W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Mar 31, 2021 – 04:13 pm BST

PDB ID	:	7AO7
Title	:	Structure of CYP153A from Polaromonas sp. in complex with octan-1-ol
Authors	:	Zukic, E.; Rowlinson, B.; Sharma, M.; Hoffmann, S.; Hauer, B.; Grogan, G.
Deposited on	:	2020-10-13
Resolution	:	2.55 Å(reported)

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

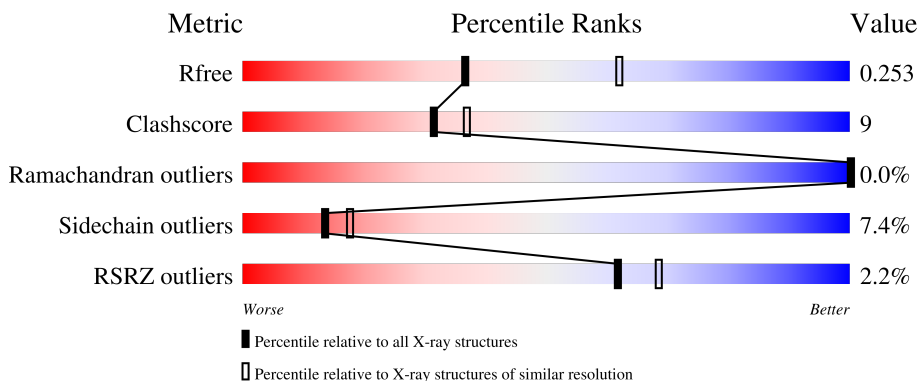|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.
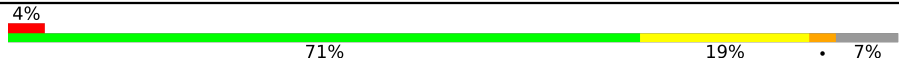
Metric	Percentile Ranks	Value
Rfree		0.253
Clashscore		9
Ramachandran outliers		0.0%
Sidechain outliers		7.4%
RSRZ outliers		2.2%

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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	418	3% / 81% / 13% · ·
1	B	418	2% / 77% / 16% · 5%
1	C	418	2% / 74% / 17% 5% ·
1	D	418	.% / 78% / 15% · 5%
1	E	418	78% / 16% · ·

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| Mol	Chain	Length	Quality of chain
1	F	418	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19048 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 Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3037	1934	524	558	21			
1	B	397	Total	C	N	O	S	0	0	0
			3061	1952	538	552	19			
1	C	401	Total	C	N	O	S	0	0	0
			3085	1965	529	571	20			
1	D	397	Total	C	N	O	S	0	0	0
			3107	1977	544	565	21			
1	E	402	Total	C	N	O	S	0	0	0
			3146	2007	544	574	21			
1	F	390	Total	C	N	O	S	0	0	0
			2947	1883	512	533	19			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
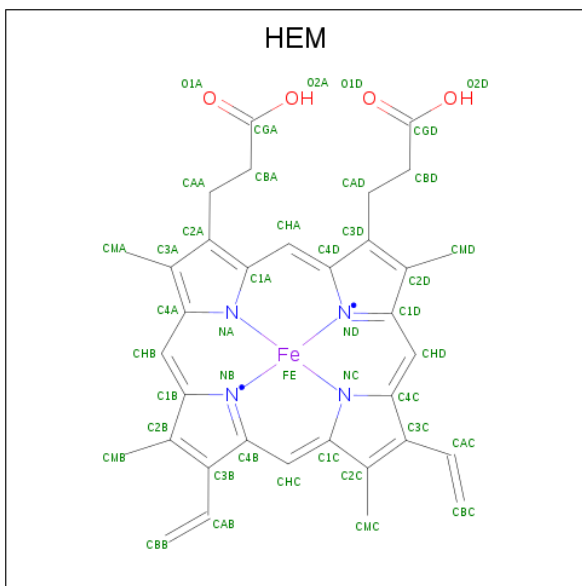
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is OCTAN-1-OL (three-letter code: OC9) (formula: $C_8H_{18}O$) (labeled as "Ligand of Interest" by depositor).
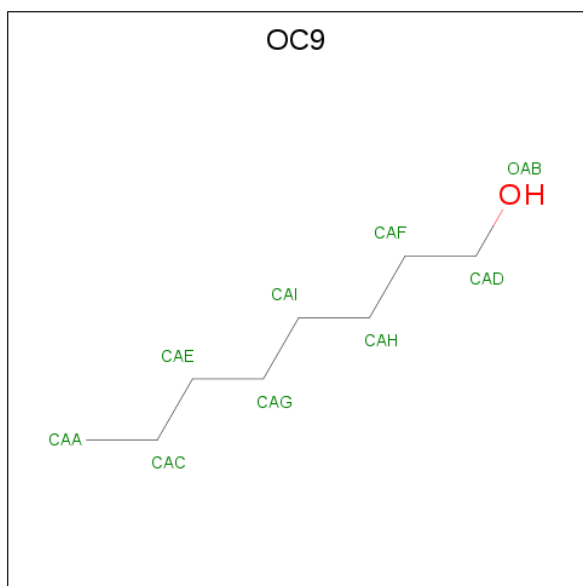
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	8	1		
3	B	1	Total	C	O	0	0
			9	8	1		
3	C	1	Total	C	O	0	0
			9	8	1		
3	D	1	Total	C	O	0	0
			9	8	1		
3	E	1	Total	C	O	0	0
			9	8	1		

• Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total 43	O 43	0	0
4	B	51	Total 51	O 51	0	0
4	C	55	Total 55	O 55	0	0
4	D	80	Total 80	O 80	0	0
4	E	105	Total 105	O 105	0	0
4	F	28	Total 28	O 28	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
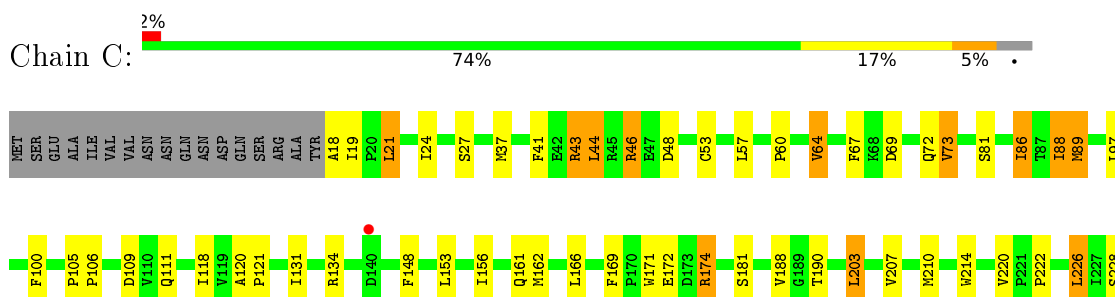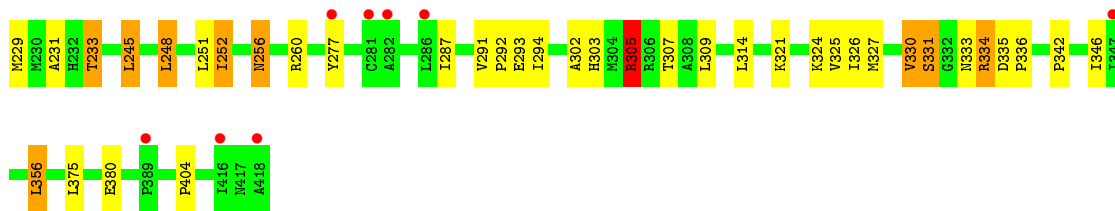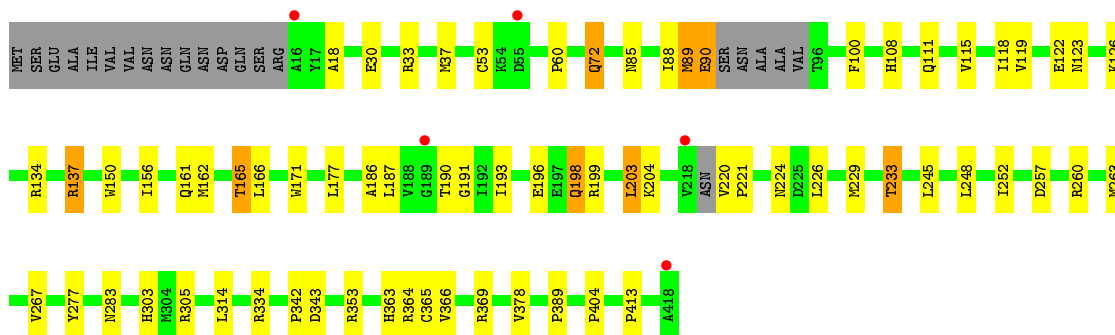
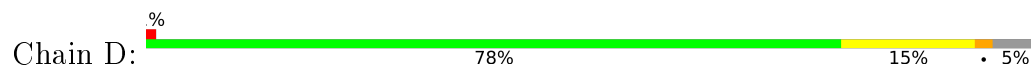- Molecule 1: Cytochrome P450
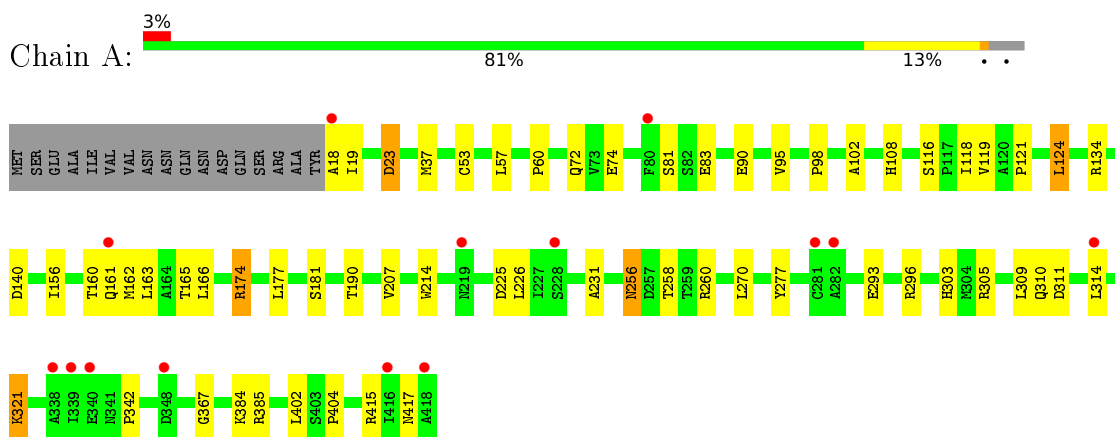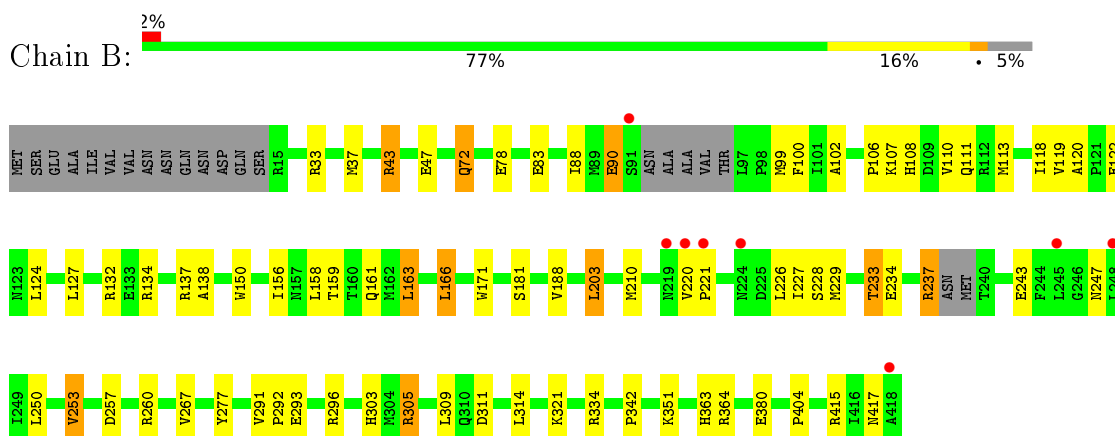
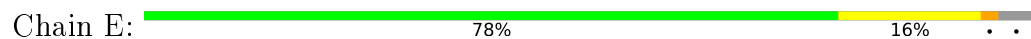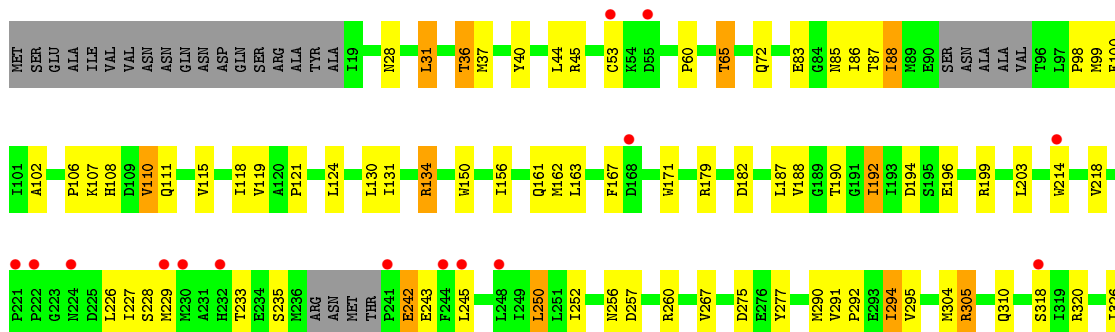
- Molecule 1: Cytochrome P450

- Molecule 1: Cytochrome P450

- Molecule 1: Cytochrome P450

Chain D:

- Molecule 1: Cytochrome P450

Chain E:

- Molecule 1: Cytochrome P450

Chain F:

R334 P342 I346 R349 H363 R369 Q374 L375 K384 E393 R415 I416 N417 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.50Å 116.19Å 288.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 2.55 45.13 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.17-2.55) 99.9 (45.13-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.205 , 0.254 0.208 , 0.253	Depositor DCC
R_{free} test set	4029 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19048	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.29% 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 $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OC9, HEM

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	0.71	0/3111	0.82	0/4254
1	B	0.70	0/3135	0.83	2/4273 (0.0%)
1	C	0.74	1/3160 (0.0%)	0.86	2/4317 (0.0%)
1	D	0.71	0/3181	0.86	0/4330
1	E	0.73	0/3222	0.85	2/4388 (0.0%)
1	F	0.70	0/3020	0.86	2/4123 (0.0%)
All	All	0.72	1/18829 (0.0%)	0.85	8/25685 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	PRO	C-N	7.72	1.49	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	305	ARG	CG-CD-NE	5.79	123.95	111.80
1	C	305	ARG	CG-CD-NE	-5.73	99.76	111.80
1	B	305	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	174	ARG	CB-CA-C	-5.34	99.72	110.40
1	B	90	GLU	CB-CA-C	5.27	120.94	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3037	0	2885	44	0
1	B	3061	0	2947	50	0
1	C	3085	0	2970	84	0
1	D	3107	0	3032	45	0
1	E	3146	0	3085	51	0
1	F	2947	0	2783	56	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0
2	D	43	0	30	1	0
2	E	43	0	30	3	0
2	F	43	0	30	3	0
3	A	9	0	18	1	0
3	B	9	0	17	0	0
3	C	9	0	18	0	0
3	D	9	0	17	0	0
3	E	9	0	18	1	0
4	A	43	0	0	3	0
4	B	51	0	0	4	0
4	C	55	0	0	3	0
4	D	80	0	0	3	0
4	E	105	0	0	4	0
4	F	28	0	0	4	0
All	All	19048	0	17970	329	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 9.

The worst 5 of 329 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLN:NE2	1:B:247:ASN:HD21	1.55	1.04
1:B:132:ARG:NH2	1:B:380:GLU:OE1	1.97	0.98
1:F:100:PHE:HB3	1:F:111:GLN:HE21	1.27	0.97
1:D:343:ASP:CB	4:D:672:HOH:O	2.16	0.93
1:C:46:ARG:HG2	1:C:46:ARG:HH11	1.32	0.93

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	399/418 (96%)	387 (97%)	12 (3%)	0	100	100
1	B	391/418 (94%)	382 (98%)	9 (2%)	0	100	100
1	C	399/418 (96%)	390 (98%)	9 (2%)	0	100	100
1	D	391/418 (94%)	383 (98%)	8 (2%)	0	100	100
1	E	400/418 (96%)	389 (97%)	10 (2%)	1 (0%)	41	51
1	F	384/418 (92%)	368 (96%)	16 (4%)	0	100	100
All	All	2364/2508 (94%)	2299 (97%)	64 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	235	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/366 (85%)	297 (96%)	14 (4%)	27	37
1	B	314/366 (86%)	291 (93%)	23 (7%)	14	18
1	C	324/366 (88%)	287 (89%)	37 (11%)	5	5
1	D	329/366 (90%)	310 (94%)	19 (6%)	20	26
1	E	334/366 (91%)	311 (93%)	23 (7%)	15	20
1	F	295/366 (81%)	270 (92%)	25 (8%)	10	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1907/2196 (87%)	1766 (93%)	141 (7%)	13 18

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	320	ARG
1	F	65	THR
1	F	196	GLU
1	C	89	MET
1	C	88	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	283	ASN
1	E	232	HIS
1	D	303	HIS
1	E	161	GLN
1	E	256	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands 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	OC9	D	502	2	8,8,8	0.23	0	7,7,7	0.59	0
3	OC9	A	502	2	8,8,8	0.35	0	7,7,7	0.59	0
2	HEM	A	501	1,3	27,50,50	1.53	6 (22%)	17,82,82	1.76	6 (35%)
3	OC9	E	502	2	8,8,8	0.30	0	7,7,7	1.10	1 (14%)
2	HEM	E	501	1,3	27,50,50	1.21	3 (11%)	17,82,82	1.28	3 (17%)
2	HEM	C	501	1,3	27,50,50	1.15	2 (7%)	17,82,82	1.42	5 (29%)
2	HEM	F	501	1	27,50,50	1.25	2 (7%)	17,82,82	1.19	2 (11%)
3	OC9	B	502	2	8,8,8	0.29	0	7,7,7	0.49	0
2	HEM	B	501	1,3	27,50,50	1.23	4 (14%)	17,82,82	1.88	4 (23%)
3	OC9	C	502	2	8,8,8	0.26	0	7,7,7	0.75	0
2	HEM	D	501	1,3	27,50,50	1.23	2 (7%)	17,82,82	1.65	4 (23%)

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	OC9	D	502	2	-	4/6/6/6	-
3	OC9	A	502	2	-	0/6/6/6	-
2	HEM	A	501	1,3	-	0/6/54/54	-
3	OC9	E	502	2	-	2/6/6/6	-
2	HEM	E	501	1,3	-	0/6/54/54	-
2	HEM	C	501	1,3	-	0/6/54/54	-
2	HEM	F	501	1	-	0/6/54/54	-
3	OC9	B	502	2	-	4/6/6/6	-
2	HEM	B	501	1,3	-	0/6/54/54	-
3	OC9	C	502	2	-	3/6/6/6	-
2	HEM	D	501	1,3	-	2/6/54/54	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-C2C	-3.63	1.35	1.40
2	A	501	HEM	C4D-C3D	3.52	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C2B	-3.24	1.35	1.40
2	A	501	HEM	C3C-C2C	-2.87	1.36	1.40
2	D	501	HEM	C3B-C2B	-2.85	1.36	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CAA-CBA-CGA	5.31	121.58	112.67
2	D	501	HEM	C4C-C3C-C2C	-4.03	104.08	106.90
2	A	501	HEM	CAD-CBD-CGD	3.35	118.29	112.67
2	A	501	HEM	C4C-C3C-C2C	-3.13	104.71	106.90
2	D	501	HEM	C1D-C2D-C3D	2.87	109.00	107.00

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
3	C	502	OC9	CAE-CAG-CAI-CAH
3	B	502	OC9	CAD-CAF-CAH-CAI
3	D	502	OC9	OAB-CAD-CAF-CAH

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	OC9	1	0
2	A	501	HEM	5	0
3	E	502	OC9	1	0
2	E	501	HEM	3	0
2	C	501	HEM	3	0
2	F	501	HEM	3	0
2	B	501	HEM	5	0
2	D	501	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 501

Bond lengths

Bond angles

Torsions

Rings

Ligand OC9 E 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM F 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand OC9 B 502	
Bond lengths	Bond angles
Torsions	Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand OC9 C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 501

Bond lengths

Bond angles

Torsions

Rings

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 (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	401/418 (95%)	0.35	14 (3%)	44	51	31, 58, 82, 101	0
1	B	397/418 (94%)	0.03	8 (2%)	65	72	30, 49, 80, 107	0
1	C	401/418 (95%)	-0.06	9 (2%)	62	68	26, 46, 72, 88	0
1	D	397/418 (94%)	-0.12	5 (1%)	77	82	24, 39, 75, 115	0
1	E	402/418 (96%)	-0.24	1 (0%)	95	97	20, 37, 56, 85	0
1	F	390/418 (93%)	0.27	15 (3%)	40	47	29, 57, 92, 114	0
All	All	2388/2508 (95%)	0.04	52 (2%)	62	68	20, 48, 80, 115	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ALA	4.2
1	A	418	ALA	4.0
1	E	418	ALA	3.7
1	F	224	ASN	3.6
1	F	248	LEU	3.5

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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	OC9	A	502	9/9	0.91	0.23	47,52,59,59	0
2	HEM	A	501	43/43	0.97	0.16	27,34,42,47	0
3	OC9	B	502	9/9	0.97	0.21	46,47,63,64	0
3	OC9	C	502	9/9	0.97	0.24	35,37,47,50	0
3	OC9	D	502	9/9	0.97	0.24	42,47,75,82	0
2	HEM	D	501	43/43	0.98	0.14	20,23,30,34	0
2	HEM	F	501	43/43	0.98	0.14	22,28,47,55	0
2	HEM	C	501	43/43	0.98	0.12	22,28,32,36	0
3	OC9	E	502	9/9	0.98	0.20	26,29,33,35	0
2	HEM	B	501	43/43	0.99	0.12	22,27,31,34	0
2	HEM	E	501	43/43	0.99	0.14	21,24,26,29	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 OC9 A 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
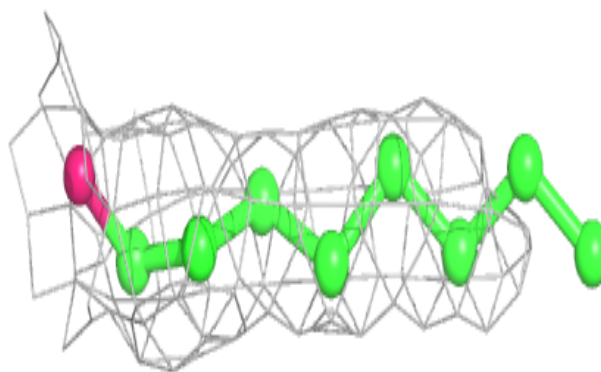$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
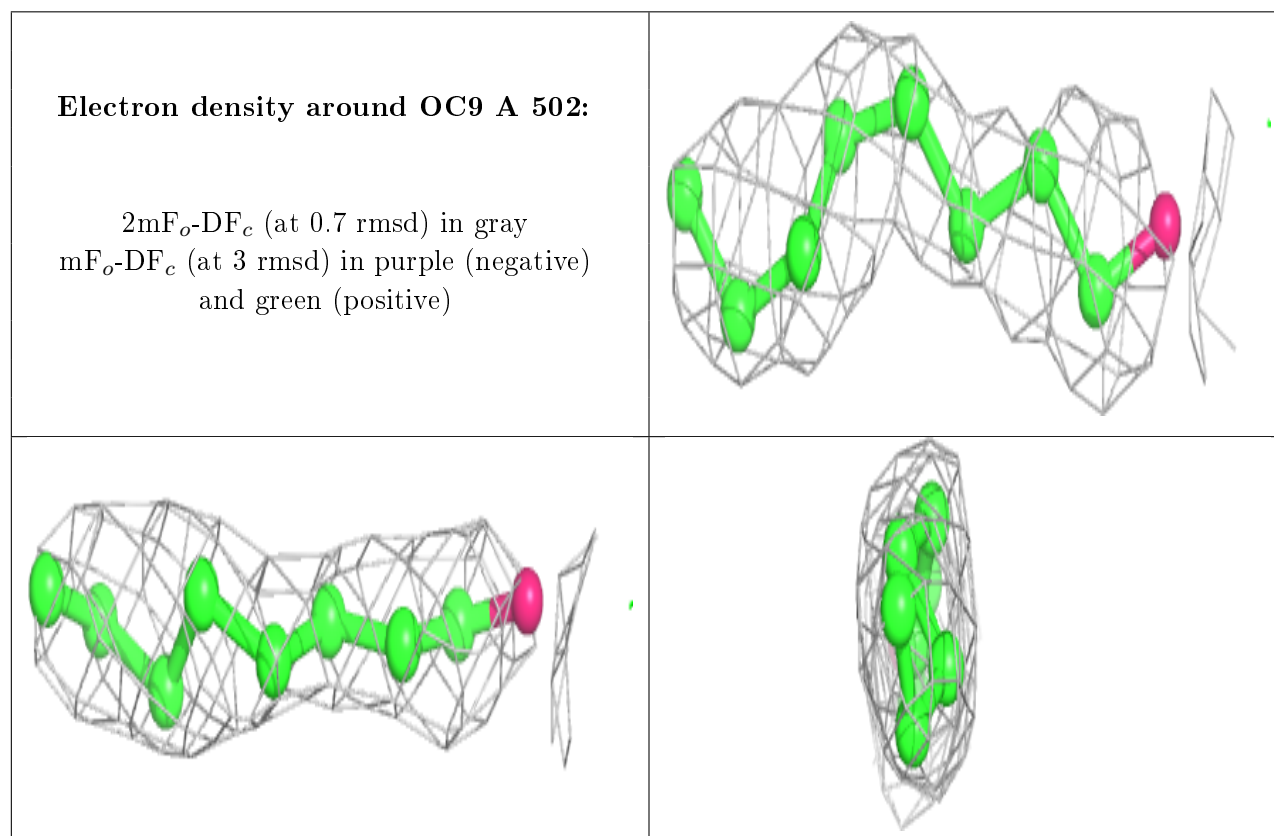
Electron density around HEM A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
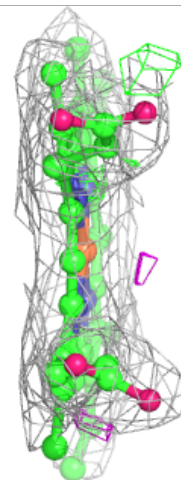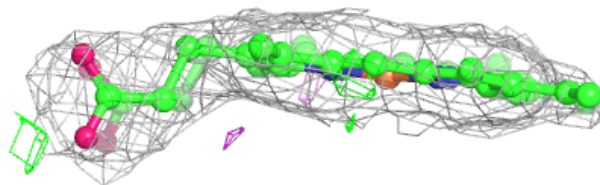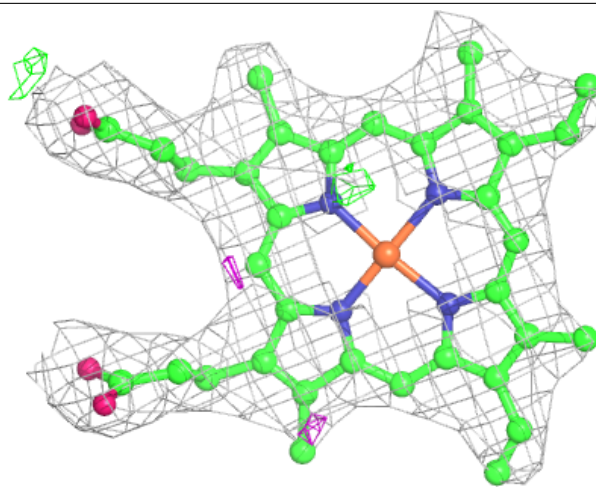
Electron density around OC9 B 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
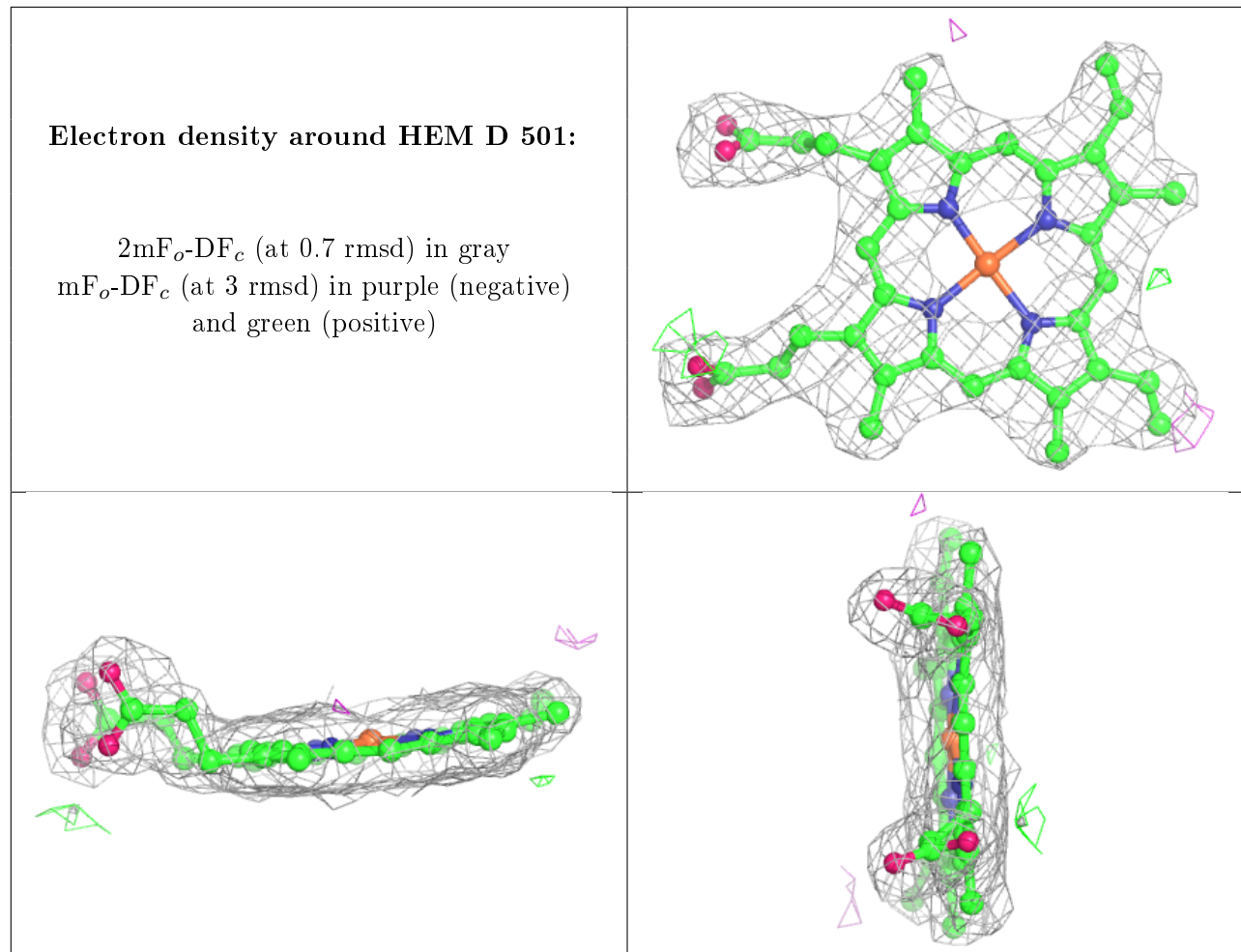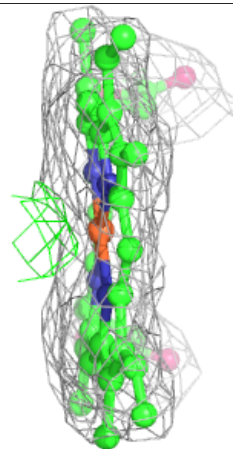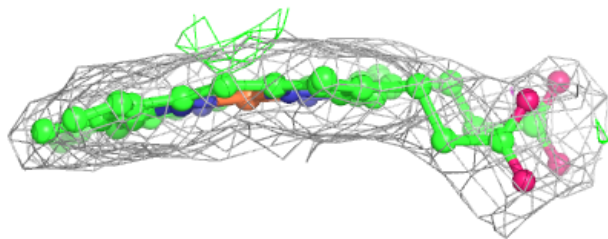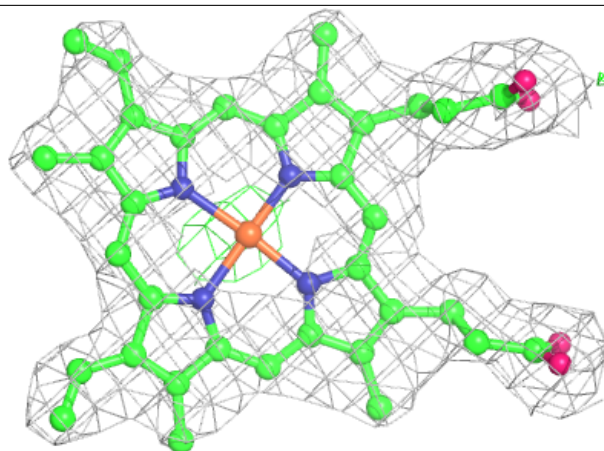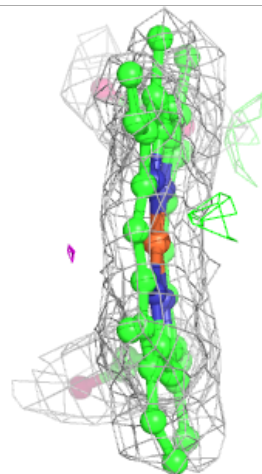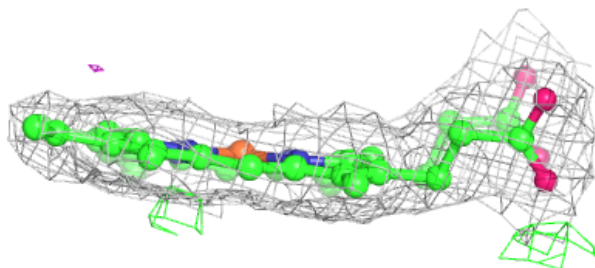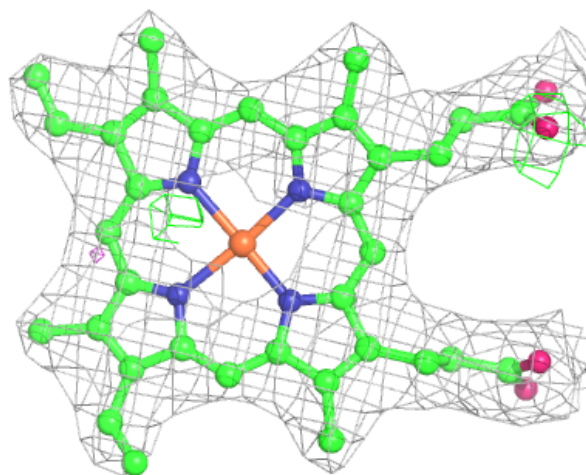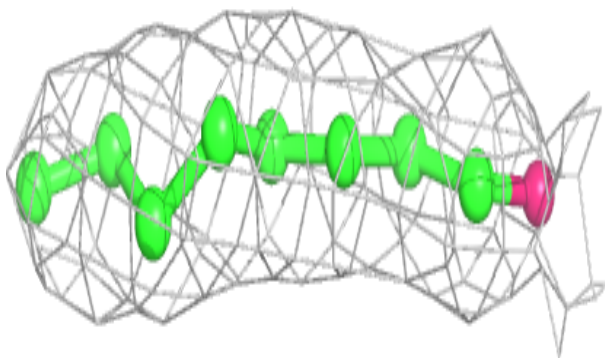and green (positive)
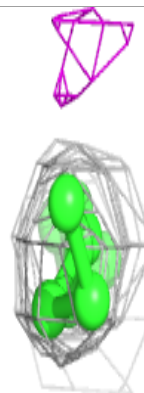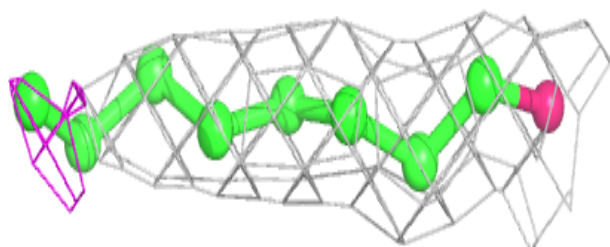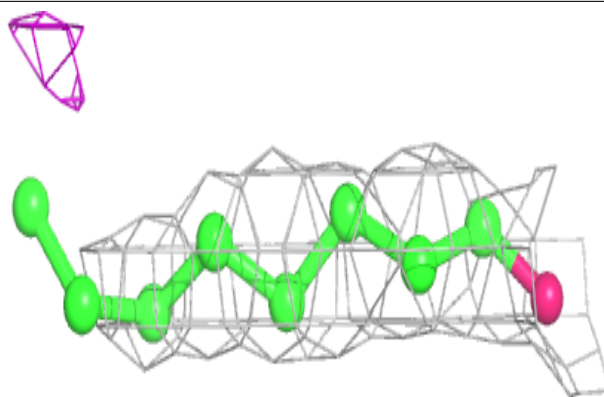
Electron density around OC9 C 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
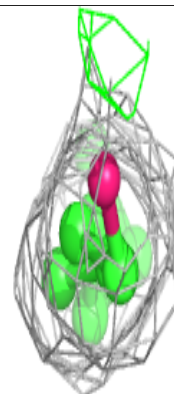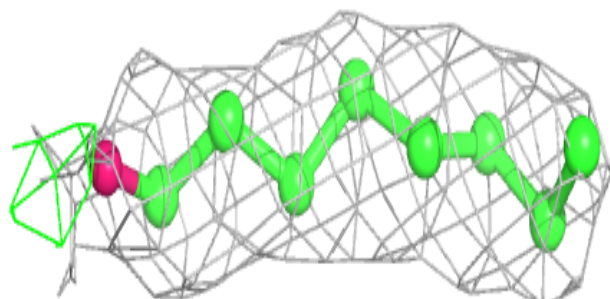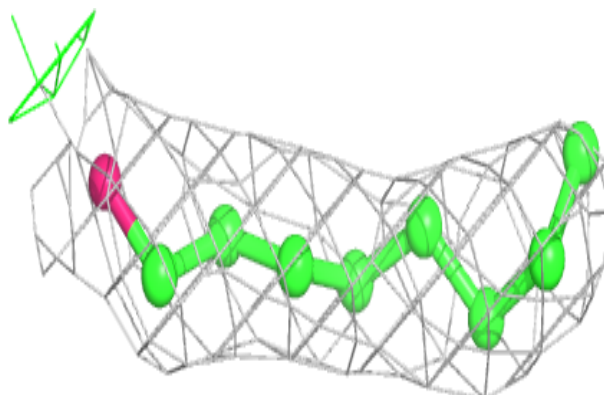
Electron density around OC9 D 502:

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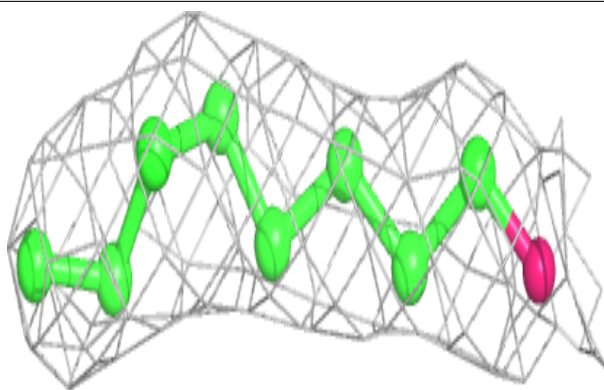mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
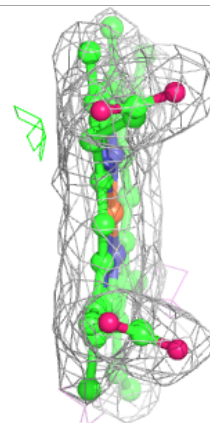mF_o-DF_c (at 3 rmsd) in purple (negative)
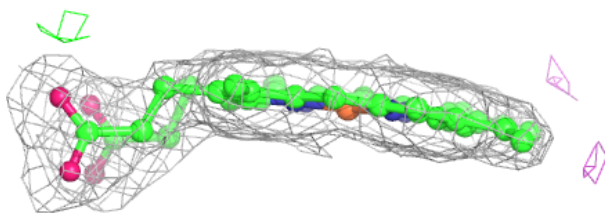and green (positive)
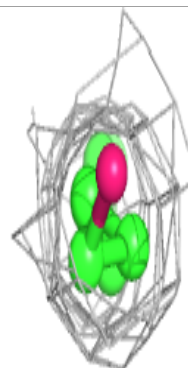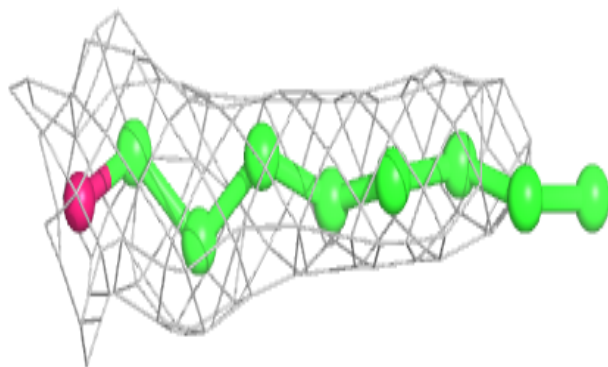
Electron density around HEM F 501:

$2mF_o$-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 C 501:

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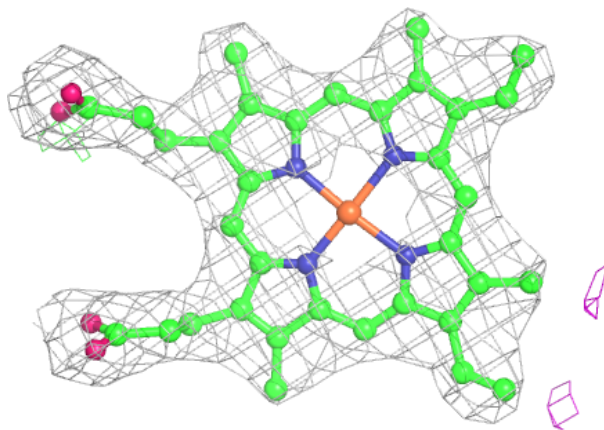and green (positive)

Electron density around OC9 E 502:

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

Electron density around HEM B 501:

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

Electron density around HEM E 501:

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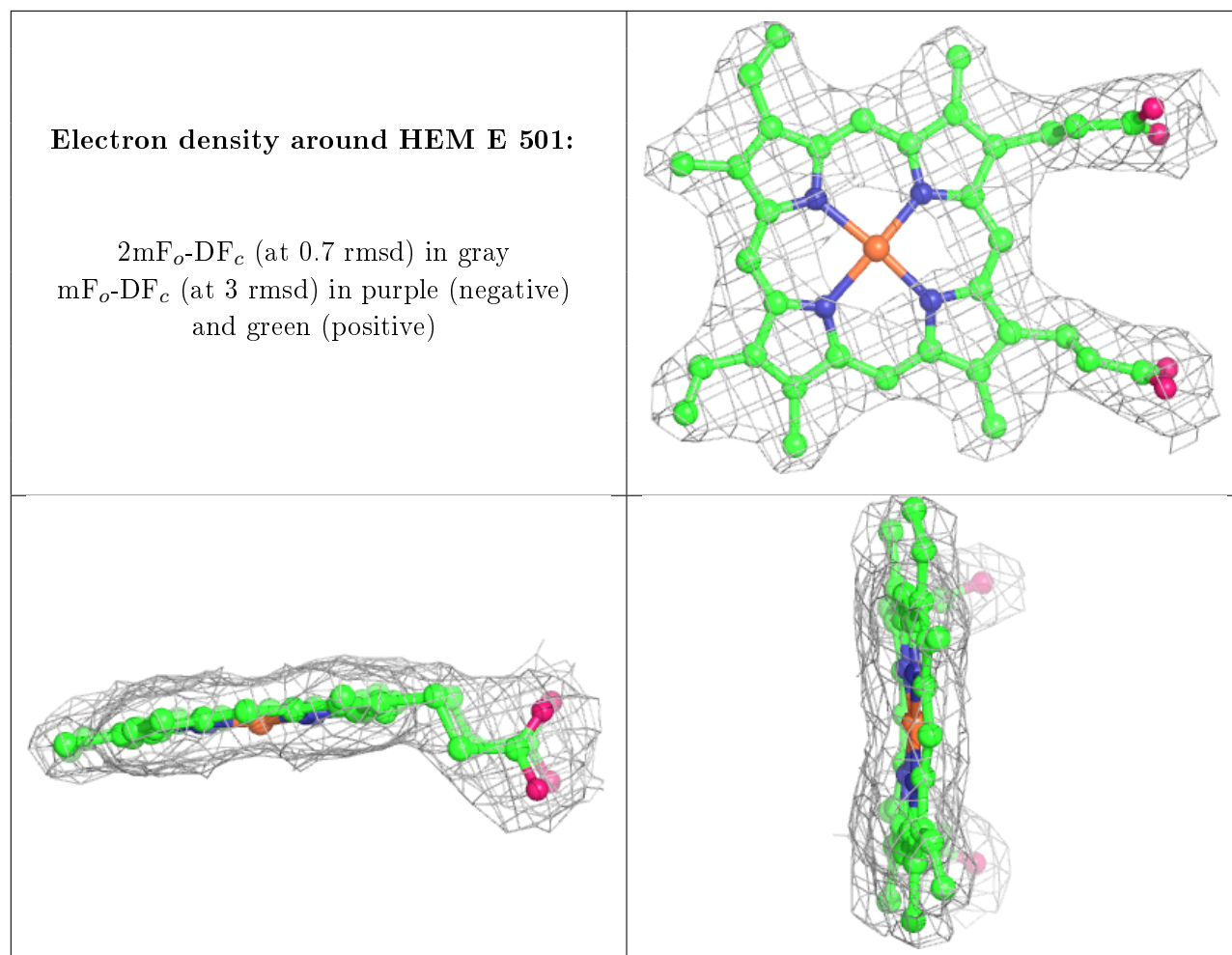mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.