Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 03:55 AM EDT

PDB ID	:	3MGX
Title	:	Crystal Structure of P450 OxyD that is involved in the Biosynthesis of Vancomycin-type Antibiotics
Authors	:	Cryle, M.J.; Schlichting, I.
Deposited on	:	2010-04-07
Resolution	:	2.10 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:

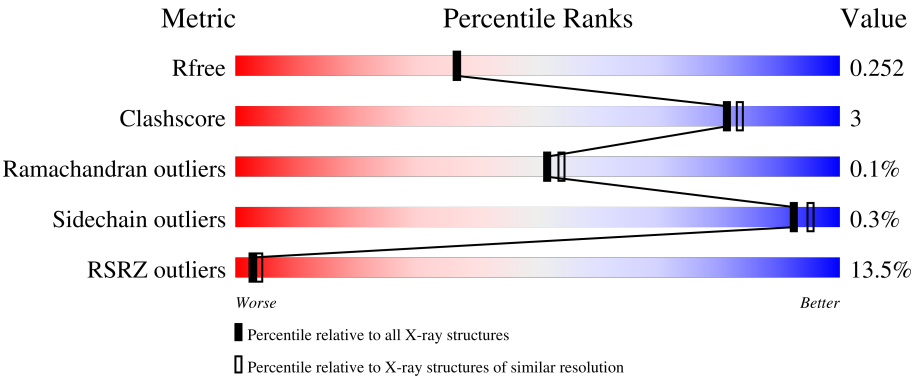
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	415	18% 86% 8% 7%
1	B	415	7% 89% 5% 6%

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
3	GOL	B	400	-	-	-	X
3	GOL	B	401	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6328 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 Putative P450 monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2966	1849	540	563	14			
1	B	391	Total	C	N	O	S	0	2	0
			3012	1879	544	575	14			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q939Y1
A	-17	SER	-	expression tag	UNP Q939Y1
A	-16	SER	-	expression tag	UNP Q939Y1
A	-15	HIS	-	expression tag	UNP Q939Y1
A	-14	HIS	-	expression tag	UNP Q939Y1
A	-13	HIS	-	expression tag	UNP Q939Y1
A	-12	HIS	-	expression tag	UNP Q939Y1
A	-11	HIS	-	expression tag	UNP Q939Y1
A	-10	HIS	-	expression tag	UNP Q939Y1
A	-9	SER	-	expression tag	UNP Q939Y1
A	-8	SER	-	expression tag	UNP Q939Y1
A	-7	GLY	-	expression tag	UNP Q939Y1
A	-6	LEU	-	expression tag	UNP Q939Y1
A	-5	VAL	-	expression tag	UNP Q939Y1
A	-4	PRO	-	expression tag	UNP Q939Y1
A	-3	ARG	-	expression tag	UNP Q939Y1
A	-2	GLY	-	expression tag	UNP Q939Y1
A	-1	SER	-	expression tag	UNP Q939Y1
A	0	HIS	-	expression tag	UNP Q939Y1
B	-18	GLY	-	expression tag	UNP Q939Y1
B	-17	SER	-	expression tag	UNP Q939Y1
B	-16	SER	-	expression tag	UNP Q939Y1
B	-15	HIS	-	expression tag	UNP Q939Y1
B	-14	HIS	-	expression tag	UNP Q939Y1
B	-13	HIS	-	expression tag	UNP Q939Y1

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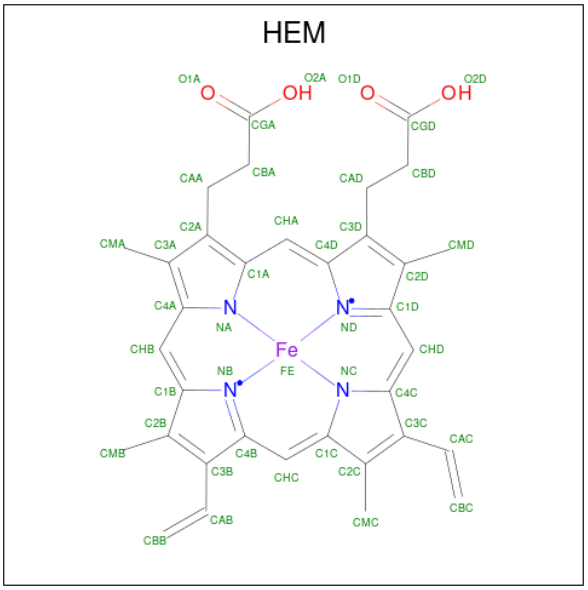
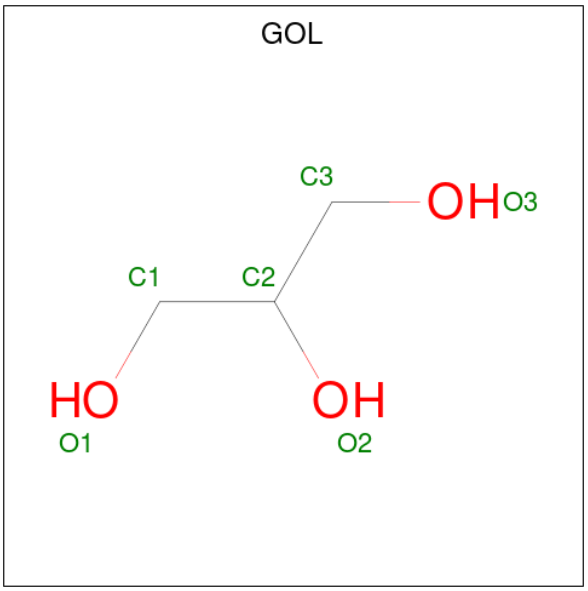
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP Q939Y1
B	-11	HIS	-	expression tag	UNP Q939Y1
B	-10	HIS	-	expression tag	UNP Q939Y1
B	-9	SER	-	expression tag	UNP Q939Y1
B	-8	SER	-	expression tag	UNP Q939Y1
B	-7	GLY	-	expression tag	UNP Q939Y1
B	-6	LEU	-	expression tag	UNP Q939Y1
B	-5	VAL	-	expression tag	UNP Q939Y1
B	-4	PRO	-	expression tag	UNP Q939Y1
B	-3	ARG	-	expression tag	UNP Q939Y1
B	-2	GLY	-	expression tag	UNP Q939Y1
B	-1	SER	-	expression tag	UNP Q939Y1
B	0	HIS	-	expression tag	UNP Q939Y1

- 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		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

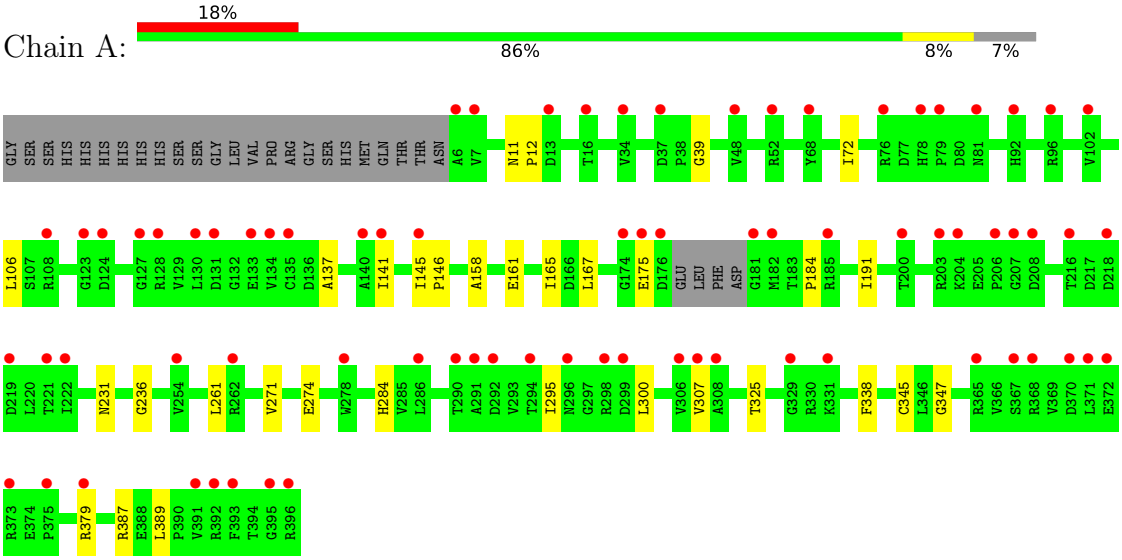
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0
4	B	136	Total O 136 136	0	0

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.

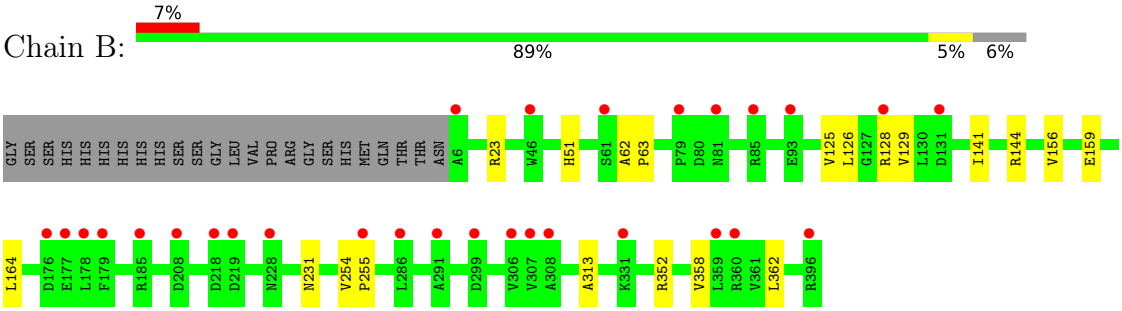
• Molecule 1: Putative P450 monooxygenase

Chain A:



• Molecule 1: Putative P450 monooxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.85Å 61.05Å 100.64Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	19.75 – 2.10 19.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.75-2.10) 99.9 (19.75-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.208 , 0.233 0.228 , 0.252	Depositor DCC
R_{free} test set	2286 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6328	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.30	0/3026	0.47	0/4123
1	B	0.30	0/3080	0.47	0/4199
All	All	0.30	0/6106	0.47	0/8322

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

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	2966	0	2928	20	0
1	B	3012	0	2967	11	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	30	0	40	0	0
3	B	30	0	40	2	0
4	A	68	0	0	0	0
4	B	136	0	0	0	0
All	All	6328	0	6035	31	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 3.

All (31) 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:A:161:GLU:O	1:A:165:ILE:HG12	1.99	0.62
1:B:128:ARG:HH21	1:B:144:ARG:HH12	1.49	0.58
1:B:358:VAL:O	1:B:362:LEU:HB2	2.04	0.58
1:A:261:LEU:HD21	1:A:271:VAL:HG21	1.88	0.55
1:A:145:ILE:HB	1:A:146:PRO:HD3	1.90	0.54
1:A:379:ARG:H	1:A:387:ARG:HH21	1.55	0.53
1:A:72:ILE:HG12	1:A:284:HIS:NE2	2.24	0.52
1:A:236:GLY:HA3	2:A:397:HEM:HBC2	1.93	0.51
1:A:175:GLU:HA	1:A:184:PRO:HG2	1.93	0.49
1:B:352:ARG:HB3	3:B:401:GOL:H31	1.94	0.48
1:B:156:VAL:HG21	1:B:164:LEU:HD12	1.95	0.48
1:A:325:THR:HG23	1:B:23:ARG:HH12	1.78	0.48
1:B:125:VAL:HG11	1:B:141:ILE:HG12	1.97	0.47
1:A:106:LEU:HD13	2:A:397:HEM:HAC	1.96	0.46
1:A:167:LEU:HB2	1:A:191:ILE:HD11	1.97	0.46
1:A:338:PHE:HB3	1:A:345:CYS:HB3	1.98	0.45
1:A:158:ALA:HA	1:A:161:GLU:HG3	1.97	0.45
1:A:137:ALA:HA	1:A:141:ILE:HG13	1.99	0.45
1:A:295:ILE:HD12	1:A:300:LEU:HD22	2.00	0.44
2:B:397:HEM:C4D	3:B:399:GOL:H11	2.52	0.44
1:A:137:ALA:HB3	1:A:389:LEU:HD23	2.00	0.44
1:A:137:ALA:HB3	1:A:389:LEU:HB3	2.00	0.44
1:A:347:GLY:HA3	2:A:397:HEM:C3C	2.53	0.43
1:A:72:ILE:HD11	1:A:307:VAL:HG21	1.99	0.43
1:B:51:HIS:HA	1:B:313:ALA:HB1	2.01	0.43
1:B:126:LEU:HA	1:B:129:VAL:HG22	2.01	0.42
1:B:254:VAL:HA	1:B:255:PRO:HD3	1.93	0.41
1:A:274:GLU:HA	1:A:274:GLU:OE1	2.21	0.41
1:B:159:GLU:H	1:B:159:GLU:CD	2.23	0.41
1:A:11:ASN:HA	1:A:12:PRO:HD3	1.89	0.41
1:B:62:ALA:HA	1:B:63:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	383/415 (92%)	368 (96%)	14 (4%)	1 (0%)	41 41
1	B	391/415 (94%)	384 (98%)	7 (2%)	0	100 100
All	All	774/830 (93%)	752 (97%)	21 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLY

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	317/342 (93%)	316 (100%)	1 (0%)	92 95
1	B	323/342 (94%)	322 (100%)	1 (0%)	92 95
All	All	640/684 (94%)	638 (100%)	2 (0%)	92 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	B	231	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	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)

12 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	GOL	A	398	-	5,5,5	0.39	0	5,5,5	0.25	0
3	GOL	B	399	-	5,5,5	0.34	0	5,5,5	0.43	0
3	GOL	B	398	-	5,5,5	0.36	0	5,5,5	0.26	0
2	HEM	A	397	1,4	41,50,50	1.99	9 (21%)	45,82,82	1.69	5 (11%)
3	GOL	A	400	-	5,5,5	0.37	0	5,5,5	0.35	0
2	HEM	B	397	1,4	41,50,50	1.93	8 (19%)	45,82,82	1.67	6 (13%)
3	GOL	A	399	-	5,5,5	0.41	0	5,5,5	0.17	0
3	GOL	A	402	-	5,5,5	0.38	0	5,5,5	0.22	0
3	GOL	A	401	-	5,5,5	0.36	0	5,5,5	0.33	0
3	GOL	B	401	-	5,5,5	0.35	0	5,5,5	0.27	0
3	GOL	B	400	-	5,5,5	0.36	0	5,5,5	0.26	0
3	GOL	B	402	-	5,5,5	0.37	0	5,5,5	0.27	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
3	GOL	A	398	-	-	0/4/4/4	-
3	GOL	B	399	-	-	4/4/4/4	-
3	GOL	B	398	-	-	0/4/4/4	-
2	HEM	A	397	1,4	-	3/12/54/54	-
3	GOL	A	400	-	-	2/4/4/4	-
2	HEM	B	397	1,4	-	0/12/54/54	-
3	GOL	A	399	-	-	2/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	A	401	-	-	2/4/4/4	-
3	GOL	B	401	-	-	4/4/4/4	-
3	GOL	B	400	-	-	2/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	397	HEM	C3D-C2D	7.99	1.53	1.36
2	B	397	HEM	C3D-C2D	7.91	1.53	1.36
2	A	397	HEM	C3C-C2C	-4.14	1.34	1.40
2	B	397	HEM	C3C-CAC	3.84	1.55	1.47
2	A	397	HEM	C3C-CAC	3.75	1.55	1.47
2	B	397	HEM	C3C-C2C	-3.75	1.35	1.40
2	A	397	HEM	FE-ND	3.04	2.11	1.96
2	A	397	HEM	CAB-C3B	2.93	1.55	1.47
2	B	397	HEM	CAB-C3B	2.80	1.55	1.47
2	B	397	HEM	FE-ND	2.36	2.08	1.96
2	B	397	HEM	CAA-C2A	2.23	1.55	1.52
2	A	397	HEM	FE-NB	2.18	2.07	1.96
2	B	397	HEM	CMB-C2B	2.16	1.55	1.50
2	A	397	HEM	CMD-C2D	2.08	1.55	1.50
2	A	397	HEM	CAA-C2A	2.05	1.55	1.52
2	B	397	HEM	CMD-C2D	2.05	1.55	1.50
2	A	397	HEM	CMB-C2B	2.01	1.55	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	397	HEM	C4D-ND-C1D	6.43	111.72	105.07
2	B	397	HEM	C4D-ND-C1D	6.20	111.48	105.07
2	A	397	HEM	C4C-CHD-C1D	3.54	127.23	122.56
2	A	397	HEM	C1B-NB-C4B	3.48	108.66	105.07
2	B	397	HEM	C4B-CHC-C1C	3.24	126.83	122.56
2	B	397	HEM	C1B-NB-C4B	3.08	108.25	105.07
2	B	397	HEM	C4C-CHD-C1D	3.07	126.60	122.56
2	A	397	HEM	C4B-CHC-C1C	2.98	126.49	122.56
2	A	397	HEM	C3B-C2B-C1B	2.23	108.14	106.49
2	B	397	HEM	C3B-C2B-C1B	2.13	108.06	106.49
2	B	397	HEM	CMA-C3A-C4A	-2.10	125.23	128.46

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	399	GOL	C1-C2-C3-O3
3	A	400	GOL	C1-C2-C3-O3
3	A	401	GOL	C1-C2-C3-O3
3	B	399	GOL	C1-C2-C3-O3
3	B	400	GOL	O1-C1-C2-C3
3	B	401	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	B	402	GOL	O1-C1-C2-O2
3	B	399	GOL	O1-C1-C2-C3
3	B	401	GOL	O1-C1-C2-C3
3	A	401	GOL	O2-C2-C3-O3
3	B	399	GOL	O2-C2-C3-O3
3	B	401	GOL	O2-C2-C3-O3
3	A	400	GOL	O2-C2-C3-O3
2	A	397	HEM	C2B-C3B-CAB-CBB
3	A	399	GOL	O2-C2-C3-O3
3	B	399	GOL	O1-C1-C2-O2
3	B	400	GOL	O1-C1-C2-O2
3	B	401	GOL	O1-C1-C2-O2
2	A	397	HEM	C4B-C3B-CAB-CBB
2	A	397	HEM	CAA-CBA-CGA-O2A

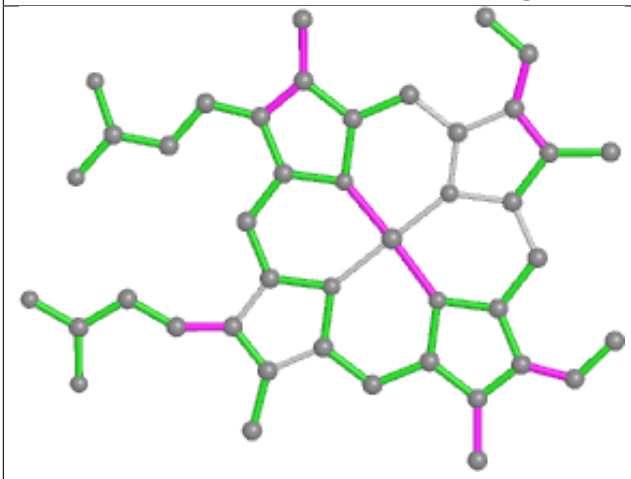
There are no ring outliers.

4 monomers are involved in 5 short contacts:

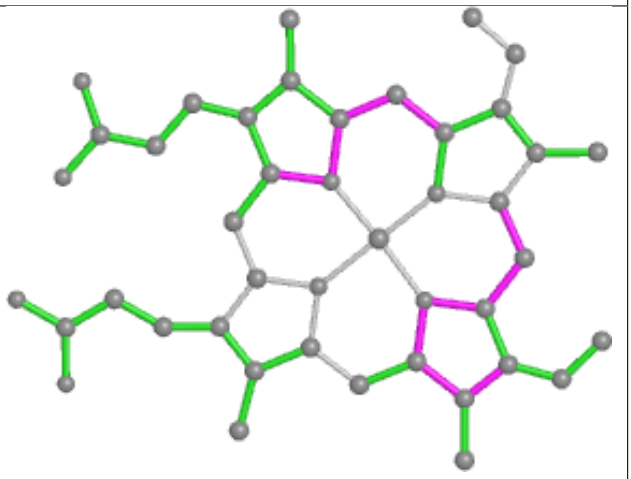
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	399	GOL	1	0
2	A	397	HEM	3	0
2	B	397	HEM	1	0
3	B	401	GOL	1	0

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.

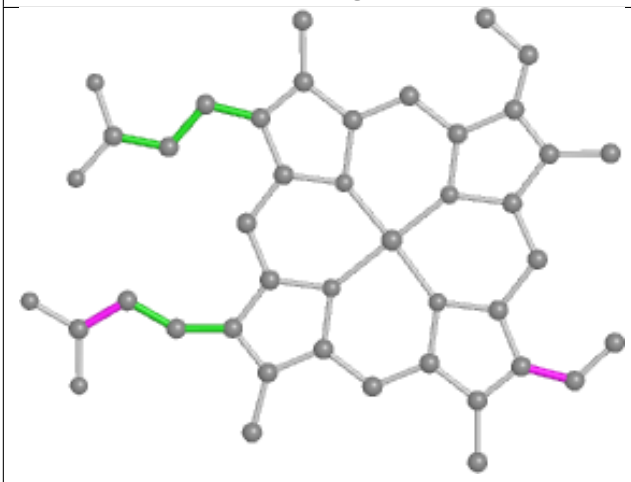
Ligand HEM A 397



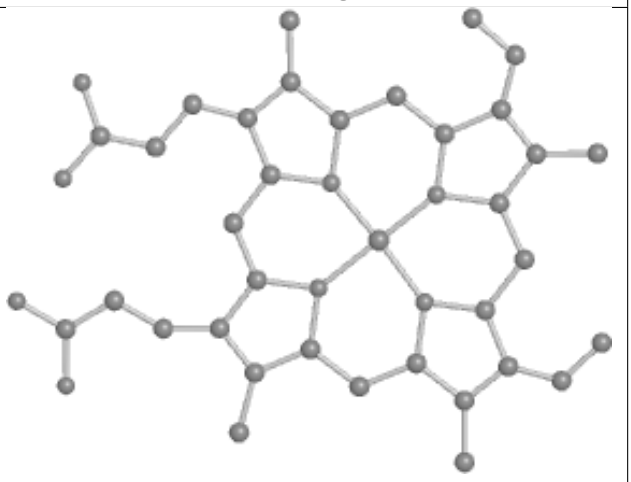
Bond lengths



Bond angles

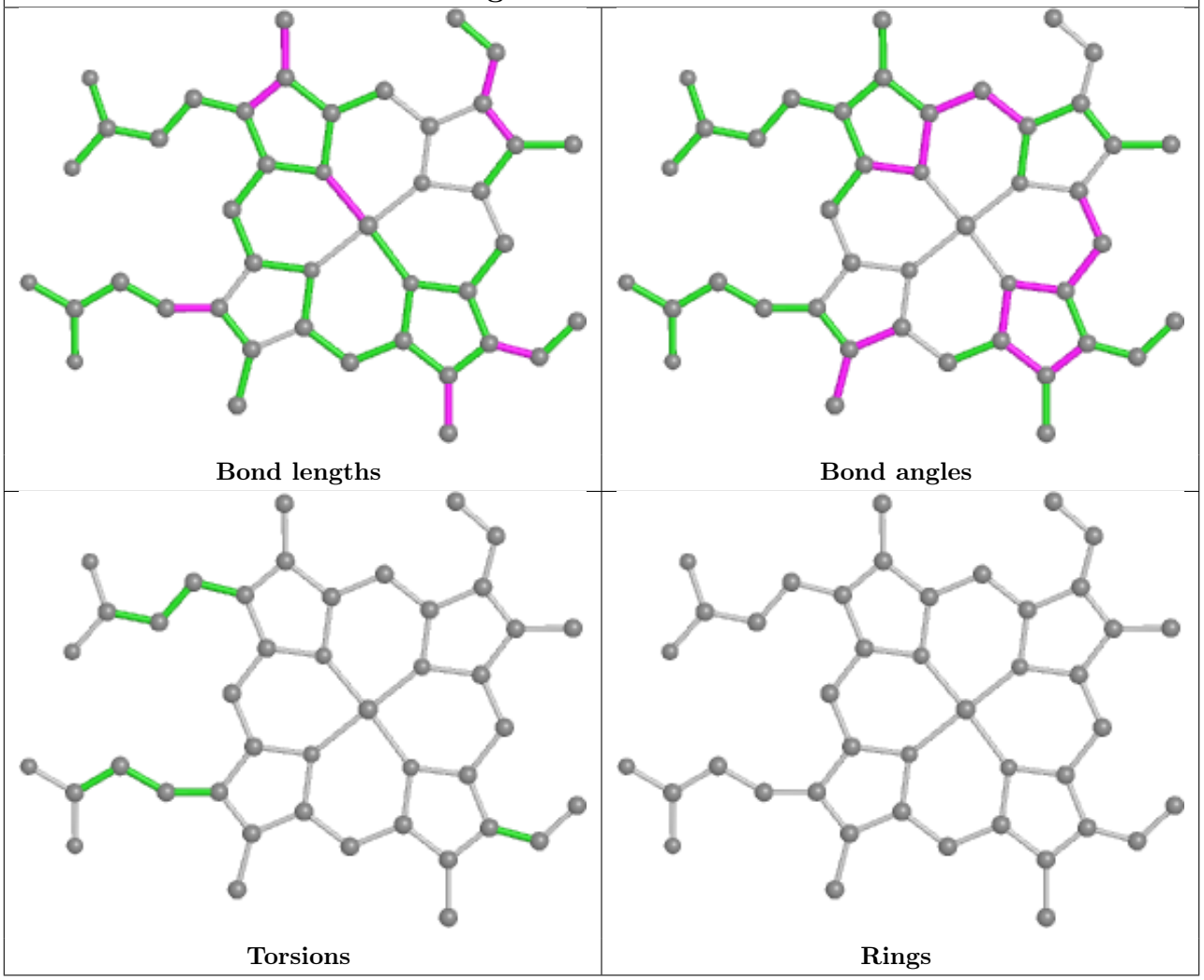


Torsions



Rings

Ligand HEM B 397



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	387/415 (93%)	1.18	76 (19%) 1 1	30, 50, 80, 95	0
1	B	391/415 (94%)	0.61	29 (7%) 14 18	19, 35, 60, 76	0
All	All	778/830 (93%)	0.89	105 (13%) 3 4	19, 43, 72, 95	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	GLY	7.4
1	A	396	ARG	7.0
1	A	128	ARG	6.8
1	A	174	GLY	6.6
1	A	6	ALA	5.8
1	A	292	ASP	5.4
1	A	204	LYS	5.3
1	A	176	ASP	5.1
1	A	134	VAL	5.1
1	A	208	ASP	5.0
1	B	176	ASP	4.8
1	A	127	GLY	4.8
1	A	203	ARG	4.7
1	A	307	VAL	4.7
1	B	131	ASP	4.2
1	A	140	ALA	4.1
1	A	131	ASP	4.1
1	A	133	GLU	3.9
1	B	219	ASP	3.9
1	B	396	ARG	3.9
1	A	370	ASP	3.8
1	B	307	VAL	3.7
1	A	368	ARG	3.7
1	B	218	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	306	VAL	3.6
1	A	373	ARG	3.5
1	B	299	ASP	3.5
1	A	218	ASP	3.4
1	A	81	ASN	3.4
1	A	207	GLY	3.4
1	A	219	ASP	3.3
1	B	306	VAL	3.3
1	A	291	ALA	3.3
1	A	7	VAL	3.2
1	B	291	ALA	3.2
1	A	372	GLU	3.1
1	A	367	SER	3.1
1	A	206	PRO	3.1
1	B	93	GLU	3.1
1	A	68	TYR	3.1
1	B	6	ALA	3.0
1	A	278	TRP	3.0
1	B	81	ASN	3.0
1	A	392	ARG	2.9
1	A	185	ARG	2.9
1	A	298	ARG	2.9
1	A	48	VAL	2.8
1	A	182	MET	2.8
1	A	222	ILE	2.8
1	A	108	ARG	2.8
1	A	92	HIS	2.8
1	A	329	GLY	2.8
1	A	76	ARG	2.7
1	B	185	ARG	2.7
1	B	61	SER	2.7
1	A	141	ILE	2.7
1	A	299	ASP	2.7
1	B	331	LYS	2.7
1	B	255	PRO	2.7
1	A	391	VAL	2.7
1	B	208	ASP	2.7
1	A	96	ARG	2.7
1	B	128	ARG	2.7
1	B	179	PHE	2.7
1	A	52	ARG	2.6
1	A	175	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	294	THR	2.6
1	A	130	LEU	2.6
1	A	379	ARG	2.6
1	A	375	PRO	2.6
1	A	365	ARG	2.6
1	A	16	THR	2.5
1	A	13	ASP	2.5
1	A	200	THR	2.5
1	A	221	THR	2.5
1	A	123	GLY	2.5
1	A	181	GLY	2.5
1	A	135	CYS	2.4
1	A	124	ASP	2.4
1	B	308	ALA	2.4
1	A	216	THR	2.4
1	A	254	VAL	2.4
1	A	262	ARG	2.4
1	A	393	PHE	2.4
1	A	290	THR	2.4
1	A	296	ASN	2.3
1	B	359	LEU	2.3
1	A	34	VAL	2.3
1	B	360	ARG	2.2
1	A	102	VAL	2.2
1	A	145	ILE	2.2
1	A	286	LEU	2.2
1	B	178	LEU	2.2
1	B	228	ASN	2.2
1	A	331	LYS	2.2
1	B	46	TRP	2.1
1	A	78	HIS	2.1
1	B	79	PRO	2.1
1	A	308	ALA	2.1
1	A	371	LEU	2.0
1	B	286	LEU	2.0
1	A	79	PRO	2.0
1	B	177	GLU	2.0
1	A	37	ASP	2.0
1	B	85	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

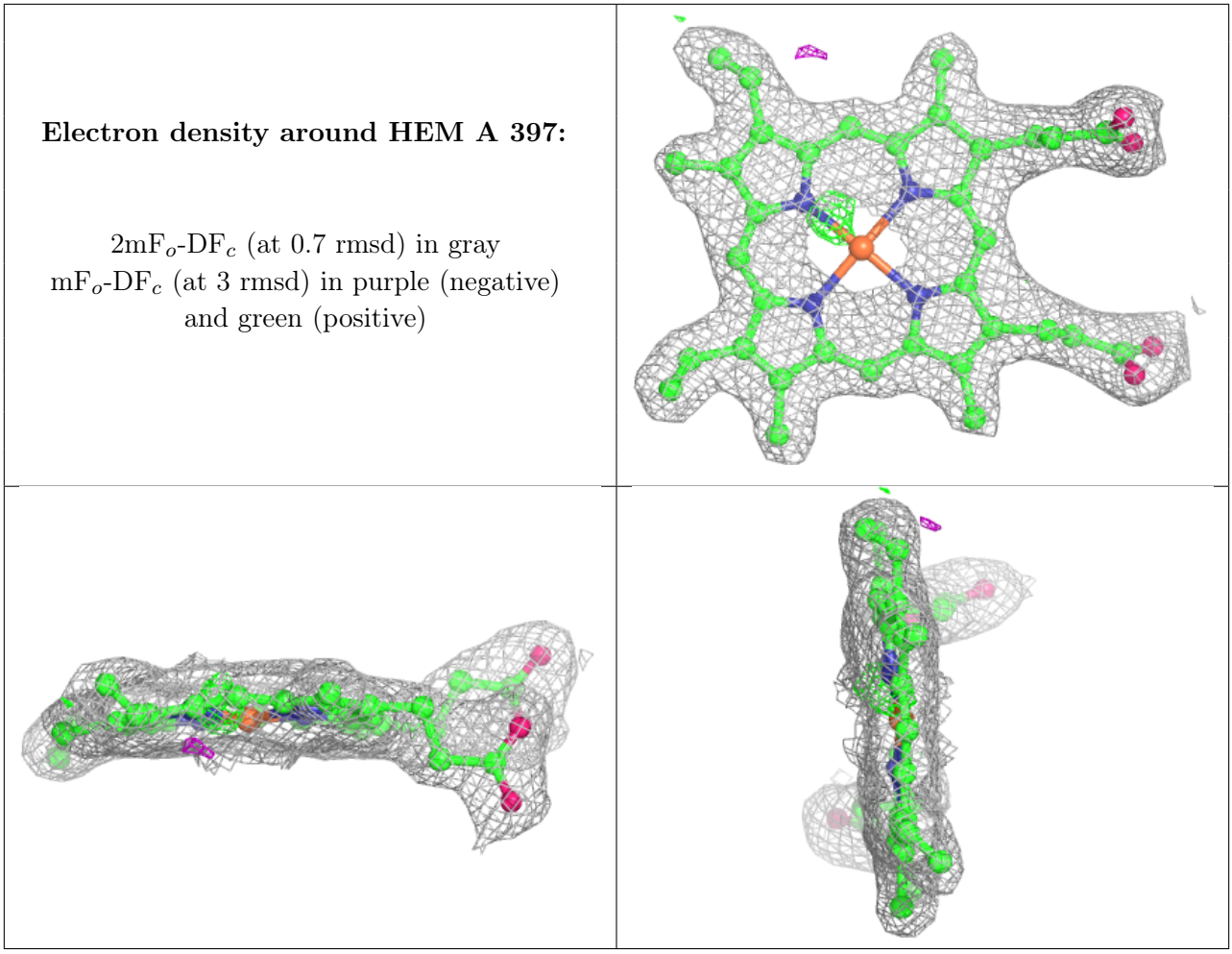
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GOL	B	401	6/6	0.13	0.56	78,78,78,79	0
3	GOL	B	402	6/6	0.56	0.23	73,73,73,73	0
3	GOL	B	400	6/6	0.59	0.52	74,74,74,74	0
3	GOL	A	402	6/6	0.71	0.38	80,80,80,81	0
3	GOL	A	401	6/6	0.80	0.35	58,58,58,59	0
3	GOL	A	400	6/6	0.84	0.20	57,57,57,57	0
3	GOL	B	399	6/6	0.88	0.21	48,48,49,49	0
3	GOL	A	398	6/6	0.89	0.26	46,46,46,46	0
3	GOL	B	398	6/6	0.92	0.15	37,38,38,38	0
3	GOL	A	399	6/6	0.93	0.18	53,53,53,53	0
2	HEM	A	397	43/43	0.97	0.11	26,28,31,33	0
2	HEM	B	397	43/43	0.98	0.10	16,18,21,21	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.

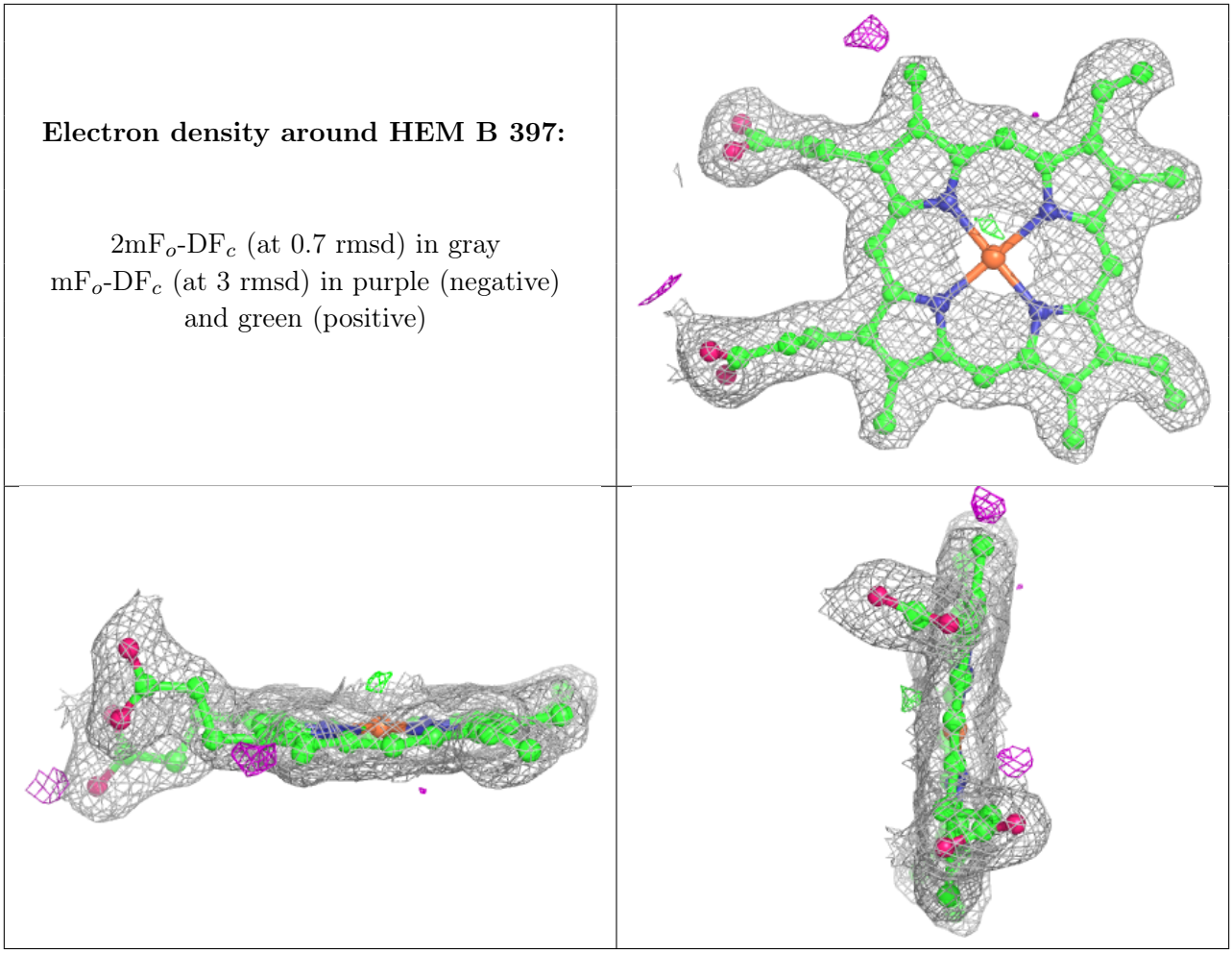
Electron density around HEM A 397:

$2mF_o$-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 397:

$2mF_o$-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

There are no such residues in this entry.