Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:56 AM EDT

PDB ID	:	6NH7
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-(3-(dimethylamino)propyl)-2,5,6-trifluorophenethyl)-4-methylpyridin-2-amine
Authors	:	Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on	:	2018-12-21
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

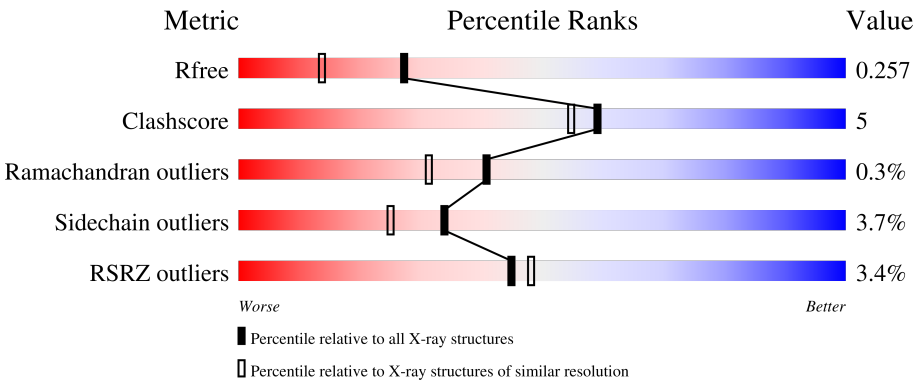
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	440	3% 81% 10% 9%
1	B	440	3% 80% 11% 9%

2 Entry composition (i)

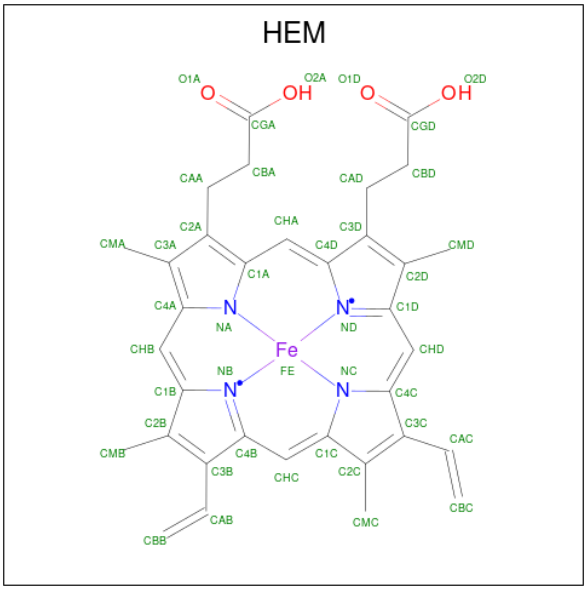
There are 7 unique types of molecules in this entry. The entry contains 7012 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endothelial nitric oxide synthase splice variant eNOS13A.

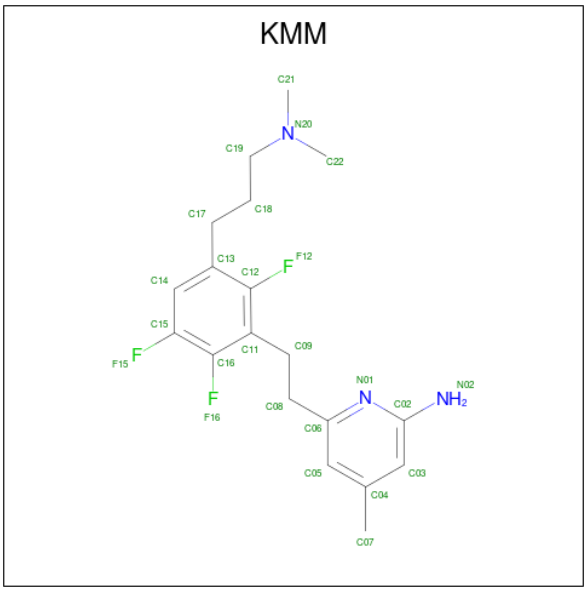
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3220	2051	566	587	16	0	4	0
1	B	402	3232	2058	569	588	17	0	5	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



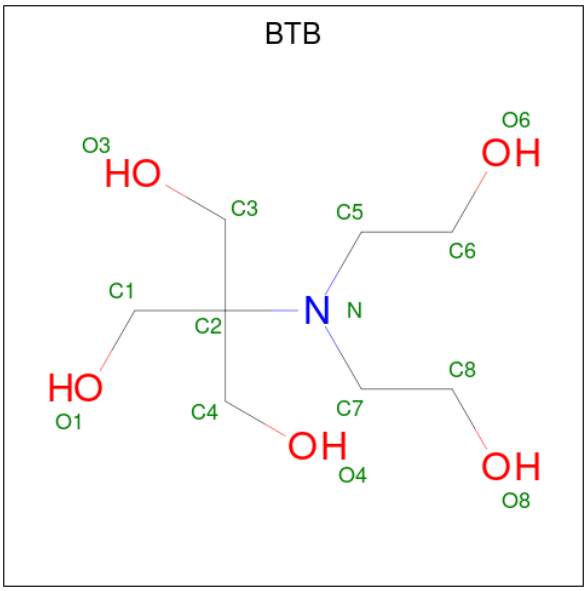
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is 6-(2-{3-[3-(dimethylamino)propyl]-2,5,6-trifluorophenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: KMM) (formula: $C_{19}H_{24}F_3N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
3	A	1	25	19	3	3	0	0
			Total	C	F	N		
3	A	1	25	19	3	3	0	0
			Total	C	F	N		
3	B	1	25	19	3	3	0	0
			Total	C	F	N		
3	B	1	25	19	3	3	0	0

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Gd		
6	A	2	2	2	0	0
6	B	2	2	2	0	0

- Molecule 7 is water.

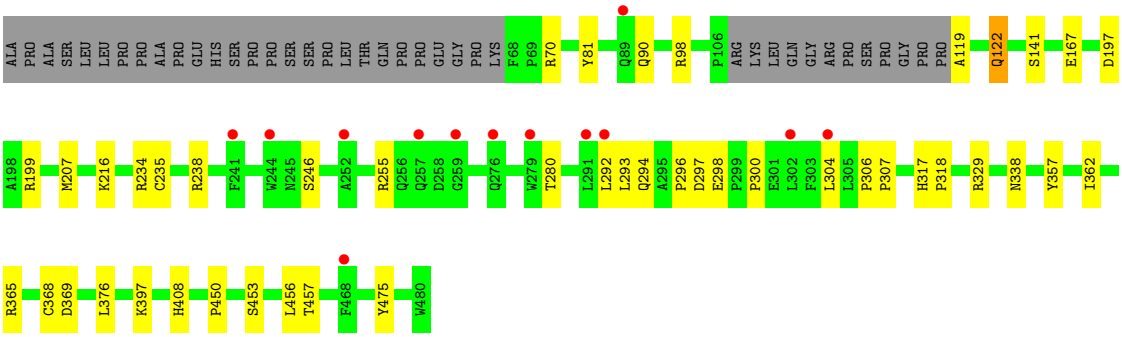
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	111	111	111	0	0
7	B	160	160	160	0	0

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.

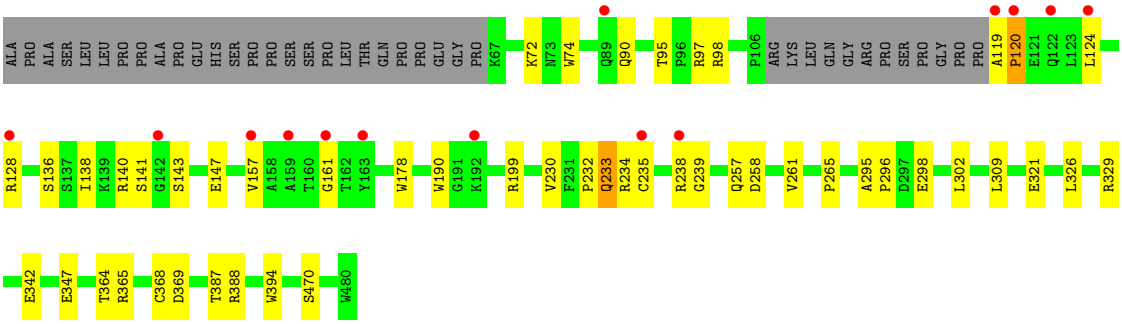
• Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A

Chain A:



• Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.96Å 109.38Å 153.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.73 – 1.90 76.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (76.73-1.90) 99.9 (76.73-1.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.210 , 0.258 0.209 , 0.257	Depositor DCC
R_{free} test set	3723 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	1.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7012	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GD, HEM, BTB, KMM, ZN

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	0.35	0/3324	0.51	0/4529
1	B	0.39	0/3336	0.54	0/4545
All	All	0.37	0/6660	0.53	0/9074

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	3220	0	3127	22	0
1	B	3232	0	3144	22	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	50	0	0	0	0
3	B	50	0	0	0	0
4	A	56	0	76	8	0
4	B	42	0	56	8	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	111	0	0	4	1
7	B	160	0	0	2	1
All	All	7012	0	6463	62	1

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 5.

All (62) 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)
4:B:504:BTB:O6	7:B:601:HOH:O	2.03	0.77
1:B:233:GLN:O	1:B:238:ARG:NH2	2.28	0.67
1:A:408:HIS:ND1	7:A:601:HOH:O	2.28	0.65
1:A:365:ARG:NH2	1:A:369:ASP:OD2	2.32	0.63
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.81	0.62
4:B:504:BTB:H61	7:B:683:HOH:O	2.03	0.59
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.84	0.59
1:B:365[A]:ARG:NH2	1:B:369:ASP:OD2	2.37	0.57
1:B:261:VAL:HG11	1:B:265:PRO:HA	1.87	0.57
1:B:234:ARG:NH1	1:B:347:GLU:OE1	2.36	0.56
1:B:321:GLU:OE2	4:B:504:BTB:O4	2.23	0.56
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.87	0.55
1:A:296:PRO:O	1:A:298:GLU:N	2.33	0.54
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.43	0.54
1:B:295:ALA:HB3	1:B:298:GLU:HG3	1.90	0.53
1:A:246:SER:HA	1:A:338:ASN:HB3	1.91	0.53
1:A:298:GLU:OE2	4:A:507:BTB:O8	2.23	0.53
1:B:238:ARG:NH1	1:B:239:GLY:O	2.43	0.52
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.24	0.51
1:A:119:ALA:HB1	1:A:122:GLN:HB3	1.94	0.50
1:B:119:ALA:N	1:B:120:PRO:HD2	2.27	0.50
1:B:235[B]:CYS:SG	1:B:238:ARG:NE	2.80	0.49
4:A:505:BTB:H12	4:A:505:BTB:O6	2.13	0.48
1:A:207:MET:HG2	1:A:293:LEU:HD13	1.96	0.47
1:A:167:GLU:HG2	4:A:506:BTB:H51	1.96	0.47
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.50	0.47
1:B:124:LEU:HD13	1:B:128:ARG:HH22	1.80	0.47
1:B:143:SER:O	1:B:147:GLU:HG3	2.14	0.47
1:B:364:THR:O	1:B:368:CYS:HB2	2.16	0.46
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.97	0.46
1:B:124:LEU:HG	1:B:157:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HD3	1:B:74:TRP:CZ2	2.50	0.45
4:B:504:BTB:H32	4:B:504:BTB:H51	1.85	0.45
1:B:387:THR:HA	1:B:394:TRP:CD1	2.52	0.45
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.56	0.45
4:B:504:BTB:H11	4:B:504:BTB:H72	1.85	0.45
1:B:199:ARG:O	1:B:232:PRO:HG3	2.17	0.44
4:B:505:BTB:H52	4:B:505:BTB:H81	1.32	0.44
4:A:506:BTB:H62	4:A:506:BTB:H71	1.61	0.44
1:A:70:ARG:NH1	7:A:612:HOH:O	2.51	0.44
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.98	0.44
4:B:505:BTB:H31	4:B:505:BTB:H51	1.61	0.43
1:A:306:PRO:HA	1:A:307:PRO:HD3	1.90	0.43
4:A:505:BTB:O4	4:A:505:BTB:O1	2.27	0.43
4:B:506:BTB:H71	4:B:506:BTB:H12	1.64	0.43
1:B:138:ILE:O	1:B:140:ARG:HG2	2.17	0.43
1:A:294:GLN:HB2	1:A:300:PRO:HB3	2.01	0.43
1:B:238:ARG:HH11	1:B:296:PRO:HG3	1.84	0.42
1:A:376:LEU:HB2	7:A:613:HOH:O	2.19	0.42
1:A:70:ARG:HB2	1:A:81:TYR:CE2	2.54	0.42
4:A:507:BTB:H72	4:A:507:BTB:H41	1.56	0.42
4:A:505:BTB:H31	4:A:505:BTB:H52	1.32	0.41
4:A:504:BTB:H32	4:A:504:BTB:H51	1.77	0.41
1:B:157:VAL:O	1:B:161:GLY:N	2.46	0.41
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.38	0.41
2:B:501:HEM:HBB2	2:B:501:HEM:CHC	2.48	0.41
1:A:357:TYR:CD2	1:A:362:ILE:HD11	2.57	0.40
1:A:397:LYS:NZ	7:A:615:HOH:O	2.53	0.40
1:B:95:THR:OG1	1:B:97:ARG:HG2	2.20	0.40
1:B:342:GLU:OE1	1:B:470:SER:OG	2.34	0.40
2:B:501:HEM:CMC	2:B:501:HEM:HBC2	2.51	0.40
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:606:HOH:O	7:B:601:HOH:O[4_555]	1.89	0.31

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	401/440 (91%)	393 (98%)	7 (2%)	1 (0%)	47	38
1	B	403/440 (92%)	392 (97%)	10 (2%)	1 (0%)	47	38
All	All	804/880 (91%)	785 (98%)	17 (2%)	2 (0%)	41	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	PRO
1	A	297	ASP

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	344/373 (92%)	332 (96%)	12 (4%)	36	27
1	B	346/373 (93%)	331 (96%)	15 (4%)	29	19
All	All	690/746 (92%)	663 (96%)	27 (4%)	34	23

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	98	ARG
1	A	122	GLN
1	A	141	SER

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Mol	Chain	Res	Type
1	A	216	LYS
1	A	234	ARG
1	A	235	CYS
1	A	238	ARG
1	A	255	ARG
1	A	280	THR
1	A	304	LEU
1	A	329	ARG
1	B	90	GLN
1	B	98	ARG
1	B	136[A]	SER
1	B	136[B]	SER
1	B	141[A]	SER
1	B	141[B]	SER
1	B	230	VAL
1	B	233	GLN
1	B	257	GLN
1	B	258	ASP
1	B	302	LEU
1	B	309	LEU
1	B	326	LEU
1	B	329	ARG
1	B	388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
4	BTB	B	506	-	13,13,13	0.57	0	7,16,16	0.68	0
3	KMM	A	503	-	26,26,26	0.38	0	36,36,36	2.14	9 (25%)
4	BTB	A	504	6	13,13,13	0.43	0	7,16,16	0.68	0
4	BTB	A	506	-	13,13,13	0.56	0	7,16,16	0.76	0
3	KMM	B	502	-	26,26,26	0.63	0	36,36,36	2.25	10 (27%)
4	BTB	A	505	-	13,13,13	0.46	0	7,16,16	0.56	0
3	KMM	A	502	-	26,26,26	0.42	0	36,36,36	2.63	10 (27%)
3	KMM	B	503	-	26,26,26	0.45	0	36,36,36	1.94	6 (16%)
4	BTB	B	505	6	13,13,13	0.53	0	7,16,16	1.06	1 (14%)
2	HEM	A	501	1	41,50,50	1.57	5 (12%)	45,82,82	1.79	12 (26%)
4	BTB	A	507	-	13,13,13	0.54	0	7,16,16	0.79	0
2	HEM	B	501	1	41,50,50	1.52	7 (17%)	45,82,82	1.61	13 (28%)
4	BTB	B	504	6	13,13,13	0.51	0	7,16,16	0.51	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
4	BTB	B	506	-	-	2/21/21/21	-
3	KMM	A	503	-	-	6/11/11/11	0/2/2/2
4	BTB	A	504	6	-	5/21/21/21	-
4	BTB	A	506	-	-	11/21/21/21	-
3	KMM	B	502	-	-	6/11/11/11	0/2/2/2
4	BTB	A	505	-	-	8/21/21/21	-
3	KMM	A	502	-	-	3/11/11/11	0/2/2/2
3	KMM	B	503	-	-	4/11/11/11	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	B	505	6	-	16/21/21/21	-
2	HEM	A	501	1	-	1/12/54/54	-
4	BTB	A	507	-	-	4/21/21/21	-
2	HEM	B	501	1	-	1/12/54/54	-
4	BTB	B	504	6	-	0/21/21/21	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	4.29	2.18	1.96
2	B	501	HEM	C3C-C2C	-3.54	1.35	1.40
2	A	501	HEM	C3C-CAC	3.41	1.54	1.47
2	A	501	HEM	C3C-C2C	-3.26	1.35	1.40
2	B	501	HEM	CAB-C3B	3.25	1.56	1.47
2	A	501	HEM	CAB-C3B	2.95	1.55	1.47
2	B	501	HEM	FE-NB	2.74	2.10	1.96
2	B	501	HEM	C3C-CAC	2.71	1.53	1.47
2	B	501	HEM	CMA-C3A	2.38	1.56	1.51
2	B	501	HEM	CMB-C2B	2.21	1.55	1.50
2	A	501	HEM	CMB-C2B	2.17	1.55	1.50
2	B	501	HEM	CMD-C2D	2.17	1.55	1.50

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	KMM	C11-C12-C13	-8.67	119.71	124.98
3	A	503	KMM	C11-C12-C13	-7.85	120.21	124.98
3	B	502	KMM	C11-C12-C13	-7.63	120.34	124.98
3	A	502	KMM	C02-N01-C06	7.61	123.87	118.10
3	B	503	KMM	C11-C12-C13	-7.11	120.66	124.98
3	B	502	KMM	C02-N01-C06	5.76	122.47	118.10
3	A	502	KMM	C08-C09-C11	-4.79	103.66	112.49
3	A	503	KMM	C02-N01-C06	4.37	121.41	118.10
3	B	503	KMM	C02-N01-C06	4.24	121.31	118.10
2	B	501	HEM	C1B-NB-C4B	3.99	109.19	105.07
3	B	502	KMM	C08-C09-C11	-3.97	105.17	112.49
3	A	503	KMM	C09-C11-C12	-3.83	118.29	122.06
3	A	502	KMM	C09-C11-C16	-3.80	118.33	122.06
3	B	502	KMM	C05-C06-N01	-3.75	118.92	122.90
2	A	501	HEM	C4D-ND-C1D	3.75	108.95	105.07
2	A	501	HEM	C4B-CHC-C1C	3.74	127.50	122.56
3	A	502	KMM	C05-C06-N01	-3.71	118.96	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	KMM	C14-C13-C12	3.68	120.13	116.76
2	A	501	HEM	CBA-CAA-C2A	-3.66	106.37	112.62
3	A	502	KMM	C14-C13-C12	3.65	120.11	116.76
3	A	503	KMM	C14-C13-C12	3.63	120.08	116.76
3	B	503	KMM	C05-C06-N01	-3.55	119.14	122.90
2	A	501	HEM	C1B-NB-C4B	3.37	108.56	105.07
3	A	502	KMM	C16-C11-C12	3.36	119.88	115.90
3	B	502	KMM	C14-C13-C12	3.26	119.74	116.76
2	B	501	HEM	C4D-ND-C1D	3.13	108.31	105.07
3	B	502	KMM	C16-C11-C12	3.09	119.56	115.90
3	A	503	KMM	C16-C11-C12	3.01	119.46	115.90
3	B	502	KMM	C08-C06-C05	2.93	125.10	121.22
3	B	503	KMM	C08-C06-N01	2.90	120.26	115.95
2	A	501	HEM	CHC-C4B-C3B	2.87	128.96	124.57
2	A	501	HEM	C4C-CHD-C1D	2.77	126.21	122.56
2	B	501	HEM	C4C-CHD-C1D	2.75	126.19	122.56
2	B	501	HEM	CBA-CAA-C2A	-2.75	107.93	112.62
2	B	501	HEM	C4B-CHC-C1C	2.71	126.13	122.56
3	A	503	KMM	C05-C06-N01	-2.67	120.07	122.90
3	A	502	KMM	C08-C06-C05	2.60	124.66	121.22
2	B	501	HEM	CBD-CAD-C3D	-2.60	105.40	112.63
2	B	501	HEM	C3B-C2B-C1B	2.55	108.38	106.49
3	B	503	KMM	C16-C11-C12	2.54	118.91	115.90
2	A	501	HEM	CMC-C2C-C3C	2.53	129.41	124.68
2	A	501	HEM	CMA-C3A-C4A	-2.52	124.59	128.46
2	A	501	HEM	C3D-C4D-ND	-2.50	107.38	110.17
3	B	502	KMM	C11-C16-C15	-2.37	120.23	121.92
3	B	502	KMM	C09-C11-C16	-2.37	119.73	122.06
2	B	501	HEM	C2B-C1B-NB	-2.36	107.04	109.84
3	A	502	KMM	C04-C05-C06	-2.34	118.79	120.32
3	A	503	KMM	C11-C16-C15	-2.32	120.27	121.92
4	B	505	BTB	O4-C4-C2	-2.31	105.12	111.44
3	A	503	KMM	C08-C06-N01	2.29	119.36	115.95
2	A	501	HEM	CHD-C1D-C2D	2.27	128.53	124.98
3	A	503	KMM	F12-C12-C13	2.22	120.20	117.85
3	A	502	KMM	C11-C16-C15	-2.10	120.42	121.92
3	B	502	KMM	F12-C12-C13	2.08	120.05	117.85
2	B	501	HEM	CHC-C4B-C3B	2.08	127.75	124.57
2	A	501	HEM	C3B-C2B-C1B	2.08	108.03	106.49
2	B	501	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
2	B	501	HEM	C3D-C4D-ND	-2.05	107.88	110.17
2	A	501	HEM	C2D-C1D-ND	-2.04	107.44	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C2C-C3C-C4C	2.03	108.32	106.90
2	B	501	HEM	CHB-C1B-NB	2.02	126.88	124.38

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	KMM	C08-C09-C11-C12
3	A	503	KMM	C12-C13-C17-C18
3	B	503	KMM	C12-C13-C17-C18
4	A	504	BTB	O1-C1-C2-C3
4	A	504	BTB	O1-C1-C2-C4
4	A	505	BTB	O1-C1-C2-C3
4	A	505	BTB	O1-C1-C2-C4
4	A	505	BTB	O1-C1-C2-N
4	A	505	BTB	C6-C5-N-C7
4	A	506	BTB	O1-C1-C2-C3
4	A	506	BTB	O1-C1-C2-C4
4	A	506	BTB	O1-C1-C2-N
4	A	506	BTB	C1-C2-C3-O3
4	A	506	BTB	C4-C2-C3-O3
4	A	506	BTB	C6-C5-N-C7
4	A	507	BTB	C4-C2-C3-O3
4	A	507	BTB	N-C2-C3-O3
4	A	507	BTB	C6-C5-N-C7
4	B	505	BTB	O1-C1-C2-C4
4	B	505	BTB	N-C2-C3-O3
4	B	505	BTB	C1-C2-C4-O4
4	B	505	BTB	C1-C2-N-C5
4	B	505	BTB	C1-C2-N-C7
4	B	505	BTB	C3-C2-N-C5
4	B	505	BTB	C3-C2-N-C7
4	B	505	BTB	C4-C2-N-C5
4	B	505	BTB	C4-C2-N-C7
4	B	505	BTB	C8-C7-N-C5
4	B	506	BTB	C8-C7-N-C5
4	B	506	BTB	N-C7-C8-O8
3	B	502	KMM	C18-C19-N20-C22
4	A	506	BTB	N-C7-C8-O8
3	B	503	KMM	C18-C19-N20-C22
3	B	502	KMM	C17-C18-C19-N20
4	B	505	BTB	N-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
3	B	502	KMM	C18-C19-N20-C21
3	B	503	KMM	C18-C19-N20-C21
4	B	505	BTB	N-C5-C6-O6
3	A	503	KMM	C17-C18-C19-N20
3	A	502	KMM	C17-C18-C19-N20
4	A	506	BTB	N-C5-C6-O6
3	A	503	KMM	C18-C19-N20-C22
3	B	503	KMM	C17-C18-C19-N20
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
4	A	504	BTB	C1-C2-C3-O3
4	A	504	BTB	C4-C2-C3-O3
4	A	507	BTB	C1-C2-C3-O3
4	B	505	BTB	O1-C1-C2-C3
4	B	505	BTB	C1-C2-C3-O3
4	B	505	BTB	C4-C2-C3-O3
4	A	504	BTB	O1-C1-C2-N
4	A	505	BTB	N-C2-C3-O3
4	A	505	BTB	C3-C2-N-C5
4	A	506	BTB	N-C2-C3-O3
4	A	506	BTB	C1-C2-N-C5
4	A	506	BTB	C3-C2-N-C5
4	B	505	BTB	O1-C1-C2-N
3	B	502	KMM	N01-C06-C08-C09
3	A	502	KMM	C05-C06-C08-C09
3	A	503	KMM	C05-C06-C08-C09
3	B	502	KMM	C05-C06-C08-C09
3	A	502	KMM	N01-C06-C08-C09
3	A	503	KMM	N01-C06-C08-C09
3	B	502	KMM	C12-C13-C17-C18
4	A	505	BTB	C1-C2-C3-O3
4	A	505	BTB	C4-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	506	BTB	1	0
4	A	504	BTB	1	0
4	A	506	BTB	2	0
4	A	505	BTB	3	0
4	B	505	BTB	2	0

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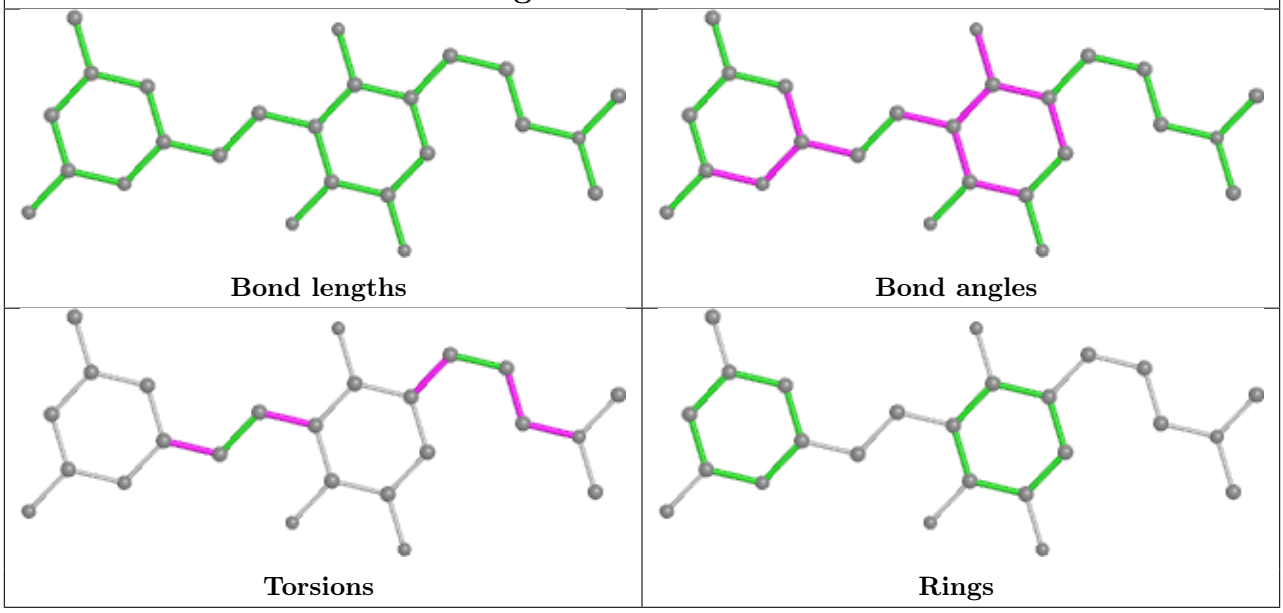
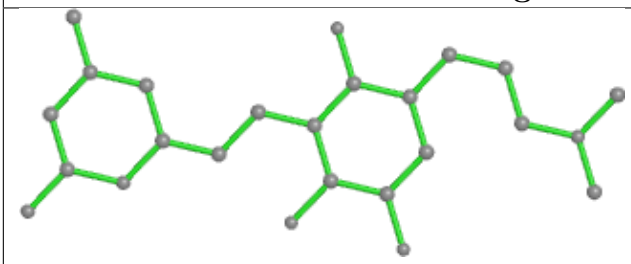
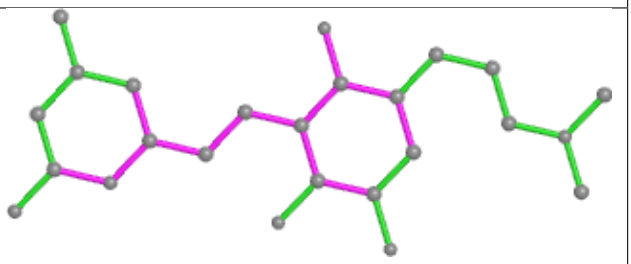
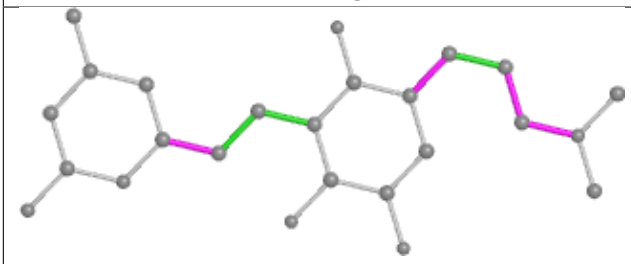
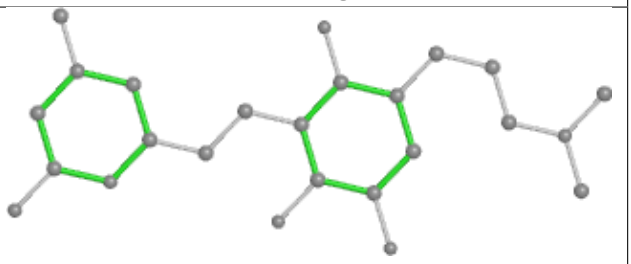
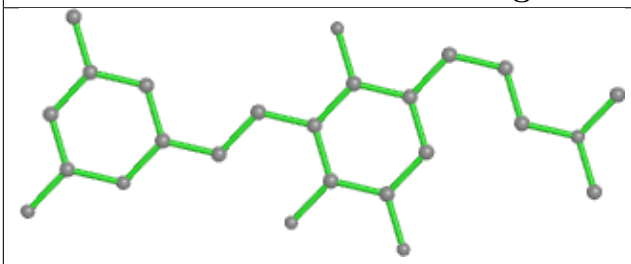
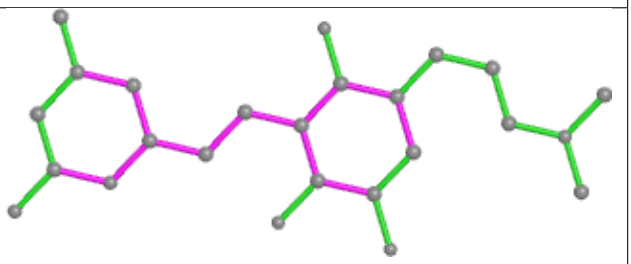
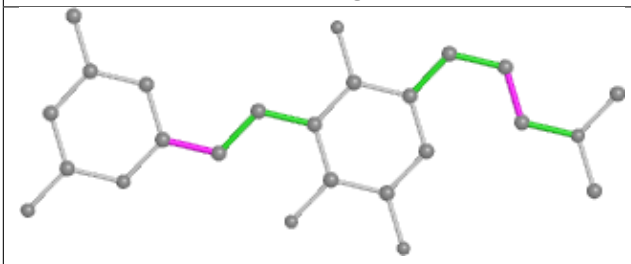
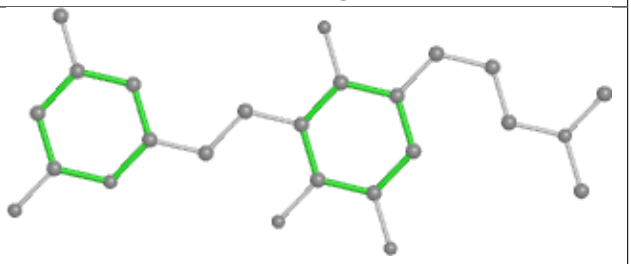
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
4	A	507	BTB	2	0
2	B	501	HEM	4	0
4	B	504	BTB	5	0

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.

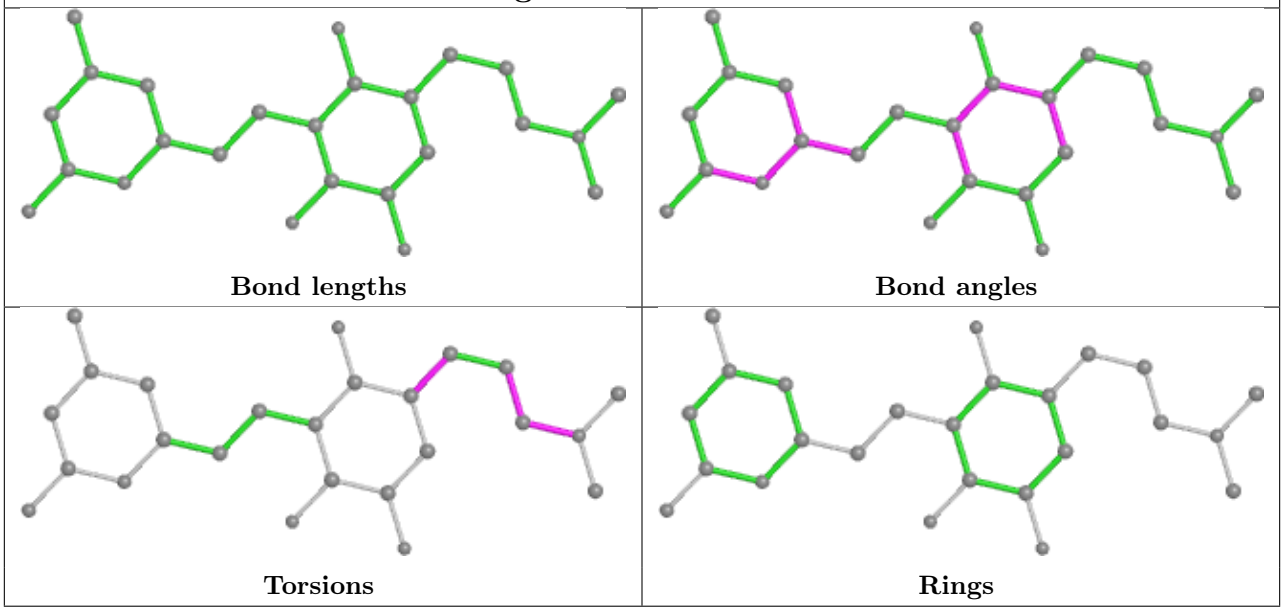
Ligand KMM A 503



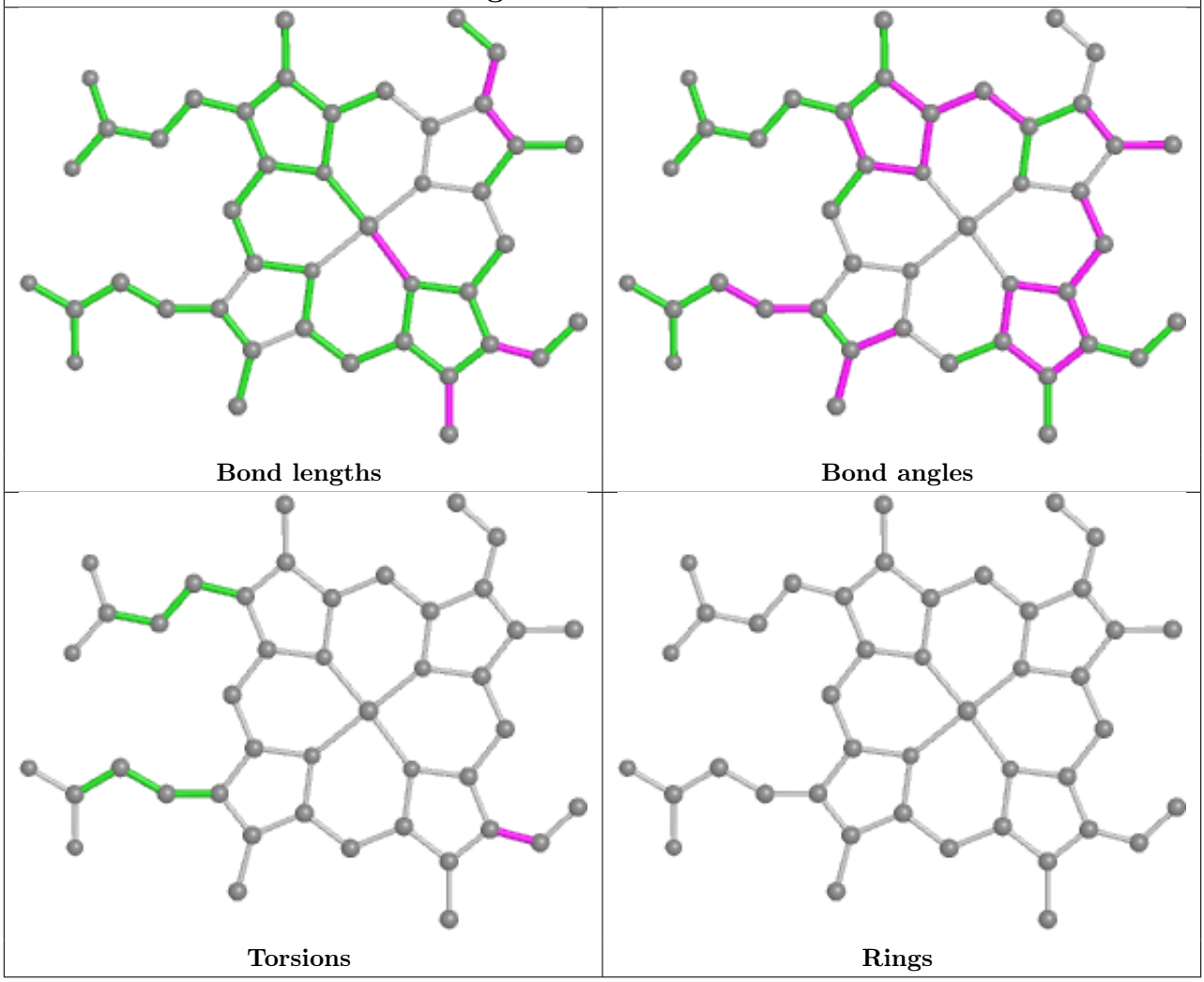
Ligand KMM B 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KMM A 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

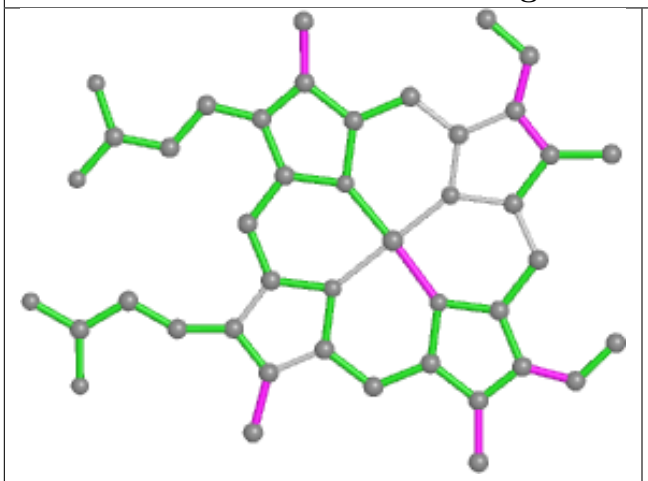
Ligand KMM B 503



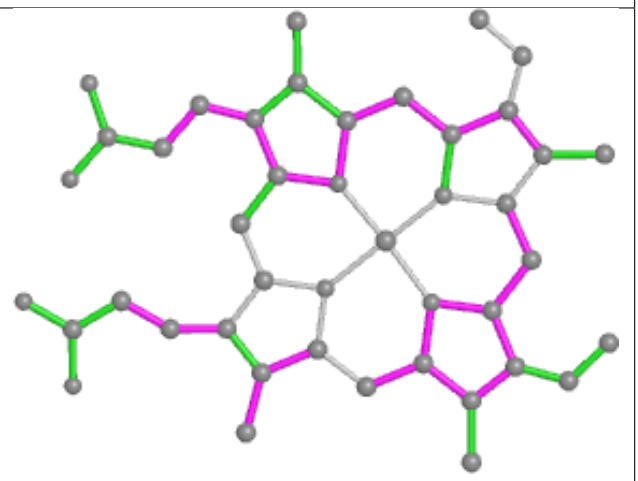
Ligand HEM A 501



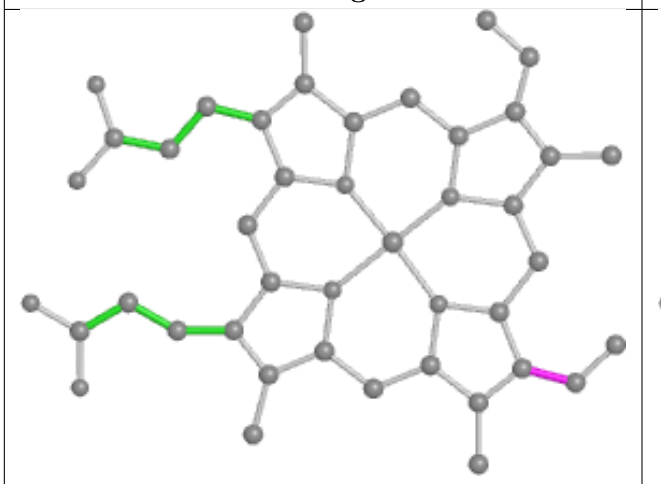
Ligand HEM B 501



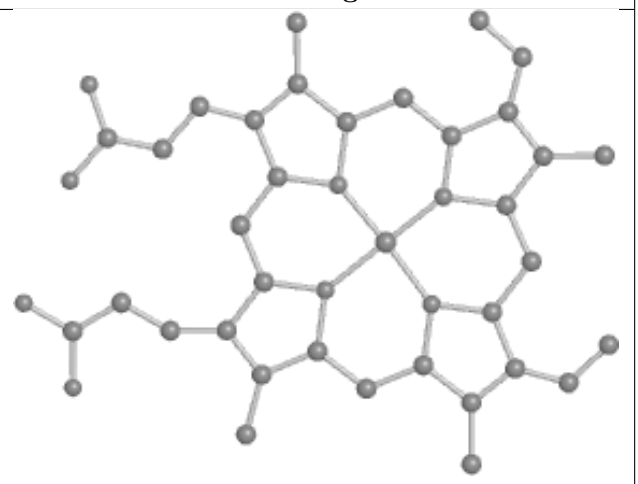
Bond lengths



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	401/440 (91%)	0.34	13 (3%)	47	50	29, 58, 105, 132	0
1	B	402/440 (91%)	0.18	14 (3%)	44	47	27, 48, 87, 145	0
All	All	803/880 (91%)	0.26	27 (3%)	45	48	27, 53, 97, 145	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	LEU	4.1
1	B	89	GLN	3.9
1	A	89	GLN	3.8
1	A	304	LEU	3.4
1	A	257	GLN	3.3
1	B	157	VAL	3.3
1	B	120	PRO	3.2
1	A	241	PHE	2.9
1	B	161	GLY	2.8
1	A	292	LEU	2.8
1	A	468	PHE	2.8
1	A	252	ALA	2.6
1	A	259	GLY	2.6
1	B	159	ALA	2.4
1	A	276	GLN	2.3
1	A	279	TRP	2.3
1	B	238	ARG	2.3
1	B	142	GLY	2.2
1	B	128	ARG	2.2
1	B	122	GLN	2.2
1	B	163	TYR	2.1
1	A	244	TRP	2.1
1	A	302	LEU	2.1
1	B	124	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	235[A]	CYS	2.1
1	B	119	ALA	2.0
1	B	192	LYS	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, 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.

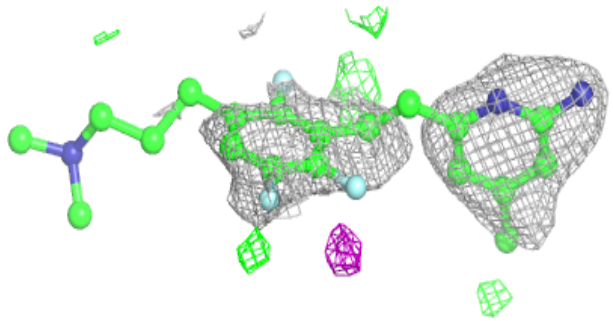
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BTB	B	506	14/14	0.70	0.16	83,93,99,99	0
4	BTB	B	505	14/14	0.79	0.16	52,76,90,90	0
4	BTB	B	504	14/14	0.80	0.17	57,72,87,92	0
4	BTB	A	507	14/14	0.84	0.12	75,83,96,97	0
4	BTB	A	504	14/14	0.85	0.20	95,101,105,106	0
4	BTB	A	505	14/14	0.85	0.14	78,84,89,90	0
3	KMM	A	503	25/25	0.86	0.28	64,108,124,125	0
4	BTB	A	506	14/14	0.89	0.20	53,79,87,87	0
3	KMM	A	502	25/25	0.91	0.17	30,71,100,105	0
3	KMM	B	503	25/25	0.92	0.19	32,81,90,91	0
3	KMM	B	502	25/25	0.93	0.13	25,52,69,74	0
2	HEM	A	501	43/43	0.97	0.11	31,42,86,97	0
2	HEM	B	501	43/43	0.98	0.10	24,30,63,80	0
6	GD	A	510	1/1	0.98	0.08	49,49,49,49	1
6	GD	B	507	1/1	0.98	0.13	45,45,45,45	0
6	GD	B	508	1/1	0.98	0.12	59,59,59,59	1
6	GD	A	509	1/1	0.99	0.11	85,85,85,85	1
5	ZN	A	508	1/1	0.99	0.09	39,39,39,39	0

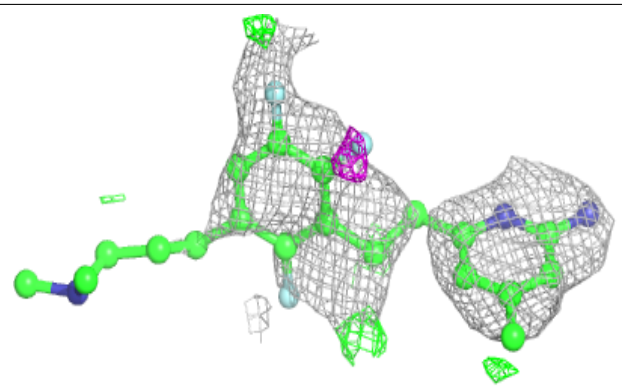
The following is a graphical depiction of the model fit to experimental electron density of all

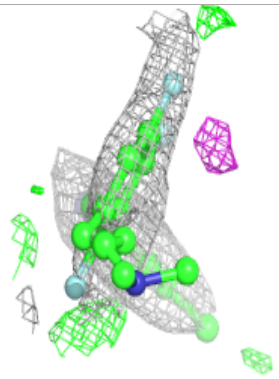
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KMM A 503:

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

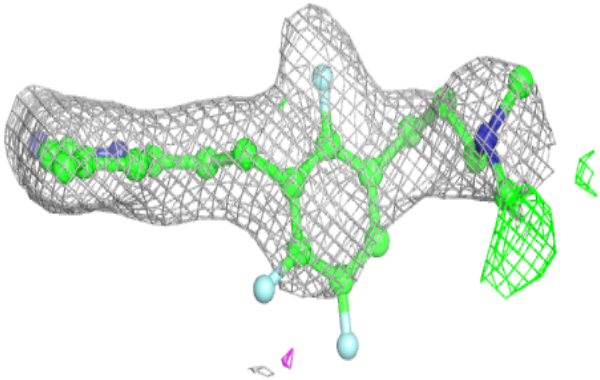


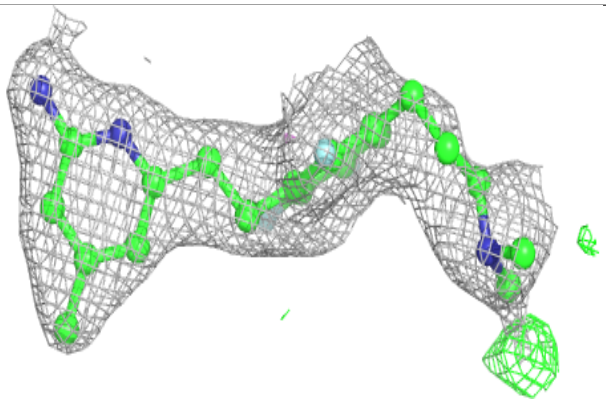


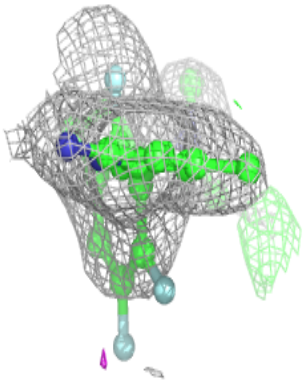


Electron density around KMM A 502:

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

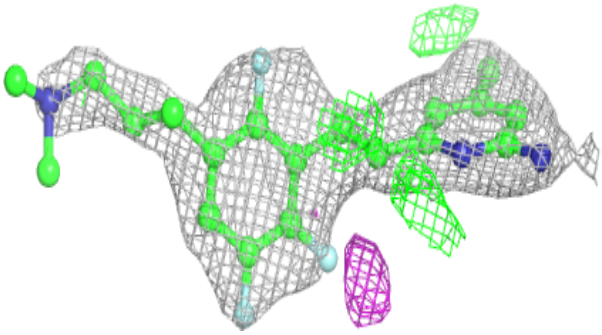


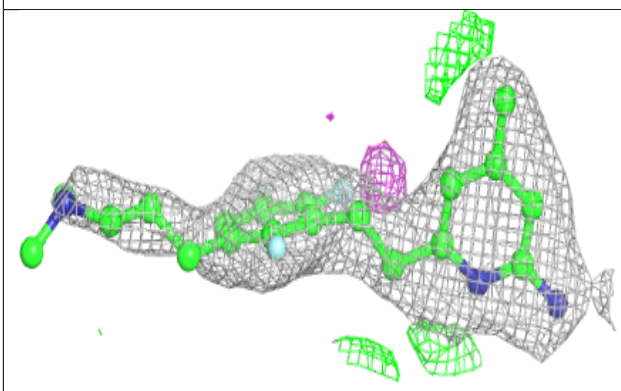


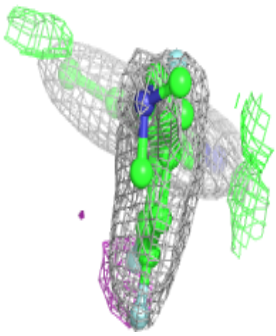


Electron density around KMM B 503:

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

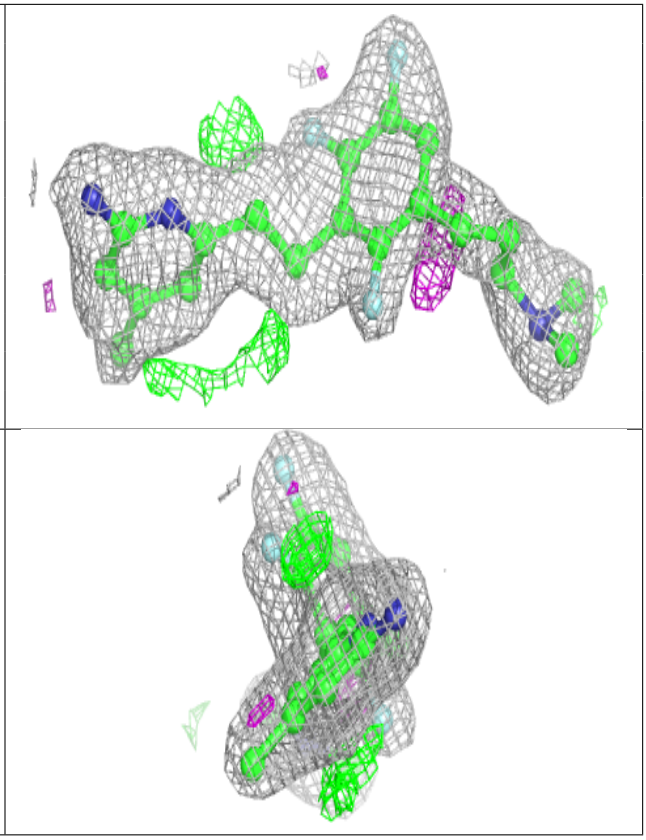






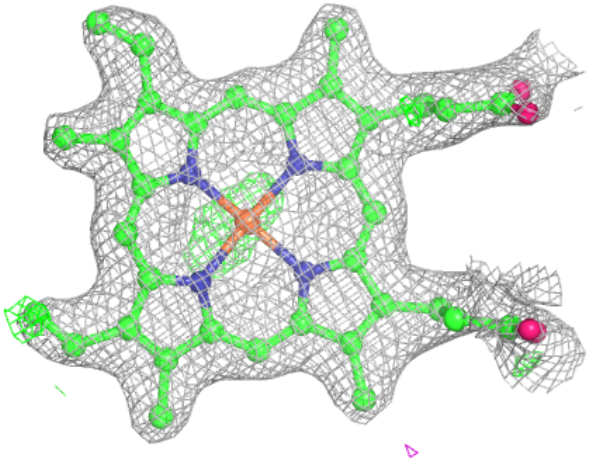
Electron density around KMM B 502:

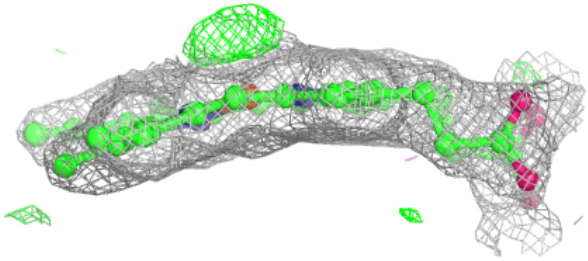
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

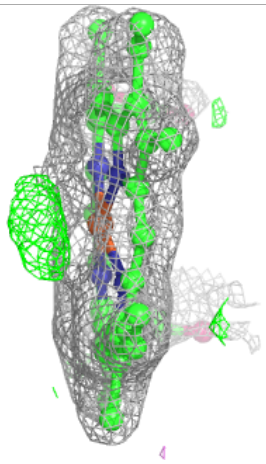


Electron density around HEM A 501:

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

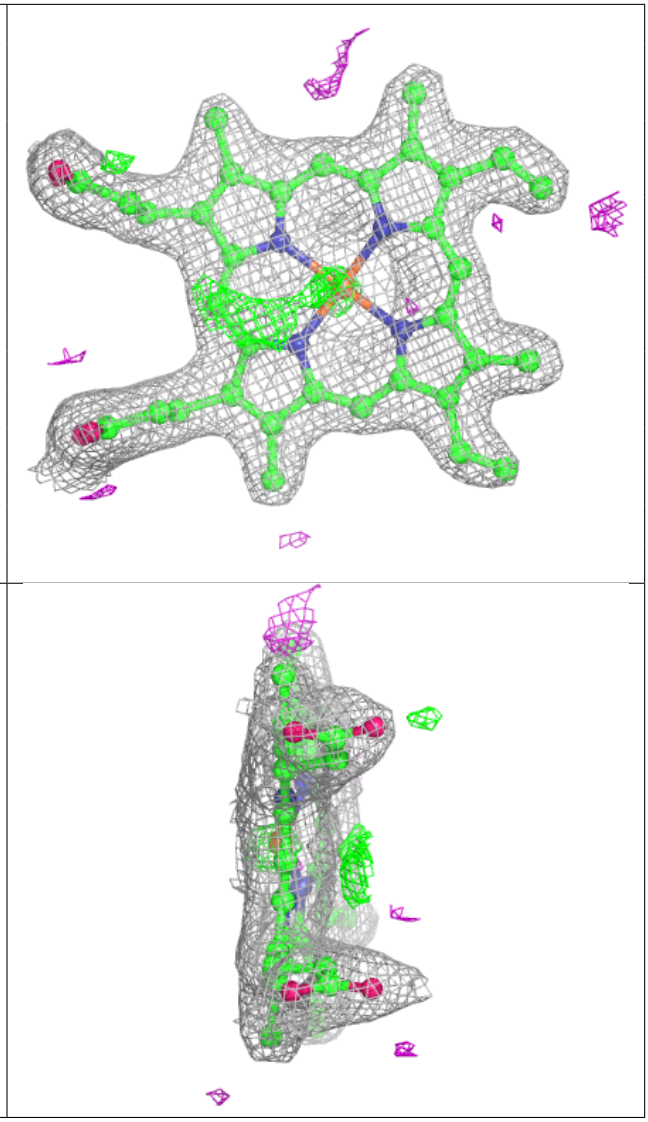






Electron density around HEM B 501:

$2mF_o$-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.