Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 02:18 AM EDT

PDB ID	:	6PMY
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 7-(3-(2-Aminoethyl)phenyl)-4-methylquinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2019-07-02
Resolution	:	1.95 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:

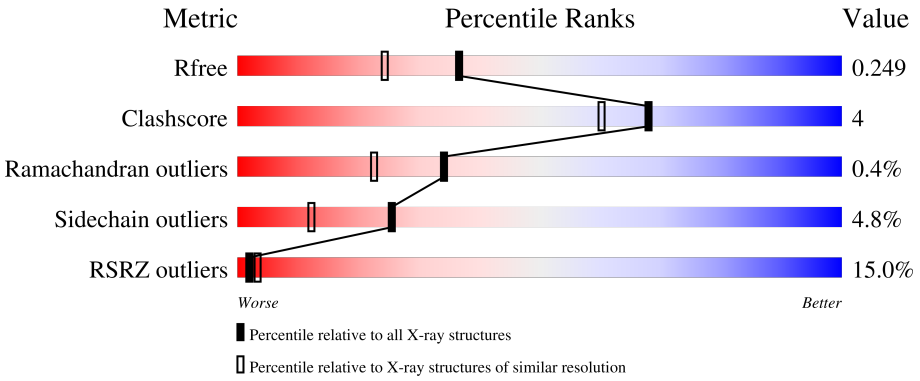
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	422	19% 83% 13%
1	B	422	10% 86% 11%

2 Entry composition

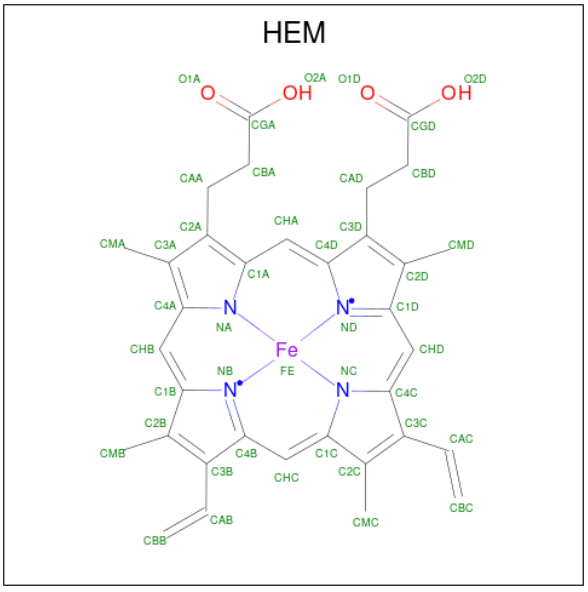
There are 7 unique types of molecules in this entry. The entry contains 7137 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

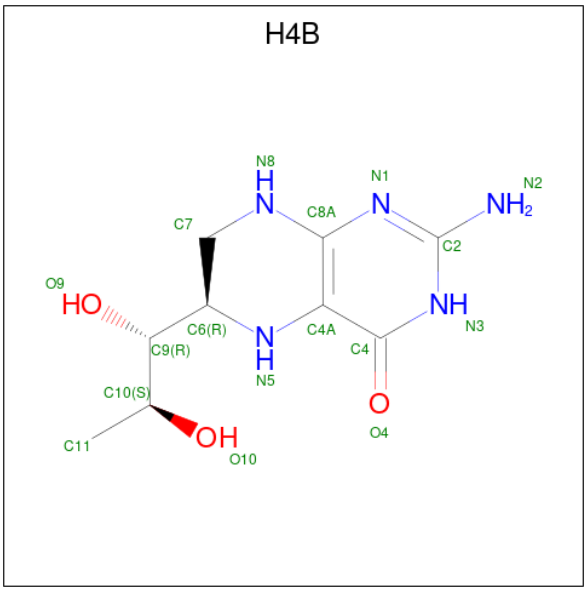
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	3	0
			3365	2154	574	615	22			
1	B	413	Total	C	N	O	S	0	2	0
			3366	2152	577	616	21			

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



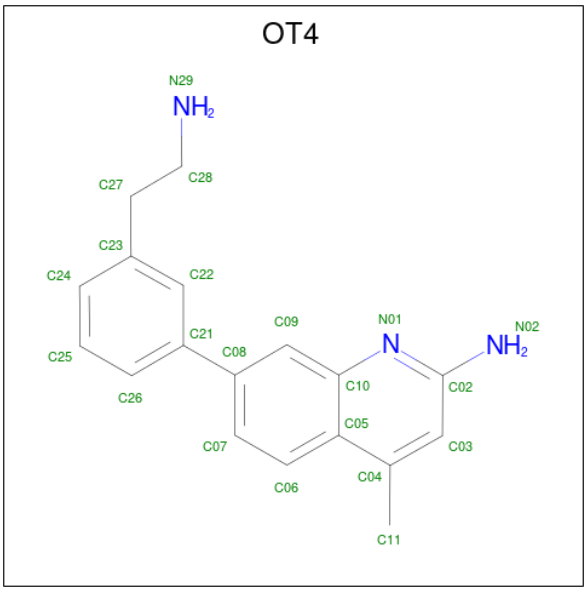
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 7-[3-(2-aminoethyl)phenyl]-4-methylquinolin-2-amine (three-letter code: OT4) (formula: $C_{18}H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 21 18 3	0	0

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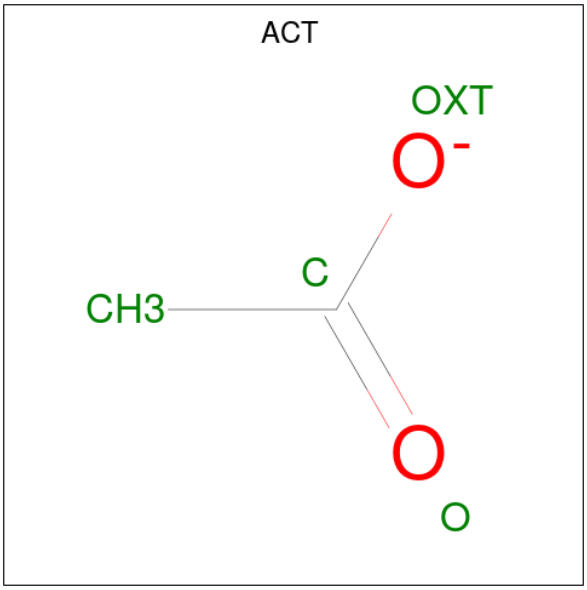
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 21 18 3	0	0

- 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.

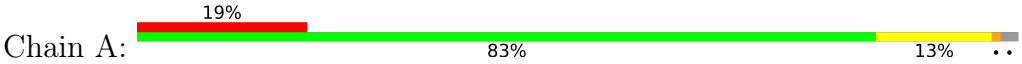
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	96	Total O 96 96	0	0
7	B	139	Total O 139 139	0	0

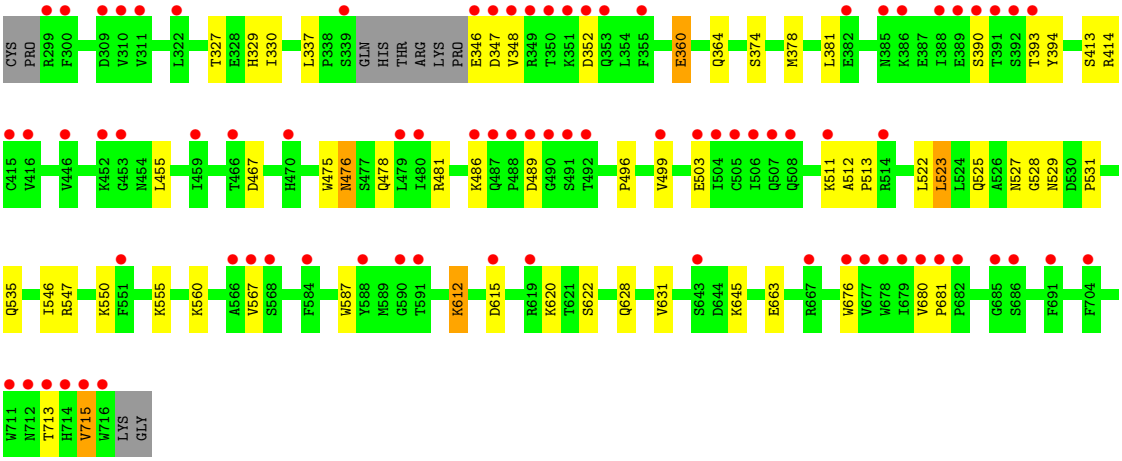
3 Residue-property plots (i)

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

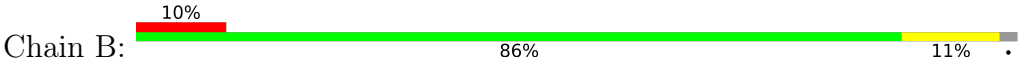
Chain A:

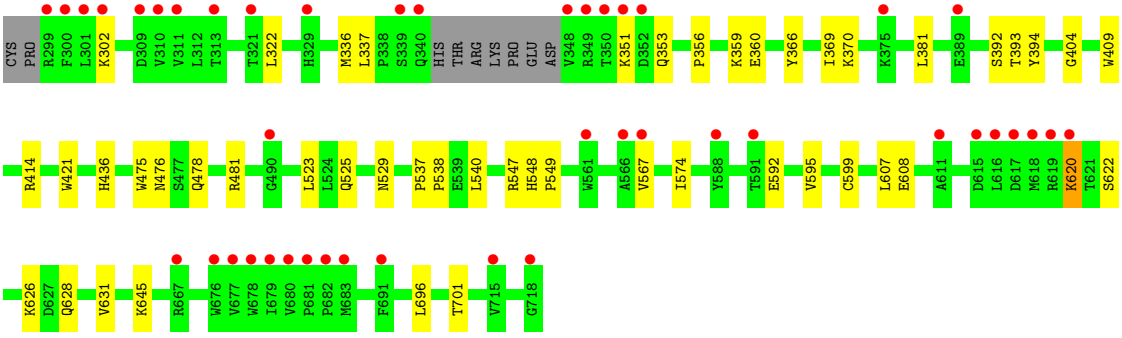




• Molecule 1: Nitric oxide synthase, brain

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	51.83Å 112.03Å 165.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.75 – 1.95 38.75 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.9 (38.75-1.95) 94.6 (38.75-1.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.247 0.204 , 0.249	Depositor DCC
R_{free} test set	3340 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.762	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.8	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	7137	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: H4B, HEM, ACT, ZN, OT4

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	0.37	0/3465	0.50	0/4701
1	B	0.38	0/3465	0.50	0/4697
All	All	0.37	0/6930	0.50	0/9398

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	3365	0	3272	27	0
1	B	3366	0	3282	23	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	21	0	0	1	0
4	B	21	0	0	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	96	0	0	1	0
7	B	139	0	0	1	0
All	All	7137	0	6650	51	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 4.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.66	0.76
1:A:414:ARG:HB2	2:A:801:HEM:HBD2	1.68	0.75
1:B:620:LYS:HD3	1:B:622:SER:H	1.54	0.73
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.72	0.72
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.75	0.68
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.75	0.67
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.77	0.66
1:B:607:LEU:HD13	1:B:626:LYS:HG2	1.77	0.66
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.81	0.63
2:B:801:HEM:O2A	4:B:803:OT4:N29	2.34	0.61
1:A:346:GLU:N	1:A:346:GLU:OE2	2.36	0.59
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.84	0.59
1:A:393:THR:OG1	1:A:394:TYR:N	2.36	0.58
1:B:414:ARG:HB2	2:B:801:HEM:HBD2	1.93	0.51
1:A:525:GLN:HE21	1:A:528:GLY:HA2	1.76	0.50
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.93	0.49
1:B:567:VAL:HG21	4:B:803:OT4:C07	2.44	0.48
1:A:567:VAL:HG21	4:A:803:OT4:C07	2.44	0.48
1:B:404:GLY:HA3	1:B:574:ILE:HD13	1.97	0.47
1:B:356:PRO:O	1:B:360:GLU:HG2	2.14	0.47
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.97	0.47
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.30	0.47
1:B:393:THR:OG1	1:B:394:TYR:N	2.48	0.46
1:A:374:SER:O	1:A:378:MET:HG2	2.16	0.45
1:B:436:HIS:HD2	7:B:1022:HOH:O	1.98	0.45
1:A:486:LYS:NZ	1:A:503:GLU:OE2	2.48	0.45
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.99	0.45
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.52	0.45
1:B:366:TYR:HA	1:B:369:ILE:HG12	1.98	0.45
1:A:546:ILE:HG12	1:A:560:LYS:HA	2.00	0.44
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.53	0.44
1:A:476:ASN:N	1:A:476:ASN:OD1	2.51	0.43
1:B:592:GLU:OE2	4:B:803:OT4:N02	2.51	0.43
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.89	0.43
1:B:351:LYS:HB3	1:B:351:LYS:HE2	1.77	0.43
1:A:612:LYS:HE3	1:A:612:LYS:HB2	1.80	0.43
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.43
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.54	0.42
1:B:595:VAL:O	1:B:599:CYS:HB2	2.19	0.42
1:B:302:LYS:HB2	1:B:302:LYS:HE3	1.72	0.42
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.03	0.41
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.92	0.41
1:A:348:VAL:HG21	1:A:467:ASP:HA	2.02	0.41
1:A:413:SER:N	7:A:905:HOH:O	2.53	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.03	0.41
1:A:476:ASN:HD21	1:A:522:LEU:HA	1.86	0.41
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.91	0.41
1:B:359:LYS:HG3	1:B:381:LEU:HD21	2.03	0.40
1:A:525:GLN:HG3	1:A:529:ASN:O	2.22	0.40
1:A:360:GLU:O	1:A:364:GLN:HG3	2.21	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	410/422 (97%)	389 (95%)	19 (5%)	2 (0%)	29 17
1	B	411/422 (97%)	399 (97%)	11 (3%)	1 (0%)	47 38
All	All	821/844 (97%)	788 (96%)	30 (4%)	3 (0%)	34 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	715	VAL
1	A	347	ASP
1	B	322	LEU

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	370/377 (98%)	347 (94%)	23 (6%)	18 7
1	B	370/377 (98%)	358 (97%)	12 (3%)	39 27
All	All	740/754 (98%)	705 (95%)	35 (5%)	25 13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	THR
1	A	329	HIS
1	A	337	LEU
1	A	352	ASP
1	A	360	GLU
1	A	381	LEU
1	A	390	SER
1	A	476	ASN
1	A	489	ASP
1	A	511	LYS
1	A	523	LEU
1	A	527	ASN
1	A	535	GLN
1	A	547	ARG
1	A	550	LYS
1	A	555	LYS
1	A	612	LYS
1	A	615	ASP
1	A	622	SER
1	A	645	LYS
1	A	663	GLU

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Mol	Chain	Res	Type
1	A	713	THR
1	A	715	VAL
1	B	336	MET
1	B	337	LEU
1	B	353	GLN
1	B	370	LYS
1	B	392	SER
1	B	476	ASN
1	B	540	LEU
1	B	547	ARG
1	B	608	GLU
1	B	620	LYS
1	B	645	LYS
1	B	701	THR

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 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	$\#\|Z\|>2$
3	H4B	A	802	-	16,18,18	0.83	0	11,26,26	2.51	6 (54%)
4	OT4	A	803	-	22,23,23	1.96	2 (9%)	30,32,32	1.47	4 (13%)
4	OT4	B	803	-	22,23,23	1.95	2 (9%)	30,32,32	1.43	4 (13%)
2	HEM	B	801	1	41,50,50	1.99	7 (17%)	45,82,82	1.87	8 (17%)
5	ACT	A	804	-	3,3,3	0.77	0	3,3,3	0.64	0
2	HEM	A	801	1	41,50,50	1.97	8 (19%)	45,82,82	1.63	8 (17%)
3	H4B	B	802	-	16,18,18	0.83	0	11,26,26	2.40	5 (45%)
5	ACT	B	804	-	3,3,3	0.75	0	3,3,3	0.81	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	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	OT4	A	803	-	-	1/7/7/7	0/3/3/3
4	OT4	B	803	-	-	3/7/7/7	0/3/3/3
2	HEM	B	801	1	-	2/12/54/54	-
2	HEM	A	801	1	-	4/12/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3D-C2D	8.26	1.54	1.36
2	B	801	HEM	C3D-C2D	7.97	1.53	1.36
4	B	803	OT4	C22-C21	-5.90	1.29	1.39
4	A	803	OT4	C22-C21	-5.87	1.29	1.39
4	B	803	OT4	C22-C23	-5.74	1.29	1.39
4	A	803	OT4	C22-C23	-5.61	1.29	1.39
2	B	801	HEM	C3C-C2C	-4.36	1.34	1.40
2	A	801	HEM	C3C-C2C	-4.19	1.34	1.40
2	B	801	HEM	C3C-CAC	3.38	1.54	1.47
2	A	801	HEM	C3C-CAC	3.12	1.54	1.47
2	A	801	HEM	CAB-C3B	2.95	1.55	1.47
2	B	801	HEM	CAB-C3B	2.69	1.54	1.47
2	B	801	HEM	FE-NB	2.53	2.09	1.96
2	A	801	HEM	FE-ND	2.52	2.09	1.96
2	A	801	HEM	FE-NB	2.37	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	CMB-C2B	2.33	1.55	1.50
2	B	801	HEM	CMD-C2D	2.30	1.55	1.50
2	A	801	HEM	CMB-C2B	2.07	1.55	1.50
2	A	801	HEM	CMD-C2D	2.06	1.55	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HEM	CBD-CAD-C3D	-5.33	97.82	112.63
2	A	801	HEM	C4D-ND-C1D	5.24	110.48	105.07
2	B	801	HEM	C4D-ND-C1D	5.17	110.42	105.07
3	B	802	H4B	C8A-C4A-C4	4.57	118.63	114.57
3	A	802	H4B	C8A-C4A-C4	4.11	118.22	114.57
4	B	803	OT4	C04-C05-C10	3.80	120.07	118.01
4	A	803	OT4	C04-C05-C10	3.72	120.03	118.01
2	A	801	HEM	CBA-CAA-C2A	-3.69	106.33	112.62
2	B	801	HEM	CBA-CAA-C2A	-3.57	106.53	112.62
3	A	802	H4B	N1-C2-N3	-3.44	120.02	125.42
3	A	802	H4B	C4-C4A-N5	3.43	122.00	119.12
4	A	803	OT4	C05-C10-N01	-3.42	119.19	122.81
2	B	801	HEM	C4B-CHC-C1C	3.16	126.73	122.56
3	B	802	H4B	N1-C2-N3	-3.15	120.48	125.42
3	B	802	H4B	C2-N3-C4	3.13	120.90	115.93
3	A	802	H4B	C2-N3-C4	2.93	120.58	115.93
2	A	801	HEM	C4C-CHD-C1D	2.89	126.38	122.56
2	B	801	HEM	CAD-C3D-C4D	2.88	129.69	124.66
3	A	802	H4B	C2-N1-C8A	2.86	120.95	114.54
2	A	801	HEM	C3B-C2B-C1B	2.72	108.50	106.49
4	B	803	OT4	C05-C10-N01	-2.67	119.97	122.81
2	B	801	HEM	CAD-CBD-CGD	2.55	119.09	113.60
2	B	801	HEM	CHD-C1D-ND	2.47	127.11	124.43
2	A	801	HEM	CMC-C2C-C3C	2.47	129.29	124.68
3	B	802	H4B	C2-N1-C8A	2.46	120.04	114.54
3	B	802	H4B	C4-C4A-N5	2.39	121.13	119.12
4	B	803	OT4	N02-C02-N01	2.23	120.11	118.26
4	A	803	OT4	N02-C02-N01	2.21	120.09	118.26
2	B	801	HEM	C4C-CHD-C1D	2.15	125.40	122.56
4	A	803	OT4	C03-C04-C05	2.09	119.84	117.78
2	A	801	HEM	C4B-CHC-C1C	2.09	125.31	122.56
2	A	801	HEM	CBD-CAD-C3D	-2.06	106.89	112.63
2	A	801	HEM	CAD-C3D-C4D	2.06	128.25	124.66
3	A	802	H4B	N2-C2-N3	2.04	120.42	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	803	OT4	C22-C21-C08	-2.02	117.52	120.86

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2A-CAA-CBA-CGA
4	A	803	OT4	C23-C27-C28-N29
4	B	803	OT4	C23-C27-C28-N29
2	B	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
2	A	801	HEM	C2D-C3D-CAD-CBD
4	B	803	OT4	C24-C23-C27-C28
4	B	803	OT4	C22-C23-C27-C28
2	A	801	HEM	C4D-C3D-CAD-CBD

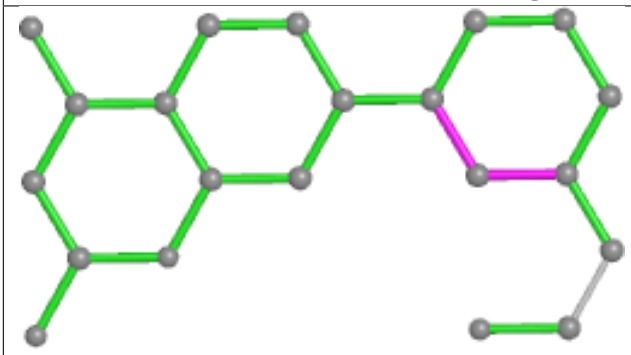
There are no ring outliers.

4 monomers are involved in 9 short contacts:

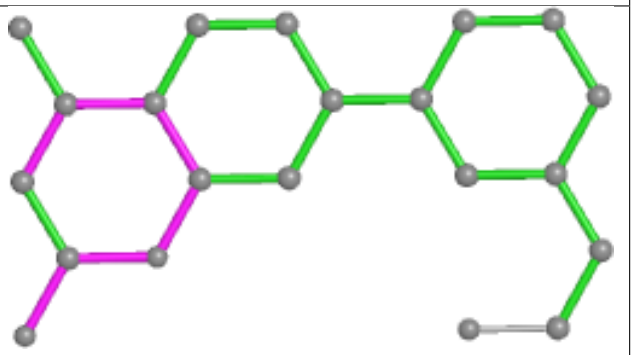
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	OT4	1	0
4	B	803	OT4	3	0
2	B	801	HEM	3	0
2	A	801	HEM	3	0

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.

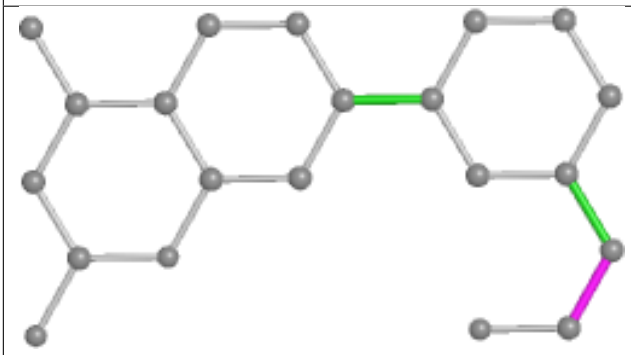
Ligand OT4 A 803



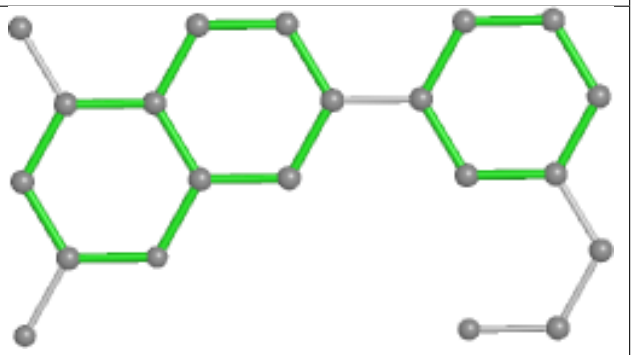
Bond lengths



Bond angles

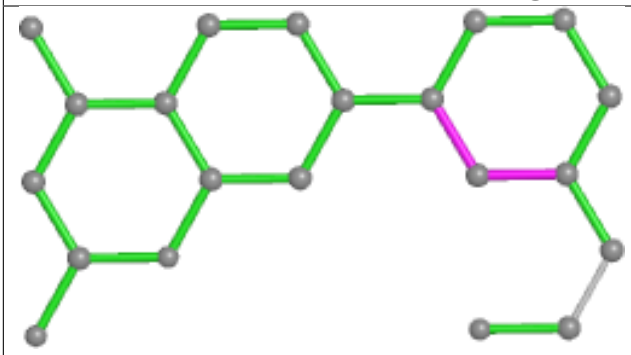


Torsions

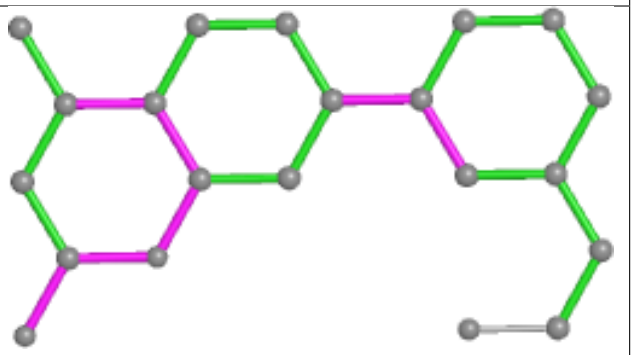


Rings

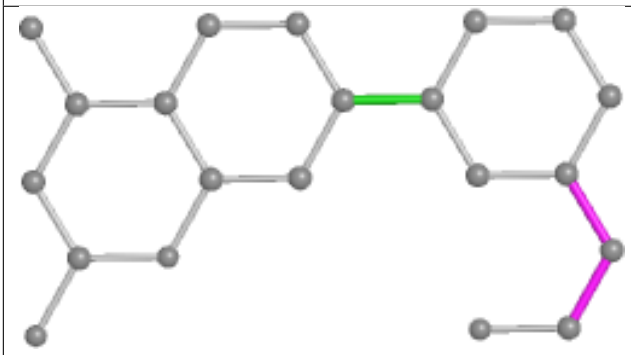
Ligand OT4 B 803



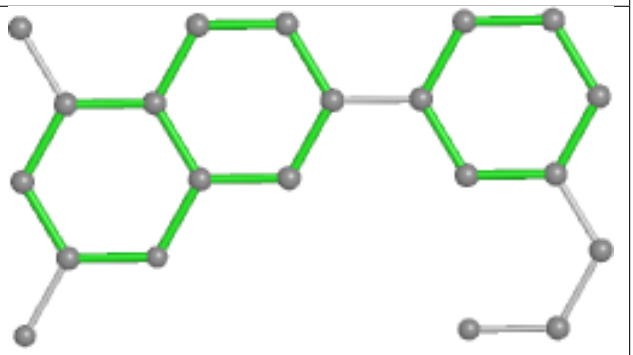
Bond lengths



Bond angles

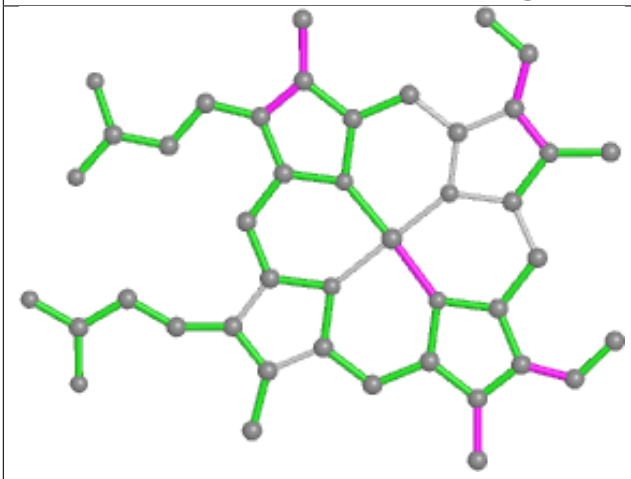


Torsions

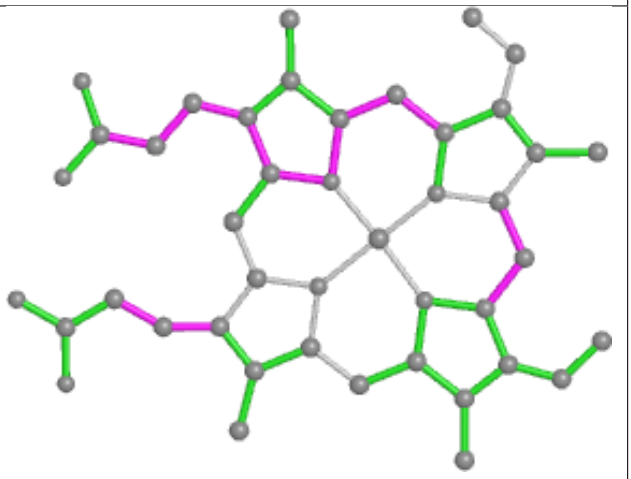


Rings

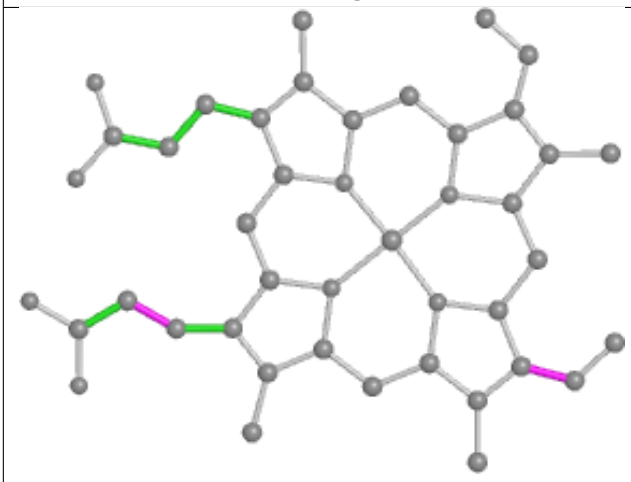
Ligand HEM B 801



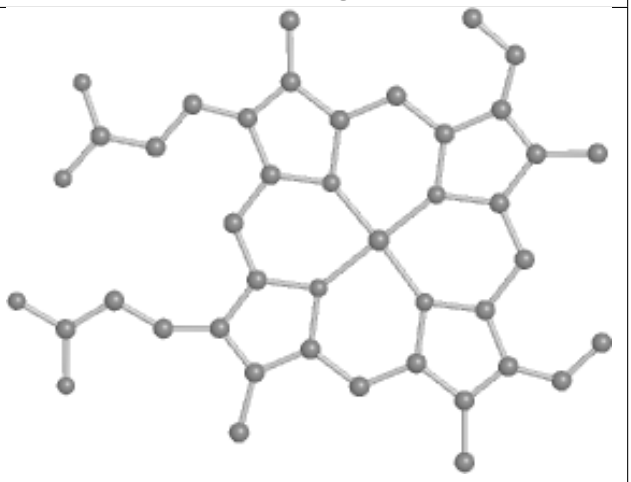
Bond lengths



Bond angles

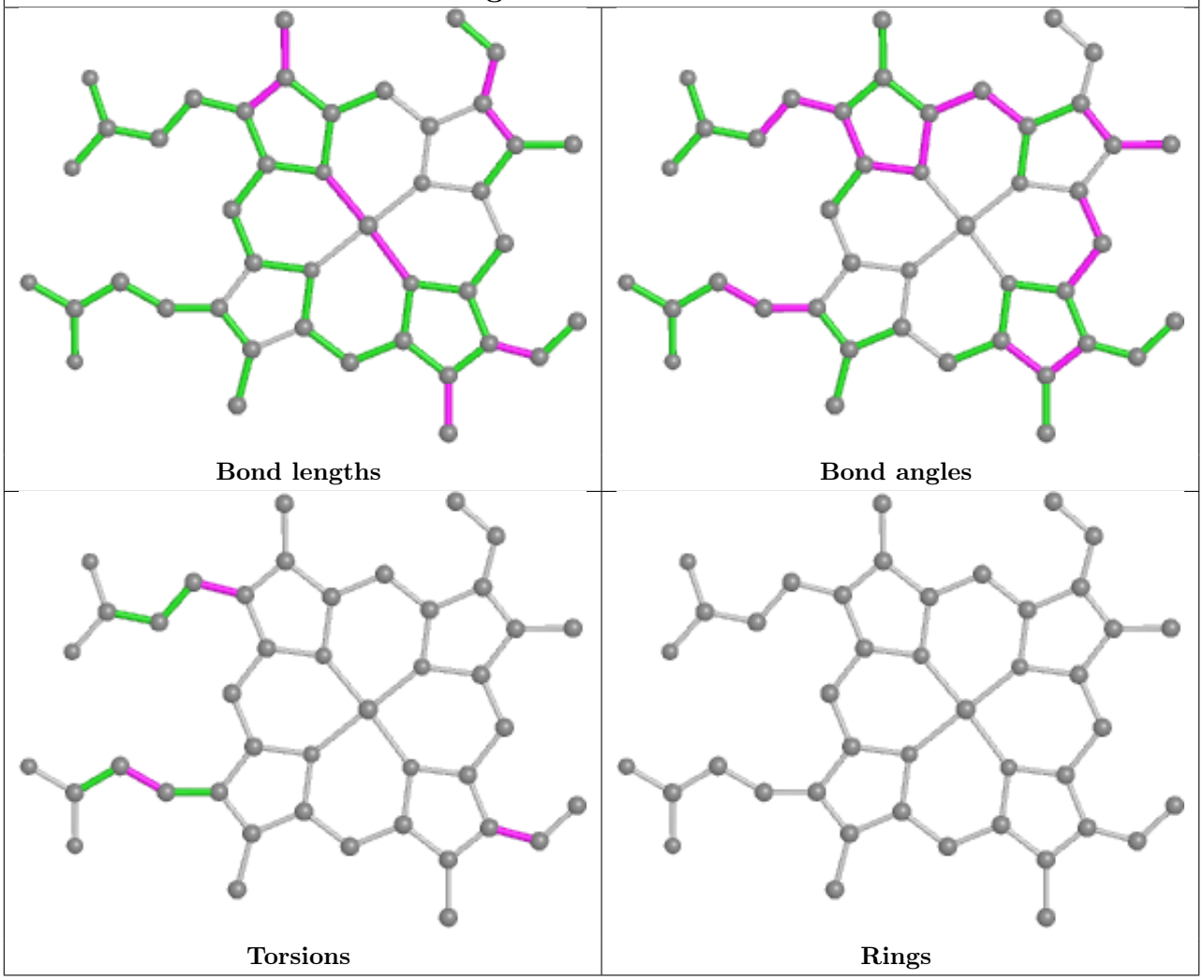


Torsions



Rings

Ligand HEM A 801



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	412/422 (97%)	1.09	80 (19%)	1	1	32, 59, 107, 150	0
1	B	413/422 (97%)	0.63	44 (10%)	6	9	31, 52, 89, 118	0
All	All	825/844 (97%)	0.86	124 (15%)	2	3	31, 54, 103, 150	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	10.7
1	B	300	PHE	9.5
1	A	488	PRO	8.1
1	A	347	ASP	7.3
1	A	506	ILE	6.4
1	A	348	VAL	6.1
1	A	489	ASP	5.5
1	B	348	VAL	5.4
1	A	346	GLU	5.0
1	A	716	TRP	4.9
1	A	352	ASP	4.9
1	A	349	ARG	4.8
1	A	713	THR	4.6
1	B	350	THR	4.6
1	A	390	SER	4.6
1	A	299	ARG	4.5
1	B	299	ARG	4.5
1	A	486	LYS	4.4
1	A	389	GLU	4.4
1	A	490	GLY	4.2
1	A	350	THR	4.1
1	B	352	ASP	3.9
1	A	391	THR	3.9
1	B	718	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	355[A]	PHE	3.9
1	A	351	LYS	3.9
1	A	551	PHE	3.8
1	A	584	PHE	3.8
1	B	309	ASP	3.8
1	A	712	ASN	3.8
1	A	491	SER	3.7
1	A	679	ILE	3.7
1	A	643	SER	3.7
1	A	388	ILE	3.7
1	A	300	PHE	3.7
1	A	385	ASN	3.6
1	A	567	VAL	3.6
1	A	508	GLN	3.6
1	A	677	VAL	3.6
1	A	678	TRP	3.4
1	A	487	GLN	3.4
1	A	322	LEU	3.4
1	A	470	HIS	3.3
1	B	677	VAL	3.3
1	B	340	GLN	3.3
1	A	676	TRP	3.3
1	B	619	ARG	3.3
1	A	615	ASP	3.2
1	A	682	PRO	3.2
1	B	680	VAL	3.2
1	A	507	GLN	3.1
1	A	415	CYS	3.1
1	A	588	TYR	3.1
1	A	503	GLU	3.0
1	A	393	THR	3.0
1	B	389	GLU	3.0
1	B	310	VAL	3.0
1	B	678	TRP	3.0
1	A	311	VAL	3.0
1	A	466	THR	2.9
1	A	681	PRO	2.9
1	B	567	VAL	2.9
1	B	301	LEU	2.9
1	B	691	PHE	2.9
1	A	353	GLN	2.8
1	A	499	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	566	ALA	2.8
1	A	310	VAL	2.8
1	A	480	ILE	2.7
1	B	679	ILE	2.7
1	A	704	PHE	2.7
1	B	615	ASP	2.7
1	A	492	THR	2.7
1	B	676	TRP	2.7
1	A	392	SER	2.7
1	A	591	THR	2.7
1	A	691	PHE	2.6
1	B	618	MET	2.6
1	B	682	PRO	2.6
1	B	617	ASP	2.6
1	A	505	CYS	2.5
1	B	321	THR	2.5
1	A	667	ARG	2.5
1	B	667	ARG	2.5
1	B	616	LEU	2.5
1	A	685	GLY	2.5
1	A	714	HIS	2.5
1	B	302	LYS	2.5
1	A	386	LYS	2.4
1	B	375	LYS	2.4
1	B	490	GLY	2.4
1	A	416	VAL	2.4
1	B	588	TYR	2.4
1	A	680	VAL	2.4
1	A	511	LYS	2.4
1	A	309	ASP	2.4
1	B	313	THR	2.4
1	A	590	GLY	2.3
1	A	382	GLU	2.3
1	A	514	ARG	2.3
1	A	619	ARG	2.3
1	A	504	ILE	2.3
1	B	311	VAL	2.3
1	B	351	LYS	2.3
1	A	339	SER	2.3
1	B	681	PRO	2.3
1	B	566	ALA	2.3
1	B	591	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	452	LYS	2.2
1	A	686	SER	2.2
1	B	611	ALA	2.2
1	A	459	ILE	2.2
1	A	568	SER	2.2
1	A	479	LEU	2.2
1	B	561	TRP	2.2
1	A	453	GLY	2.2
1	B	715	VAL	2.1
1	B	620	LYS	2.1
1	B	329	HIS	2.1
1	A	711	TRP	2.1
1	B	339	SER	2.1
1	B	349	ARG	2.1
1	B	683	MET	2.0
1	A	446	VAL	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
5	ACT	A	804	4/4	0.89	0.21	57,65,69,75	0
4	OT4	B	803	21/21	0.93	0.23	38,57,75,76	0
4	OT4	A	803	21/21	0.93	0.27	36,51,77,80	0
3	H4B	A	802	17/17	0.95	0.19	25,41,50,58	0
5	ACT	B	804	4/4	0.95	0.14	71,80,80,84	0
2	HEM	B	801	43/43	0.96	0.19	26,42,55,70	0
3	H4B	B	802	17/17	0.96	0.19	33,39,50,52	0

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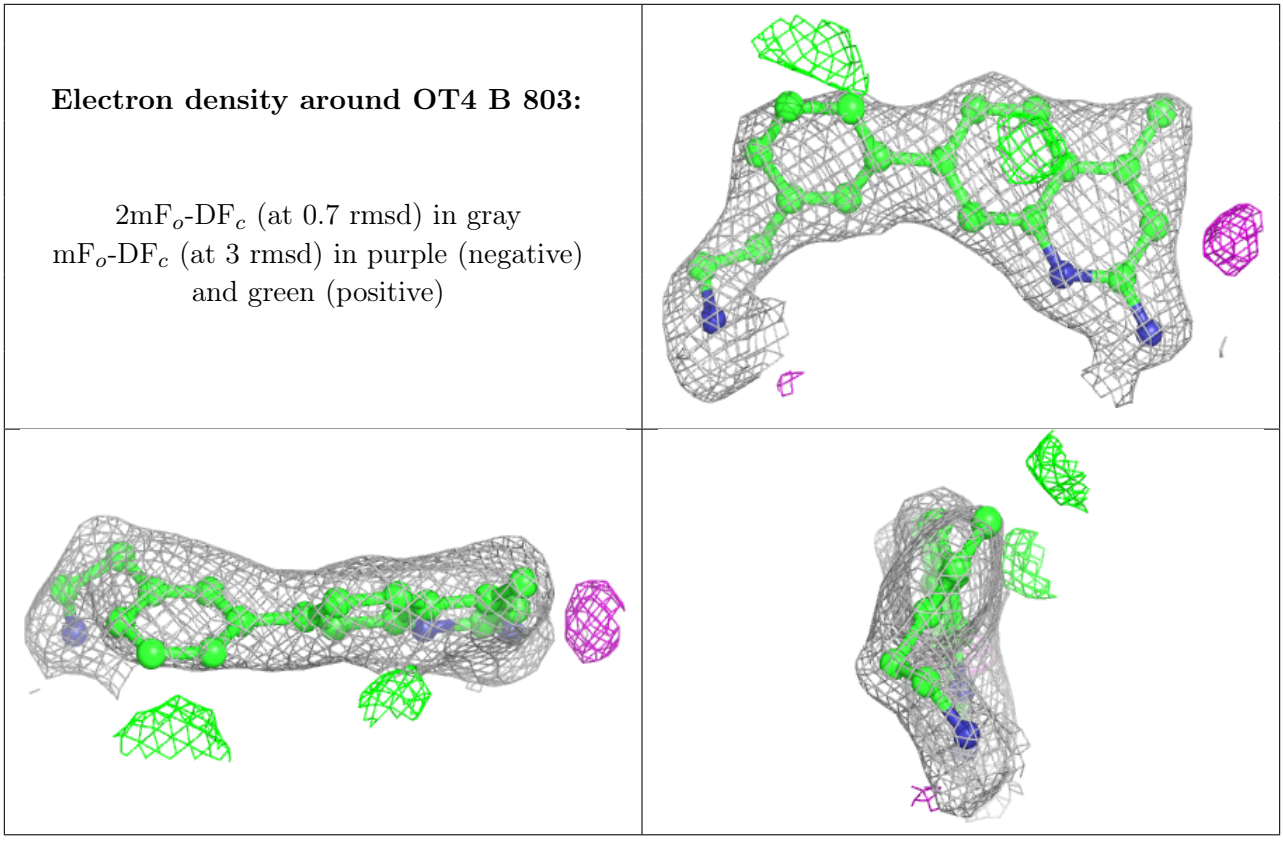
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	801	43/43	0.97	0.20	22,40,63,70	0
6	ZN	A	805	1/1	0.98	0.08	43,43,43,43	0

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.

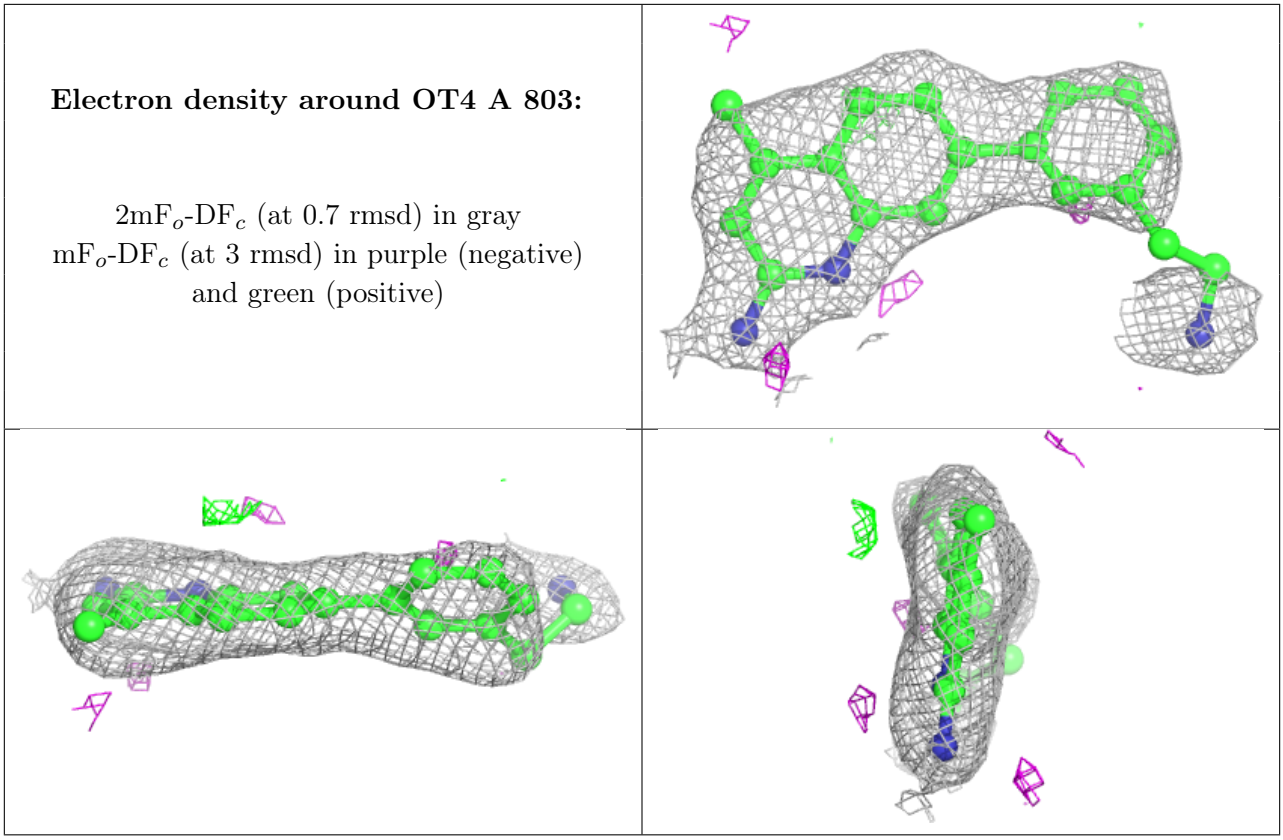
Electron density around OT4 B 803:

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



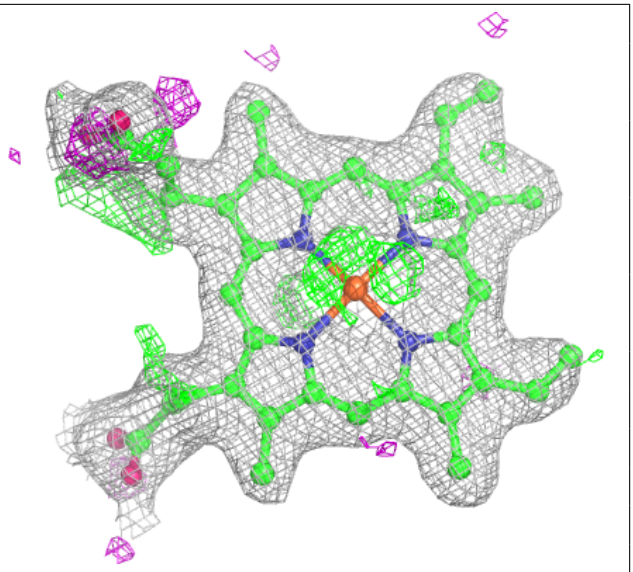
Electron density around OT4 A 803:

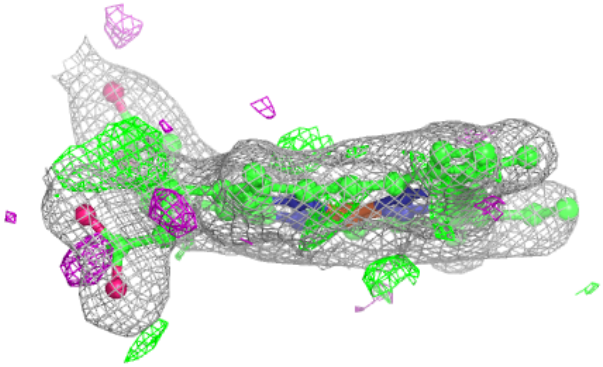
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

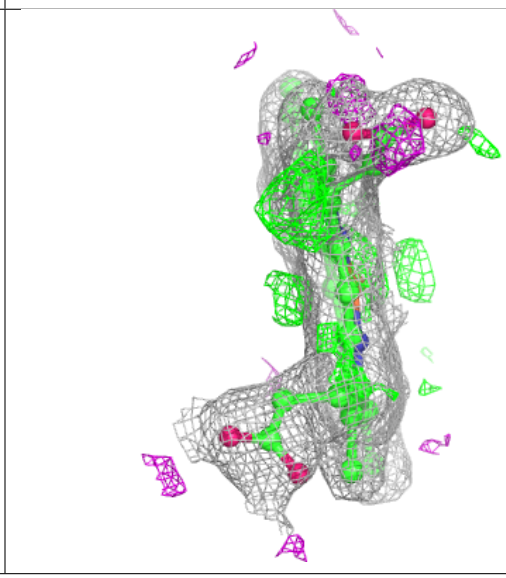


Electron density around HEM B 801:

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

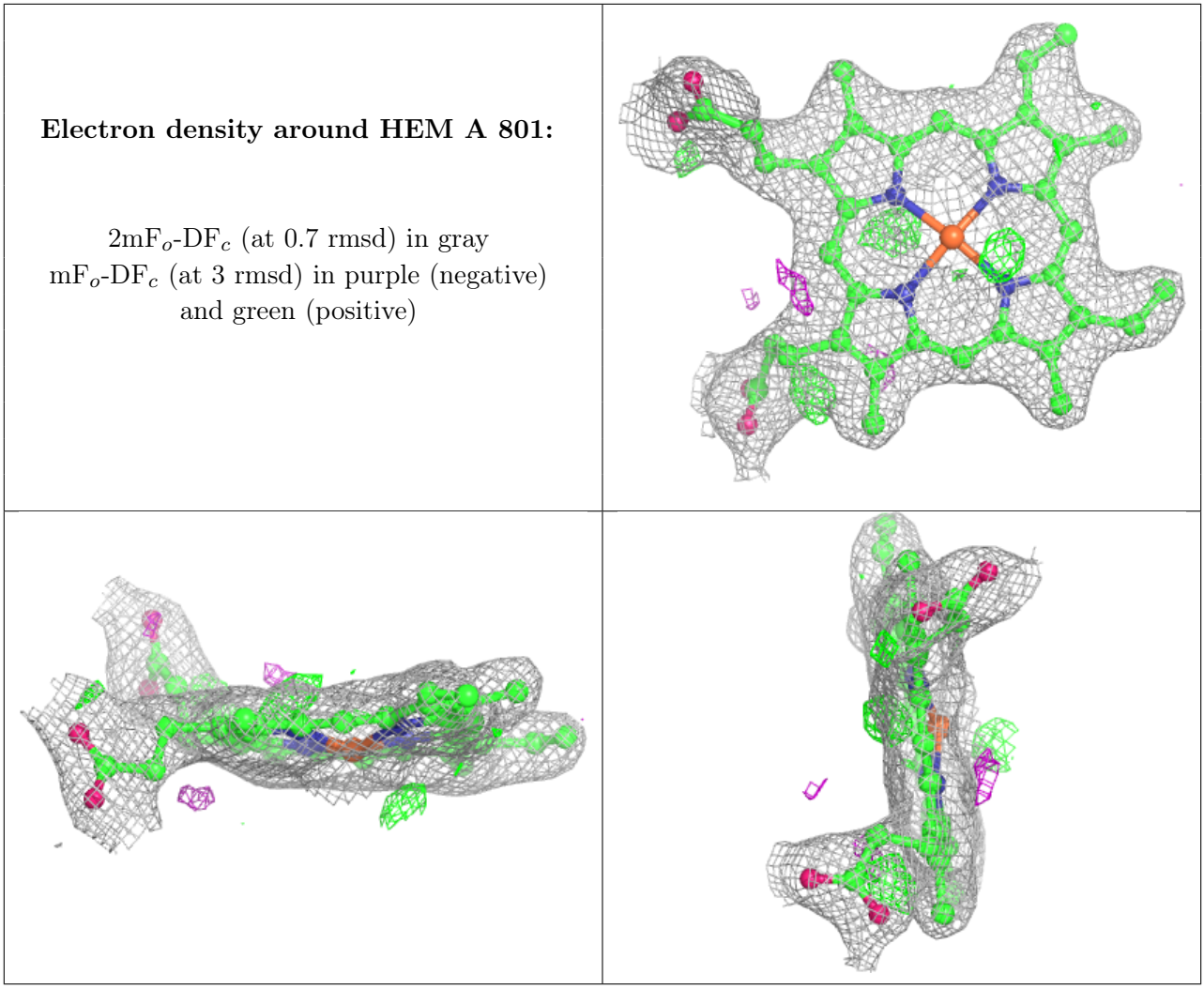






Electron density around HEM A 801:

$2mF_o$-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.