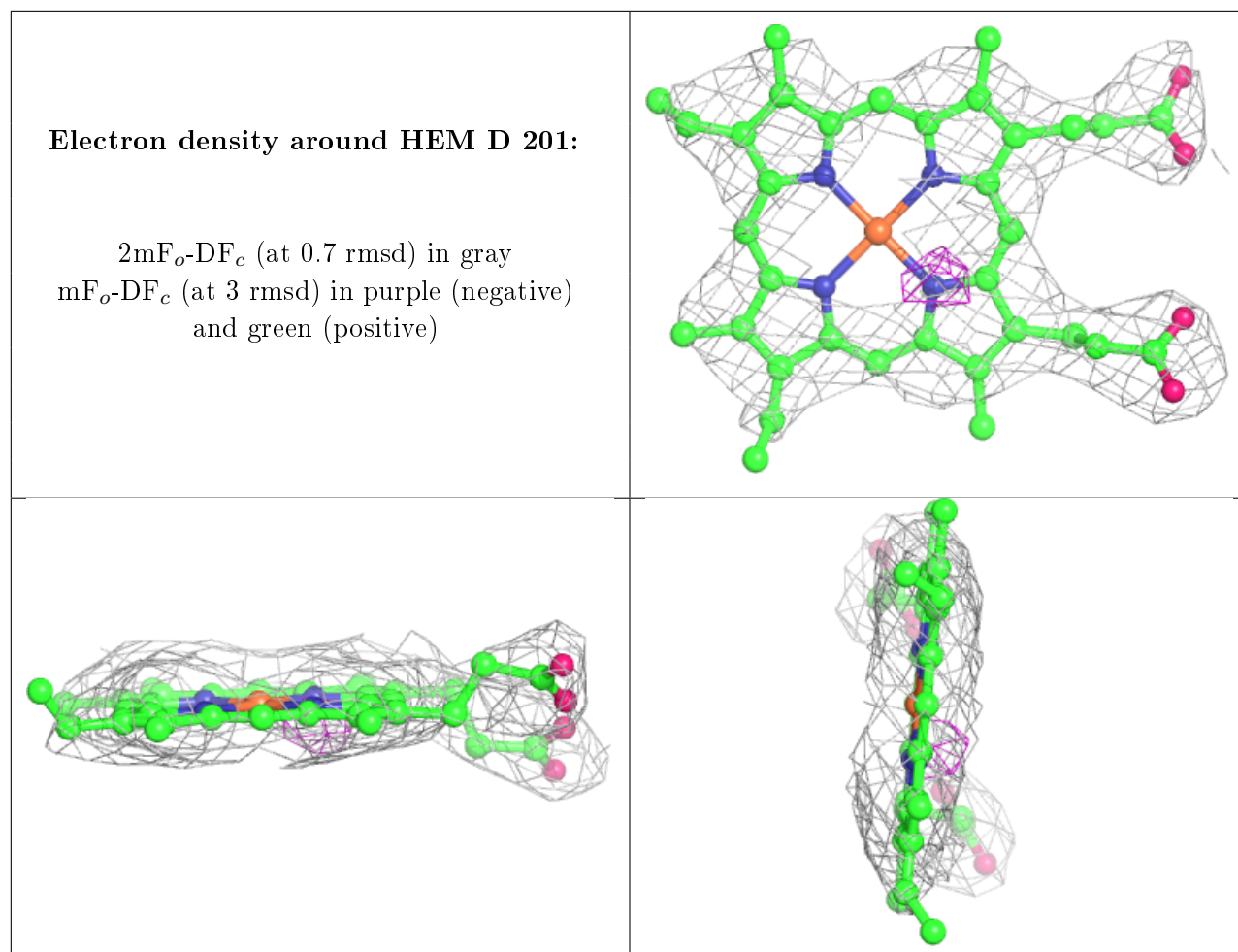**Electron density around HEM H 201:**

$2mF_o$-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 G 200:

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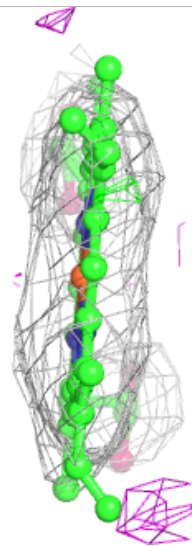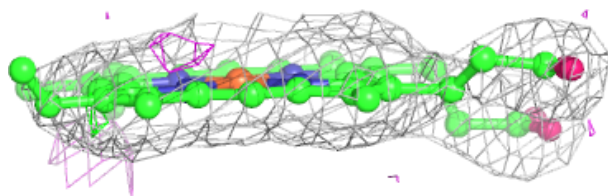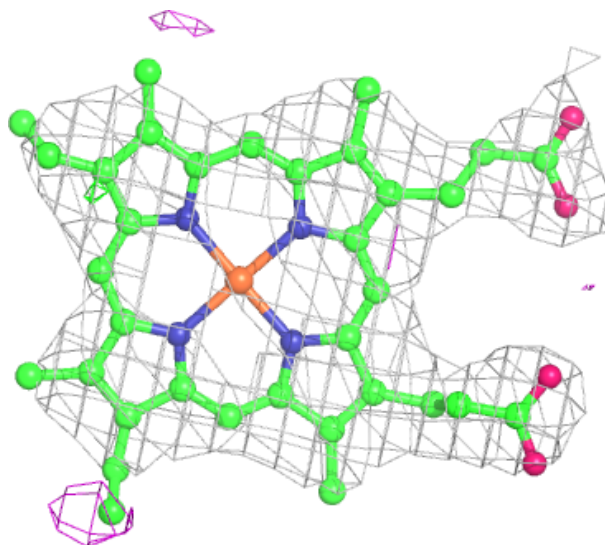mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM B 201:

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

Electron density around HEM D 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
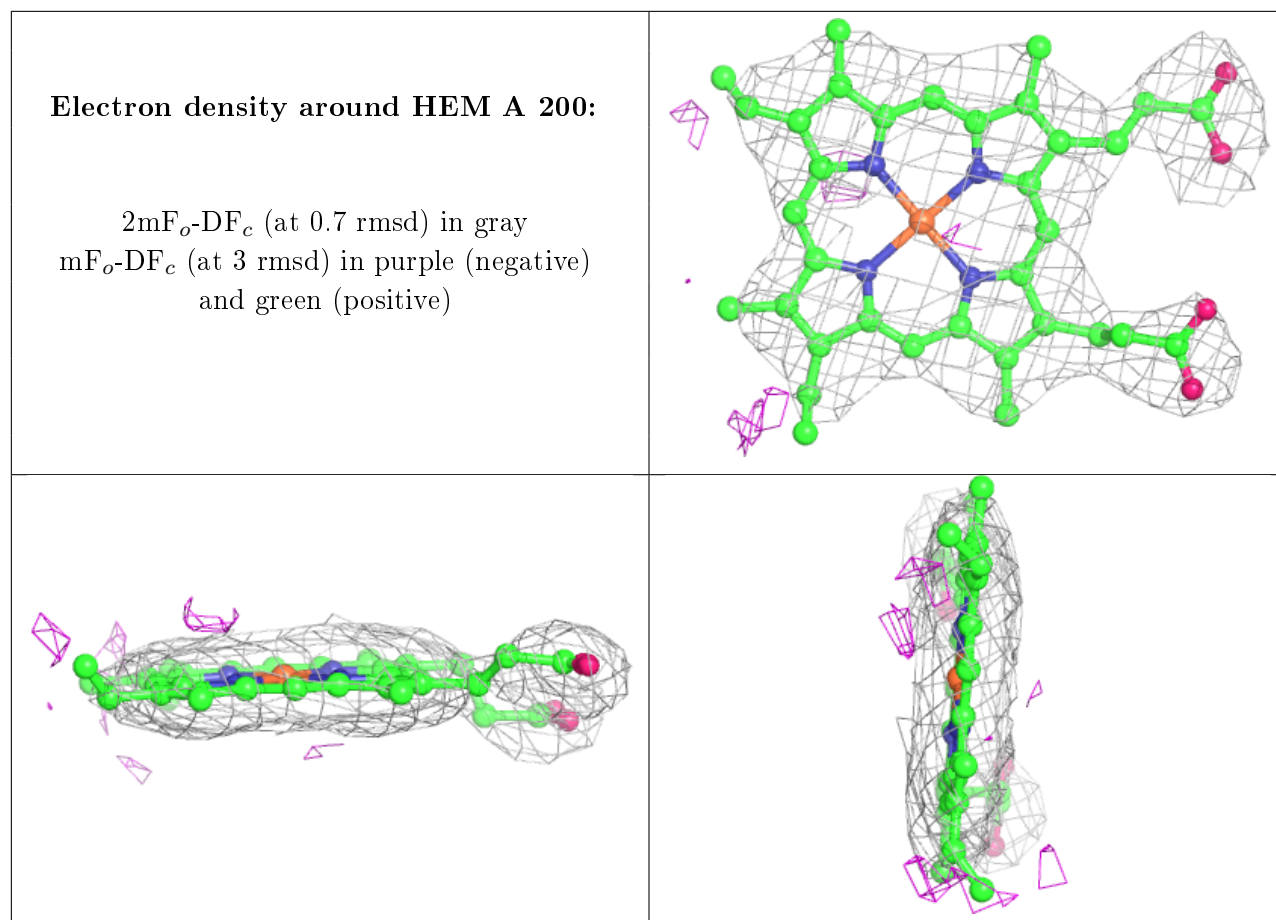
Electron density around HEM E 200:

$2mF_o$-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 F 201:

$2mF_o$-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 200:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
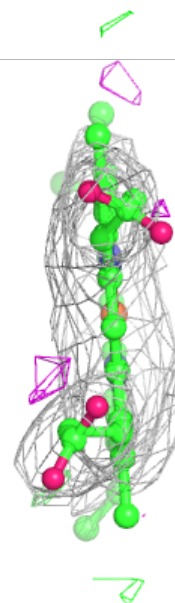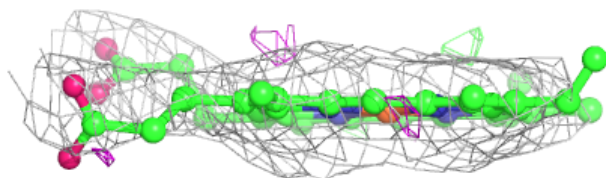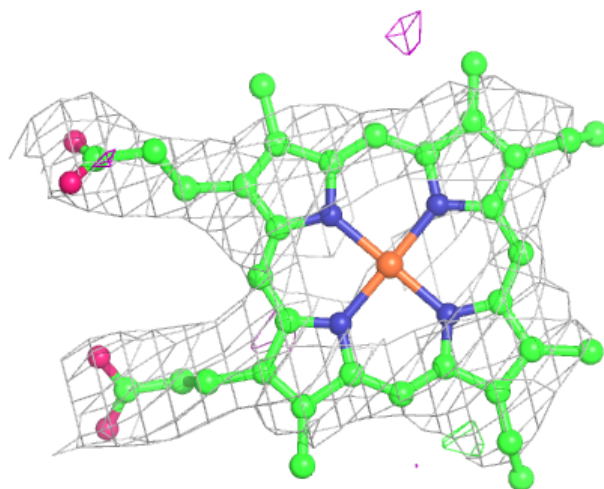
6.5 Other polymers (i)

There are no such residues in this entry.