Full wwPDB X-ray Structure Validation Report

Aug 21, 2020 – 07:04 PM BST

PDB ID	:	4CAP
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 7-(2-(3-(3-Fluorophenyl(propylamino)methyl))quinolin-2- amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2013-10-08
Resolution	:	2.06 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 following versions of software and data (see references ⓘ) were used in the production of this report:

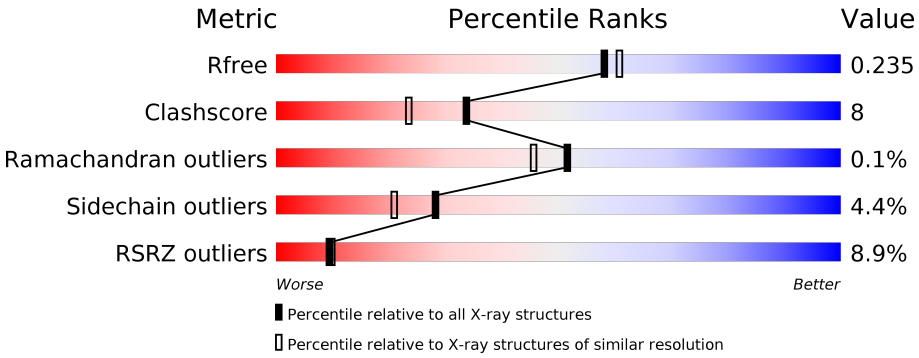
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	13% 75% 18%
1	B	422	5% 82% 15%

2 Entry composition

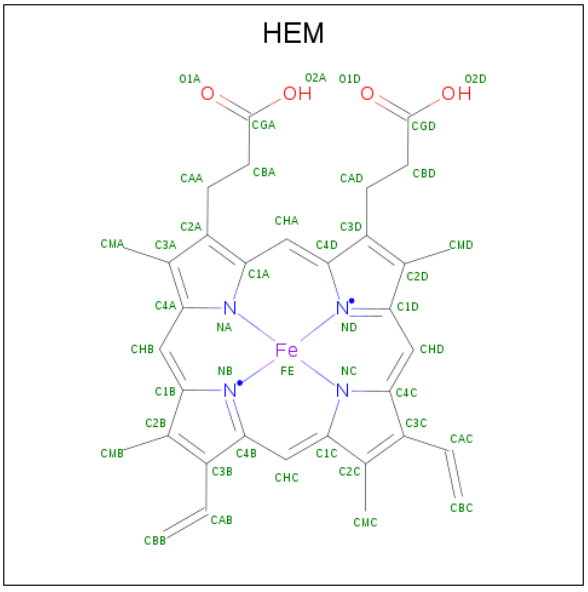
There are 7 unique types of molecules in this entry. The entry contains 7067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRIC OXIDE SYNTHASE, BRAIN.

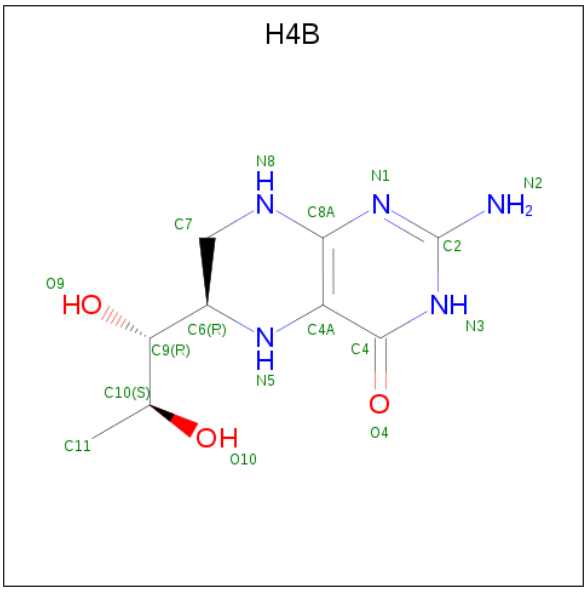
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	3	0
			3326	2130	566	609	21			
1	B	411	Total	C	N	O	S	0	1	0
			3348	2142	574	611	21			

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



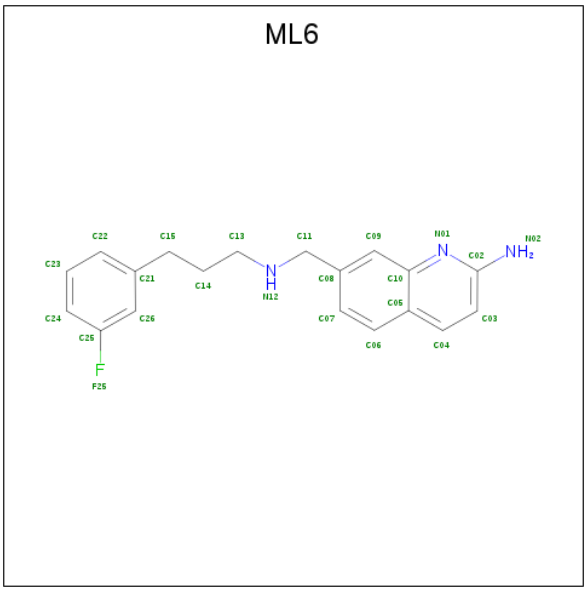
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-({[3-(3-fluorophenyl)propyl]amino}methyl)quinolin-2-amine (three-letter code: ML6) (formula: $C_{19}H_{20}FN_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			23	19	1	3		

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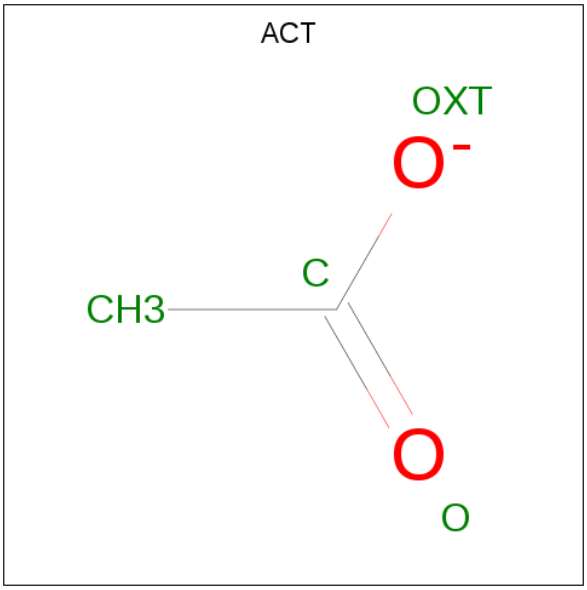
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C F N 23 19 1 3	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is water.

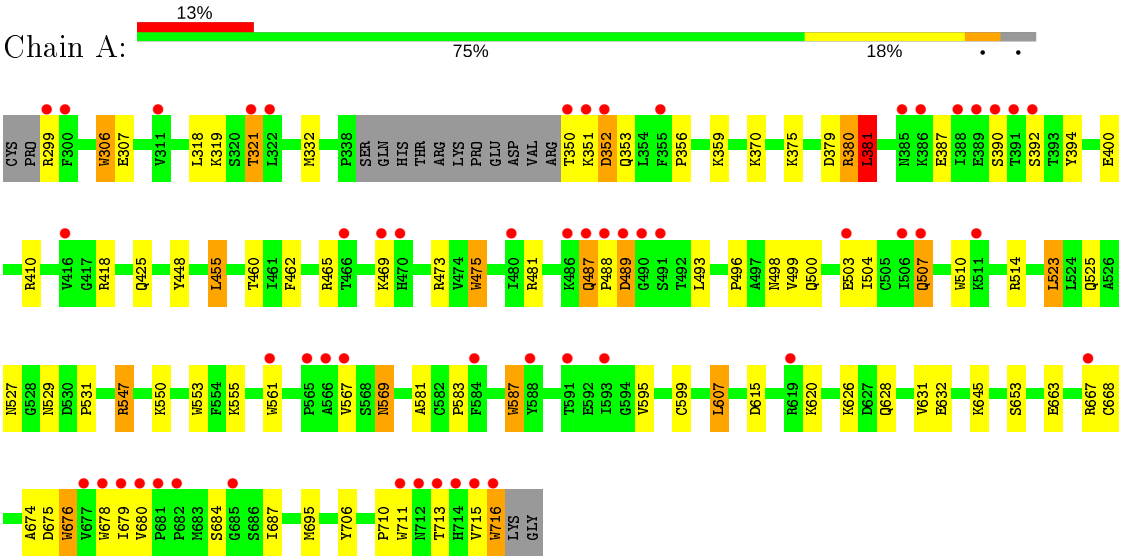
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	105	Total O 105 105	0	0
7	B	113	Total O 113 113	0	0

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.

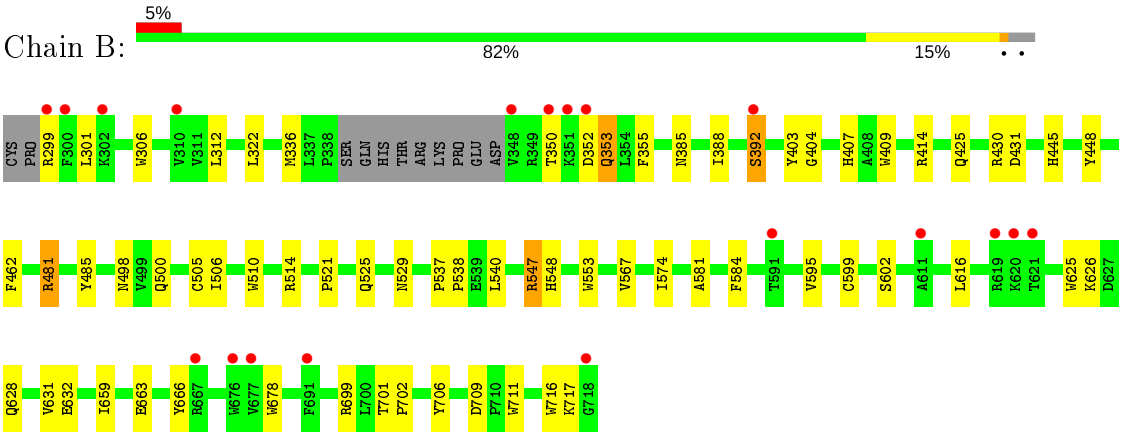
- Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain A:



- Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

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	51.77Å 110.83Å 165.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.19 – 2.06 39.06 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.7 (92.19-2.06) 98.8 (39.06-2.06)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.185 , 0.235 0.183 , 0.235	Depositor DCC
R_{free} test set	2921 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.1	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	0.97	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: HEM, ZN, ML6, H4B, ACT

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	0.91	10/3428 (0.3%)	0.88	7/4652 (0.2%)
1	B	0.98	5/3444 (0.1%)	0.93	3/4669 (0.1%)
All	All	0.95	15/6872 (0.2%)	0.91	10/9321 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	TRP	CD2-CE2	6.42	1.49	1.41
1	A	306	TRP	CD2-CE2	5.93	1.48	1.41
1	A	510	TRP	CD2-CE2	5.92	1.48	1.41
1	B	716	TRP	CD2-CE2	5.90	1.48	1.41
1	A	678	TRP	CD2-CE2	5.84	1.48	1.41
1	A	587	TRP	CD2-CE2	5.70	1.48	1.41
1	B	711	TRP	CD2-CE2	5.55	1.48	1.41
1	A	475	TRP	CD2-CE2	5.54	1.48	1.41
1	A	676	TRP	CD2-CE2	5.52	1.48	1.41
1	B	409	TRP	CD2-CE2	5.27	1.47	1.41
1	A	561	TRP	CD2-CE2	5.26	1.47	1.41
1	B	625	TRP	CD2-CE2	5.26	1.47	1.41
1	B	553	TRP	CD2-CE2	5.23	1.47	1.41
1	A	553	TRP	CD2-CE2	5.02	1.47	1.41
1	A	716	TRP	CD2-CE2	5.00	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	430	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	A	410	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	410	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	418	ARG	NE-CZ-NH1	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	709	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	547	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	607	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	455	LEU	CB-CG-CD2	5.12	119.71	111.00
1	B	431	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	381	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3326	0	3239	65	0
1	B	3348	0	3264	51	0
2	A	43	0	30	5	0
2	B	43	0	30	9	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	23	0	20	4	0
4	B	23	0	20	6	0
5	A	4	0	3	0	0
5	B	4	0	3	1	0
6	A	1	0	0	0	0
7	A	105	0	0	3	0
7	B	113	0	0	1	0
All	All	7067	0	6639	114	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 8.

All (114) 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)
5:B:860:ACT:H3	7:B:2027:HOH:O	1.37	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:VAL:HG21	4:A:800:ML6:C07	2.06	0.86
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.63	0.80
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.18	0.79
1:B:706:TYR:OH	2:B:750:HEM:O2D	2.04	0.73
2:B:750:HEM:HBC2	2:B:750:HEM:HMC2	1.73	0.71
1:B:336:MET:HG2	4:B:800:ML6:H24	1.74	0.69
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.28	0.68
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.73	0.68
1:B:567:VAL:HG21	4:B:800:ML6:C07	2.29	0.63
1:B:706:TYR:OH	2:B:750:HEM:CGD	2.47	0.63
1:A:487:GLN:HE21	1:A:488:PRO:HD2	1.65	0.61
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.83	0.60
1:A:306:TRP:CG	1:B:336:MET:CE	2.83	0.60
1:A:675:ASP:O	1:A:679:ILE:HG12	2.01	0.60
1:A:350:THR:HB	1:A:353:GLN:NE2	2.15	0.60
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.17	0.60
1:B:336:MET:HG2	4:B:800:ML6:C24	2.31	0.60
1:A:706:TYR:OH	2:A:750:HEM:O2D	2.21	0.58
1:A:306:TRP:CG	1:B:336:MET:HE2	2.38	0.58
1:A:550:LYS:HB2	1:A:550:LYS:NZ	2.16	0.58
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.84	0.58
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.04	0.58
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.38	0.58
1:A:352:ASP:O	1:A:356:PRO:HD2	2.04	0.57
1:B:481:ARG:HD3	1:B:498:ASN:ND2	2.20	0.57
1:A:375:LYS:NZ	1:A:379:ASP:OD2	2.36	0.56
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.05	0.56
1:A:306:TRP:CD2	1:B:336:MET:CE	2.88	0.56
1:A:706:TYR:OH	2:A:750:HEM:CGD	2.55	0.55
1:A:499:VAL:O	1:A:503:GLU:HG3	2.07	0.55
1:A:525:GLN:HG3	1:A:529:ASN:O	2.07	0.54
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.89	0.54
1:B:425:GLN:HG2	1:B:448:TYR:CZ	2.43	0.54
1:B:352:ASP:HB3	1:B:353:GLN:HE21	1.73	0.54
1:B:659:ILE:O	1:B:663:GLU:HG3	2.08	0.53
1:A:569:ASN:H	1:A:569:ASN:HD22	1.57	0.53
1:B:388:ILE:O	1:B:392:SER:N	2.40	0.53
1:A:359:LYS:HG3	1:A:381:LEU:HD11	1.91	0.52
1:A:307[B]:GLU:OE2	1:B:602:SER:N	2.33	0.52
1:A:493:LEU:HA	7:A:2062:HOH:O	2.09	0.52
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:HB2	1:B:581:ALA:HB3	1.93	0.51
1:A:687:ILE:HD12	1:B:626:LYS:HB3	1.92	0.51
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.94	0.50
1:B:481:ARG:HD3	1:B:498:ASN:HD21	1.77	0.49
2:B:750:HEM:C4B	4:B:800:ML6:H03	2.46	0.49
1:A:321:THR:HG22	7:A:2004:HOH:O	2.12	0.49
2:A:750:HEM:C4B	4:A:800:ML6:H03	2.48	0.49
2:B:750:HEM:CHC	2:B:750:HEM:HBB2	2.36	0.49
1:B:352:ASP:HB3	1:B:353:GLN:NE2	2.28	0.48
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.94	0.48
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.37	0.48
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.96	0.48
1:A:496:PRO:O	1:A:499:VAL:HG23	2.13	0.48
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.95	0.48
1:B:353:GLN:H	1:B:353:GLN:HE21	1.62	0.48
1:A:350:THR:HB	1:A:353:GLN:CD	2.35	0.47
1:A:350:THR:N	7:A:2010:HOH:O	2.46	0.47
1:A:550:LYS:NZ	1:A:550:LYS:CB	2.77	0.47
1:A:460:THR:O	1:A:583:PRO:HD2	2.15	0.47
1:A:332:MET:CE	1:B:301:LEU:HD22	2.45	0.47
1:A:465:ARG:HH11	1:A:465:ARG:HB2	1.80	0.47
1:A:595:VAL:O	1:A:599:CYS:HB2	2.14	0.47
1:A:531:PRO:HD2	1:A:716:TRP:HZ3	1.79	0.46
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.48	0.46
1:A:462:PHE:HB2	1:A:581:ALA:HB3	1.97	0.46
1:A:465:ARG:HB2	1:A:465:ARG:NH1	2.30	0.46
1:A:507:GLN:O	1:A:507:GLN:HG2	2.16	0.46
1:B:505:CYS:O	1:B:506:ILE:C	2.50	0.46
1:B:425:GLN:HG2	1:B:448:TYR:CE1	2.51	0.45
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.51	0.45
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.81	0.45
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.98	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.37	0.45
1:A:500:GLN:O	1:A:504:ILE:HG13	2.17	0.44
1:A:481:ARG:HD3	1:A:498:ASN:HD21	1.82	0.44
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.53	0.44
1:B:353:GLN:N	1:B:353:GLN:HE21	2.17	0.43
1:B:403:TYR:CE2	1:B:407:HIS:CE1	3.06	0.43
1:B:404:GLY:HA3	1:B:574:ILE:HD13	2.01	0.43
1:A:332:MET:HE3	1:B:301:LEU:HD22	2.01	0.42
1:A:350:THR:HB	1:A:353:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.55	0.42
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.49	0.42
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.42
1:A:607:LEU:HD13	1:A:626:LYS:HG2	2.01	0.42
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.02	0.42
1:B:595:VAL:O	1:B:599:CYS:HB2	2.20	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.42
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.97	0.42
1:A:351:LYS:HE2	1:A:392:SER:CB	2.44	0.41
1:B:388:ILE:O	1:B:392:SER:HA	2.19	0.41
1:B:299:ARG:NH1	1:B:299:ARG:HB3	2.35	0.41
1:B:312:LEU:HB3	1:B:666:TYR:CD2	2.54	0.41
2:B:750:HEM:NC	4:B:800:ML6:H04	2.35	0.41
1:A:350:THR:HB	1:A:353:GLN:CG	2.50	0.41
4:A:800:ML6:H23	1:B:306:TRP:CZ3	2.56	0.41
1:B:584:PHE:CD2	2:B:750:HEM:CAC	3.03	0.41
1:A:503:GLU:O	1:A:507:GLN:HB3	2.21	0.41
1:A:531:PRO:HD2	1:A:716:TRP:CZ3	2.55	0.41
1:A:667:ARG:NH1	1:A:668:CYS:SG	2.94	0.41
1:B:355:PHE:CE1	1:B:385:ASN:CB	3.04	0.41
1:A:475:TRP:CE2	1:A:531:PRO:HG3	2.55	0.41
4:B:800:ML6:H26	4:B:800:ML6:H14	1.91	0.41
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.56	0.41
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.56	0.41
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.86	0.41
1:A:567:VAL:HG21	4:A:800:ML6:C06	2.51	0.40
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.49	0.40
1:A:569:ASN:N	1:A:569:ASN:HD22	2.16	0.40
1:B:547:ARG:HD3	1:B:547:ARG:N	2.35	0.40
1:A:425:GLN:HG2	1:A:448:TYR:CZ	2.56	0.40
2:A:750:HEM:HBD2	2:A:750:HEM:CMD	2.52	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	406/422 (96%)	387 (95%)	18 (4%)	1 (0%)	47 39
1	B	408/422 (97%)	394 (97%)	14 (3%)	0	100 100
All	All	814/844 (96%)	781 (96%)	32 (4%)	1 (0%)	51 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	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	366/377 (97%)	342 (93%)	24 (7%)	16 9
1	B	367/377 (97%)	359 (98%)	8 (2%)	52 46
All	All	733/754 (97%)	701 (96%)	32 (4%)	28 21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	321	THR
1	A	352	ASP
1	A	370	LYS
1	A	380	ARG
1	A	381	LEU
1	A	390	SER
1	A	469	LYS
1	A	487	GLN
1	A	489	ASP
1	A	507	GLN
1	A	514	ARG

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Mol	Chain	Res	Type
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	615	ASP
1	A	620	LYS
1	A	645	LYS
1	A	653	SER
1	A	663	GLU
1	A	713	THR
1	A	715	VAL
1	B	350	THR
1	B	353	GLN
1	B	392	SER
1	B	481	ARG
1	B	500	GLN
1	B	540	LEU
1	B	547	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	487	GLN
1	A	507	GLN
1	A	508	GLN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	364	GLN
1	B	454	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ACT	B	860	-	1,3,3	0.47	0	0,3,3	0.00	-
3	H4B	A	760	-	16,18,18	1.29	2 (12%)	11,26,26	3.13	7 (63%)
4	ML6	A	800	-	25,25,25	1.63	6 (24%)	32,33,33	1.25	2 (6%)
2	HEM	A	750	1	27,50,50	2.40	9 (33%)	17,82,82	3.96	9 (52%)
2	HEM	B	750	1	27,50,50	2.26	11 (40%)	17,82,82	3.57	9 (52%)
5	ACT	A	860	-	1,3,3	3.26	1 (100%)	0,3,3	0.00	-
3	H4B	B	760	-	16,18,18	1.58	2 (12%)	11,26,26	2.28	3 (27%)
4	ML6	B	800	-	25,25,25	0.97	2 (8%)	32,33,33	1.54	6 (18%)

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	H4B	A	760	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ML6	A	800	-	-	2/8/8/8	0/3/3/3
2	HEM	A	750	1	-	2/6/54/54	-
2	HEM	B	750	1	-	0/6/54/54	-
3	H4B	B	760	-	-	1/8/17/17	0/2/2/2
4	ML6	B	800	-	-	2/8/8/8	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3C-C2C	6.77	1.49	1.40
2	B	750	HEM	C3C-C2C	6.04	1.48	1.40
2	A	750	HEM	C1A-NA	4.74	1.45	1.36
2	A	750	HEM	C4A-NA	4.30	1.45	1.36
2	B	750	HEM	C4A-NA	4.02	1.44	1.36
2	B	750	HEM	C1A-NA	3.97	1.44	1.36
4	A	800	ML6	C02-N01	3.86	1.38	1.33
3	B	760	H4B	C7-C6	3.79	1.55	1.52
2	B	750	HEM	C2A-C3A	3.47	1.47	1.37
2	A	750	HEM	C1C-C2C	3.43	1.50	1.42
2	B	750	HEM	C3B-C2B	3.36	1.45	1.40
2	A	750	HEM	C3D-C2D	3.33	1.47	1.37
5	A	860	ACT	CH3-C	3.26	1.52	1.48
4	A	800	ML6	C09-C08	3.04	1.44	1.37
4	A	800	ML6	C10-N01	3.03	1.42	1.37
2	A	750	HEM	C3B-C2B	2.95	1.44	1.40
3	A	760	H4B	C2-N2	2.94	1.39	1.33
4	A	800	ML6	C04-C03	2.92	1.42	1.36
4	A	800	ML6	C06-C07	2.80	1.42	1.36
2	A	750	HEM	C2A-C3A	2.79	1.46	1.37
2	B	750	HEM	C3D-C2D	2.73	1.45	1.37
3	B	760	H4B	C7-N8	2.63	1.49	1.44
2	B	750	HEM	C1C-C2C	2.55	1.48	1.42
2	B	750	HEM	C4D-C3D	2.54	1.48	1.42
4	B	800	ML6	C02-N01	2.53	1.36	1.33
2	A	750	HEM	C1D-CHD	2.47	1.47	1.41
2	B	750	HEM	C1A-CHA	2.35	1.47	1.41
2	A	750	HEM	C4B-CHC	2.29	1.47	1.41
3	A	760	H4B	C4-N3	2.20	1.36	1.33
4	B	800	ML6	C04-C03	2.14	1.41	1.36
4	A	800	ML6	C24-C25	2.11	1.41	1.37
2	B	750	HEM	C4B-CHC	2.10	1.46	1.41
2	B	750	HEM	C1B-C2B	2.05	1.47	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	750	HEM	C1D-C2D-C3D	-9.23	100.58	107.00
2	B	750	HEM	C1D-C2D-C3D	-9.04	100.71	107.00
2	A	750	HEM	CBA-CAA-C2A	-7.75	98.20	112.49
2	A	750	HEM	CAD-CBD-CGD	-7.40	100.25	112.67
2	B	750	HEM	CBA-CAA-C2A	-6.93	99.70	112.49
3	A	760	H4B	N3-C2-N1	-5.07	117.47	125.42
3	A	760	H4B	C4-C4A-N5	5.00	123.31	119.12
3	A	760	H4B	C4-N3-C2	4.71	123.42	115.93
3	B	760	H4B	C4-C4A-C8A	4.45	118.52	114.57
2	B	750	HEM	C3B-C4B-NB	4.32	114.80	109.21
2	B	750	HEM	CMB-C2B-C3B	4.26	132.66	124.68
4	A	800	ML6	C08-C11-N12	3.98	123.10	112.80
2	B	750	HEM	CAD-CBD-CGD	-3.86	106.19	112.67
2	A	750	HEM	C3B-C4B-NB	3.79	114.10	109.21
2	A	750	HEM	CMB-C2B-C3B	3.72	131.65	124.68
2	A	750	HEM	CMC-C2C-C3C	3.66	131.53	124.68
4	B	800	ML6	C03-C02-N01	-3.59	117.77	122.08
4	B	800	ML6	C11-C08-C09	-3.49	115.26	121.51
3	B	760	H4B	C4-N3-C2	3.25	121.10	115.93
4	B	800	ML6	C08-C11-N12	3.12	120.89	112.80
2	A	750	HEM	CBD-CAD-C3D	-3.08	106.80	112.48
3	A	760	H4B	C2-N1-C8A	3.06	121.39	114.54
2	B	750	HEM	CBD-CAD-C3D	-3.03	106.89	112.48
3	A	760	H4B	N2-C2-N1	2.84	121.67	117.25
2	B	750	HEM	C4C-C3C-C2C	2.72	108.80	106.90
3	B	760	H4B	N3-C2-N1	-2.70	121.19	125.42
2	B	750	HEM	CMC-C2C-C3C	2.53	129.41	124.68
4	B	800	ML6	C08-C09-C10	-2.49	118.90	121.08
4	B	800	ML6	C04-C03-C02	2.38	121.33	119.48
4	B	800	ML6	C24-C25-C26	-2.37	120.21	123.29
4	A	800	ML6	C09-C10-N01	2.35	122.30	118.72
3	A	760	H4B	N2-C2-N3	2.31	120.85	117.25
2	B	750	HEM	CMD-C2D-C1D	2.30	132.00	128.46
2	A	750	HEM	C4C-C3C-C2C	2.22	108.44	106.90
3	A	760	H4B	C4A-N5-C6	-2.16	115.28	121.16
2	A	750	HEM	CMD-C2D-C1D	2.08	131.67	128.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C2D-C3D-CAD-CBD
2	A	750	HEM	C4D-C3D-CAD-CBD
3	B	760	H4B	O10-C10-C9-O9
4	A	800	ML6	C14-C15-C21-C26
4	A	800	ML6	C14-C15-C21-C22
4	B	800	ML6	C14-C15-C21-C26
4	B	800	ML6	C14-C15-C21-C22

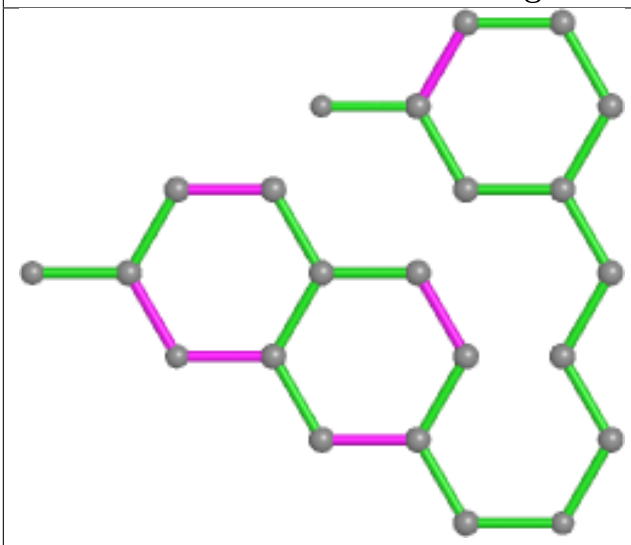
There are no ring outliers.

5 monomers are involved in 22 short contacts:

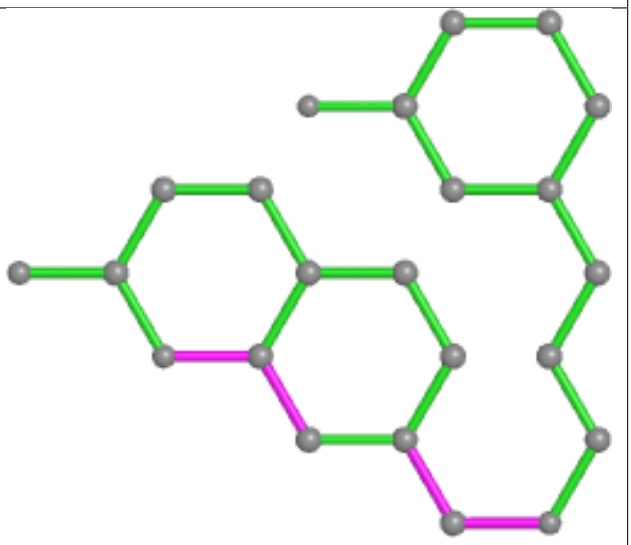
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	860	ACT	1	0
4	A	800	ML6	4	0
2	A	750	HEM	5	0
2	B	750	HEM	9	0
4	B	800	ML6	6	0

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.

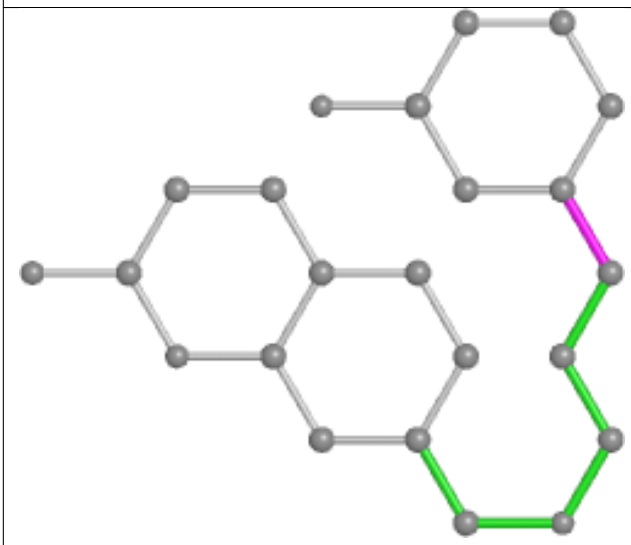
Ligand ML6 A 800



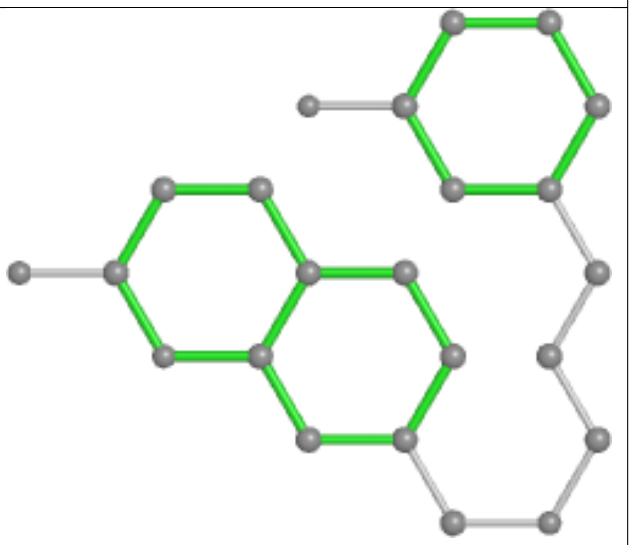
Bond lengths



Bond angles

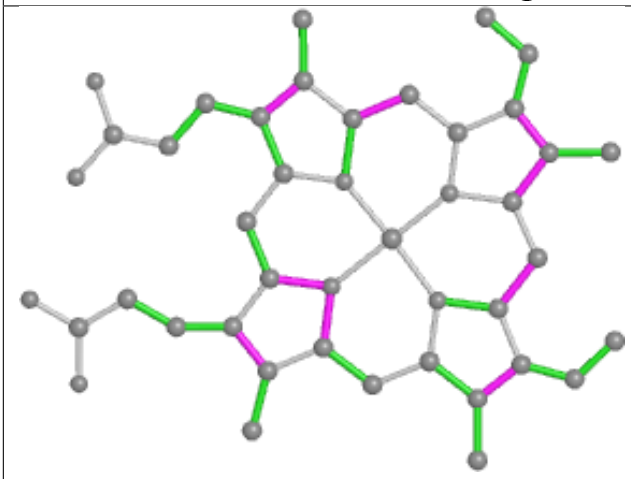


Torsions

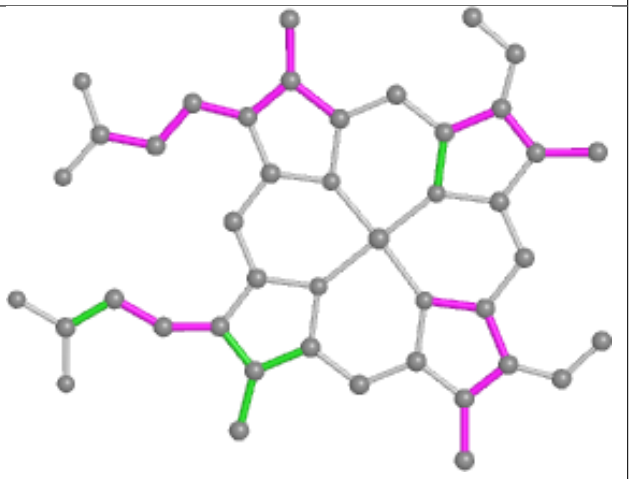


Rings

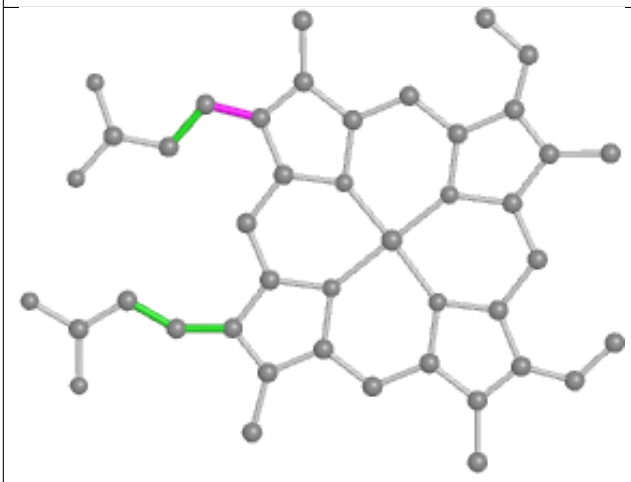
Ligand HEM A 750



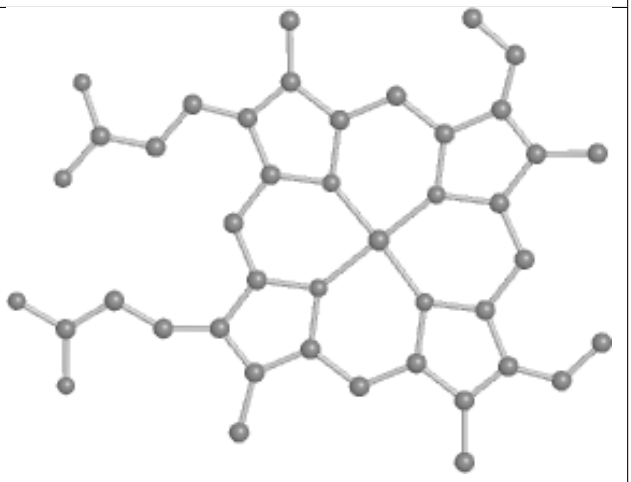
Bond lengths



Bond angles

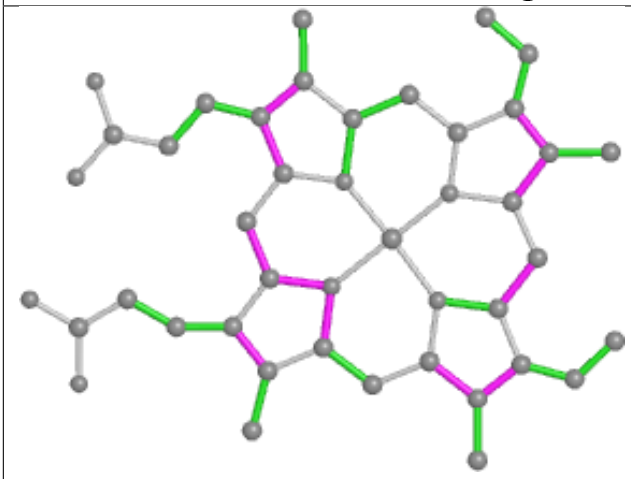


Torsions

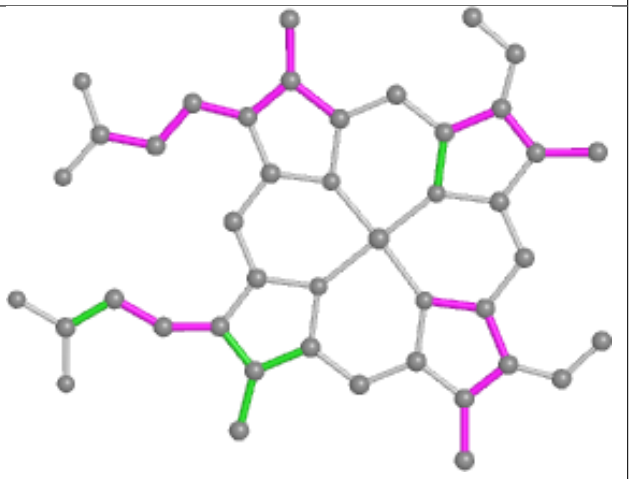


Rings

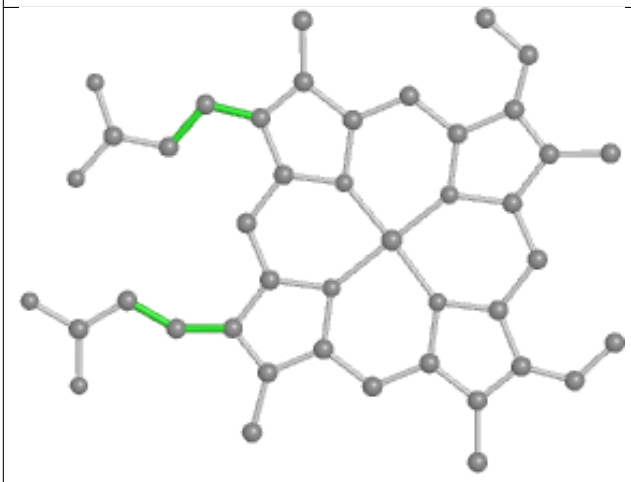
Ligand HEM B 750



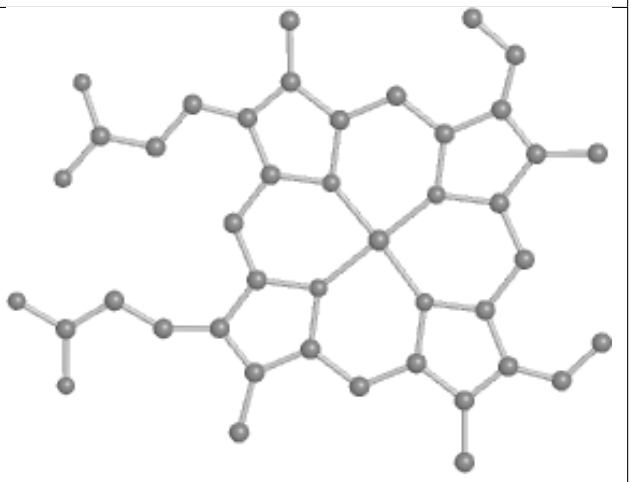
Bond lengths



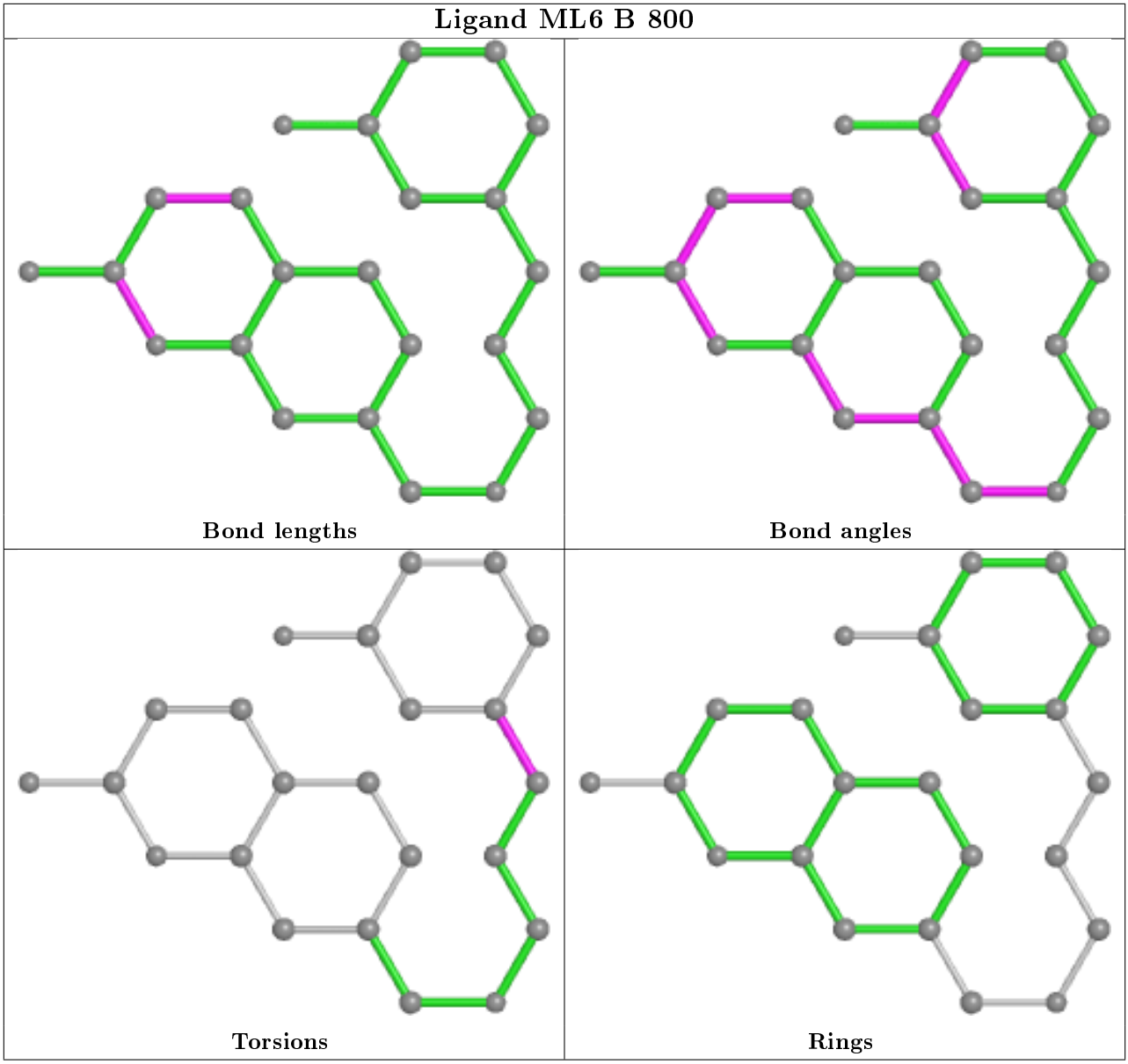
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	407/422 (96%)	0.49	54 (13%) 3 2	32, 58, 101, 140	0
1	B	411/422 (97%)	0.03	19 (4%) 32 33	30, 47, 78, 101	0
All	All	818/844 (96%)	0.26	73 (8%) 9 10	30, 52, 93, 140	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	6.3
1	A	715	VAL	6.0
1	B	348	VAL	5.9
1	B	718	GLY	5.8
1	A	488	PRO	5.7
1	B	300	PHE	5.4
1	B	619	ARG	4.8
1	A	486	LYS	4.7
1	A	352	ASP	4.5
1	A	355	PHE	4.5
1	A	713	THR	4.4
1	A	712	ASN	4.0
1	A	392	SER	3.8
1	A	487	GLN	3.7
1	A	507	GLN	3.6
1	B	350	THR	3.6
1	A	391	THR	3.5
1	A	506	ILE	3.4
1	A	351	LYS	3.4
1	A	714	HIS	3.2
1	A	491	SER	3.2
1	A	390	SER	3.1
1	A	480	ILE	3.1
1	A	490	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	3.0
1	A	677	VAL	3.0
1	A	679	ILE	3.0
1	B	310	VAL	2.9
1	A	619	ARG	2.9
1	A	489	ASP	2.9
1	A	350	THR	2.9
1	B	299	ARG	2.8
1	A	388	ILE	2.8
1	B	677	VAL	2.8
1	A	680	VAL	2.7
1	A	681	PRO	2.7
1	A	469	LYS	2.6
1	A	470	HIS	2.6
1	A	503	GLU	2.6
1	A	561	TRP	2.6
1	A	567	VAL	2.5
1	B	620	LYS	2.5
1	A	385	ASN	2.5
1	A	711	TRP	2.5
1	A	389	GLU	2.4
1	B	621	THR	2.4
1	A	593	ILE	2.4
1	B	676	TRP	2.4
1	A	466	THR	2.4
1	B	667	ARG	2.3
1	A	299	ARG	2.3
1	A	565	PRO	2.3
1	B	352	ASP	2.3
1	A	322	LEU	2.2
1	A	566	ALA	2.2
1	A	588	TYR	2.2
1	A	311	VAL	2.2
1	A	416	VAL	2.2
1	B	351	LYS	2.2
1	A	321	THR	2.2
1	B	591	THR	2.2
1	A	511	LYS	2.2
1	A	667	ARG	2.2
1	A	386	LYS	2.1
1	B	392	SER	2.1
1	B	302	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	591	THR	2.1
1	A	685	GLY	2.1
1	B	691	PHE	2.1
1	A	584	PHE	2.1
1	A	682	PRO	2.0
1	A	678	TRP	2.0
1	B	611	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

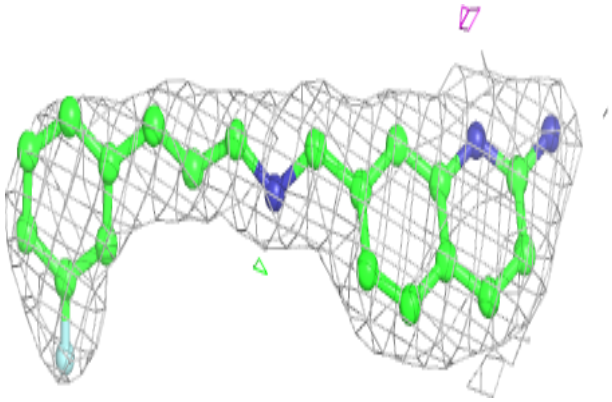
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

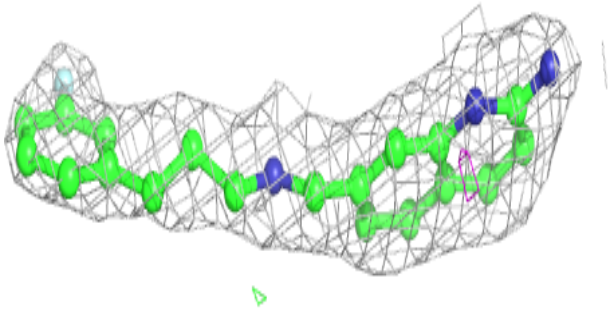
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ML6	A	800	23/23	0.88	0.26	35,42,70,77	0
5	ACT	B	860	4/4	0.91	0.15	58,67,69,70	0
4	ML6	B	800	23/23	0.95	0.20	35,47,70,71	0
3	H4B	B	760	17/17	0.96	0.20	36,38,44,48	0
3	H4B	A	760	17/17	0.96	0.19	36,41,45,48	0
5	ACT	A	860	4/4	0.97	0.17	67,67,78,78	0
2	HEM	B	750	43/43	0.98	0.18	34,39,49,59	0
2	HEM	A	750	43/43	0.98	0.21	33,38,47,60	0
6	ZN	A	1717	1/1	0.99	0.10	44,44,44,44	0

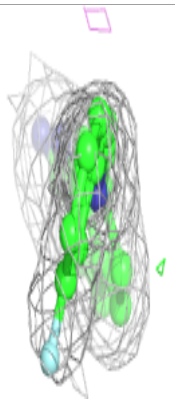
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ML6 A 800:

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

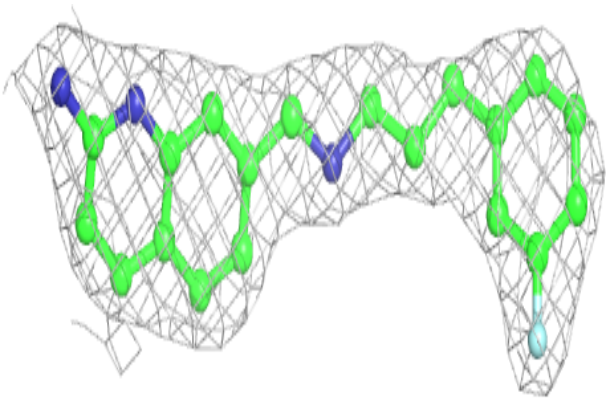


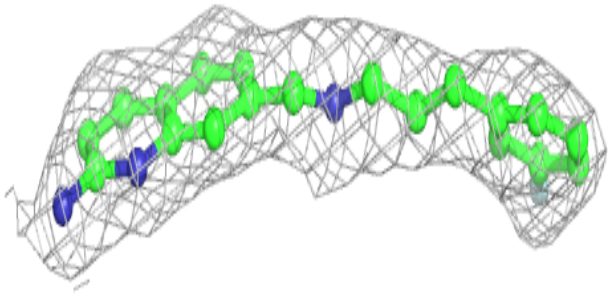


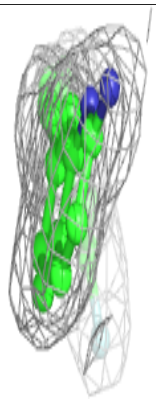


Electron density around ML6 B 800:

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

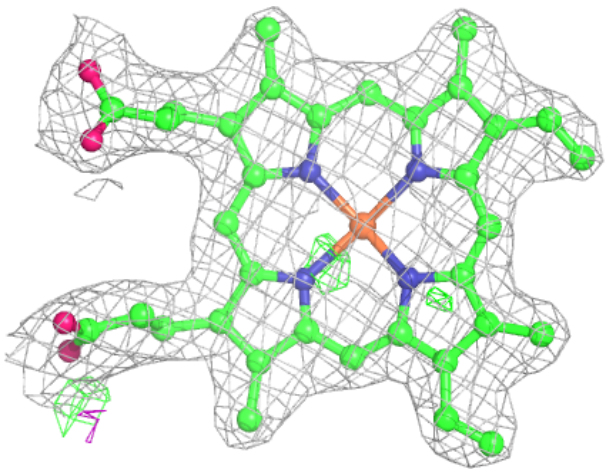


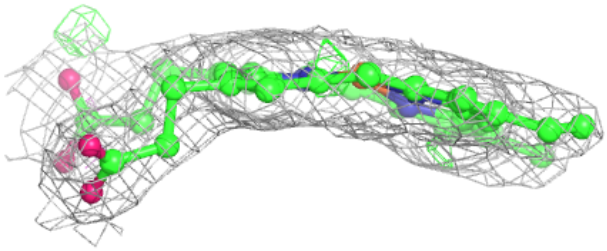


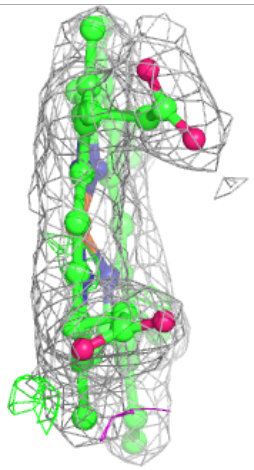


Electron density around HEM B 750:

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

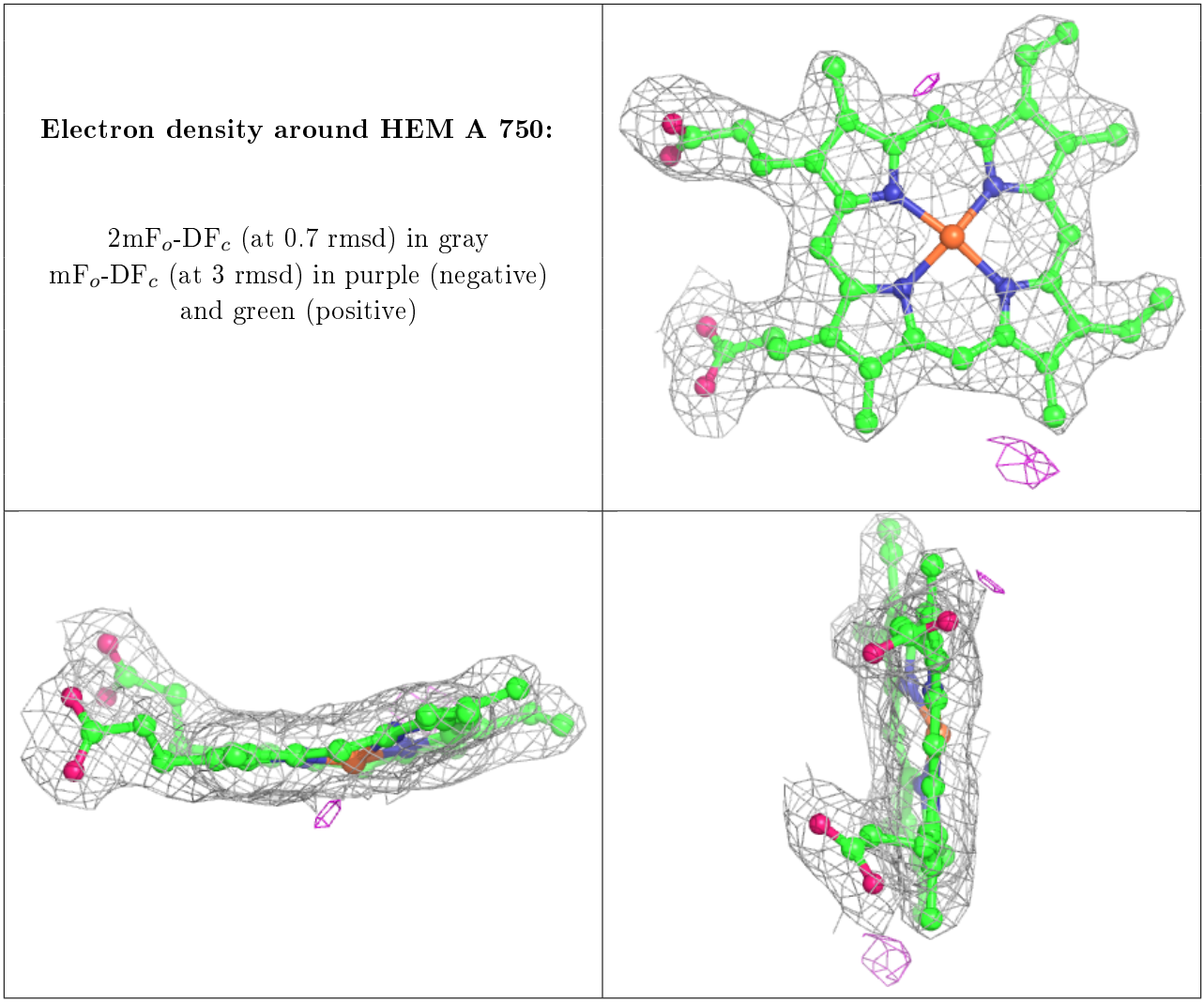






Electron density around HEM A 750:

$2mF_o$-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.