Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 11:28 PM EST

PDB ID	:	3N68
Title	:	Structure of endothelial nitric oxide synthase heme domain N368D/V106M double mutant complexed with 4-(3-(2-(6-amino-4-methylpyridin-2-yl)ethyl)phenethyl)-6-methylpyridin-2-amine
Authors	:	Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on	:	2010-05-25
Resolution	:	2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

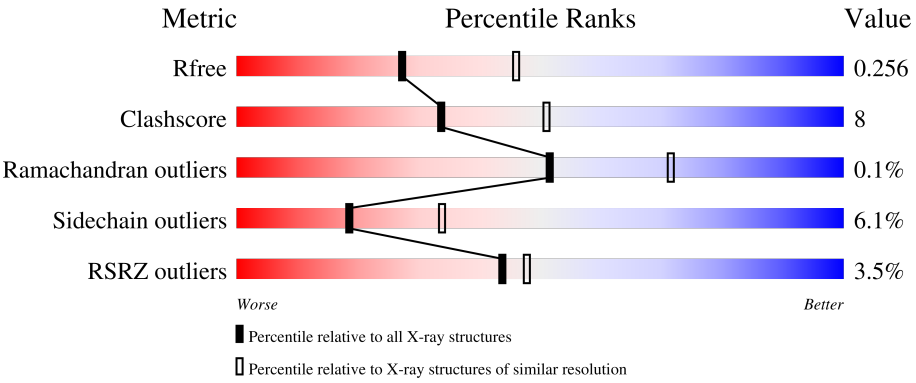
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	444	4% 76% 14% • 9%
1	B	444	3% 69% 20% • 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6715 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.

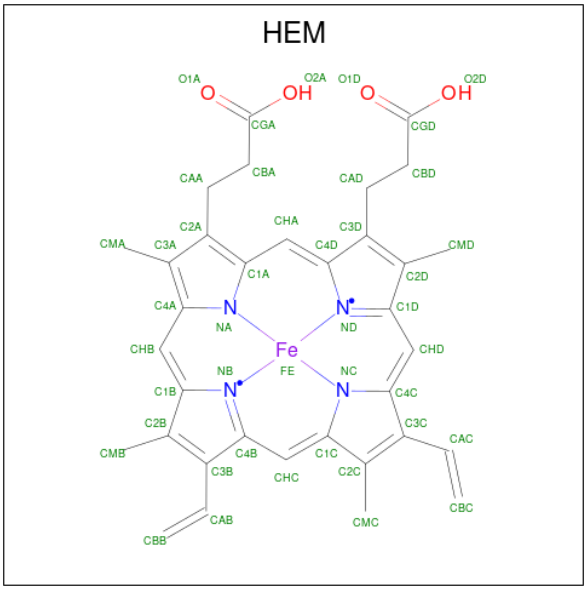
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3210	2041	563	589	17			
1	B	403	Total	C	N	O	S	0	0	0
			3210	2040	565	588	17			

There are 6 discrepancies between the modelled and reference sequences:

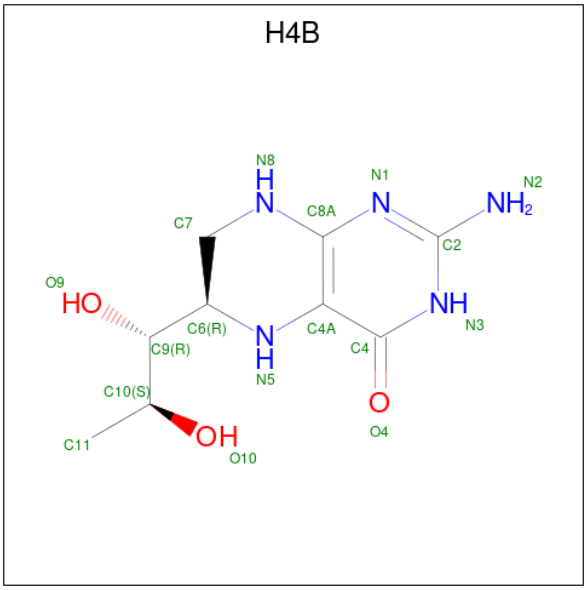
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29476
A	106	MET	VAL	engineered mutation	UNP P29476
A	368	ASP	ASN	engineered mutation	UNP P29476
B	100	ARG	CYS	SEE REMARK 999	UNP P29476
B	106	MET	VAL	engineered mutation	UNP P29476
B	368	ASP	ASN	engineered mutation	UNP P29476

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



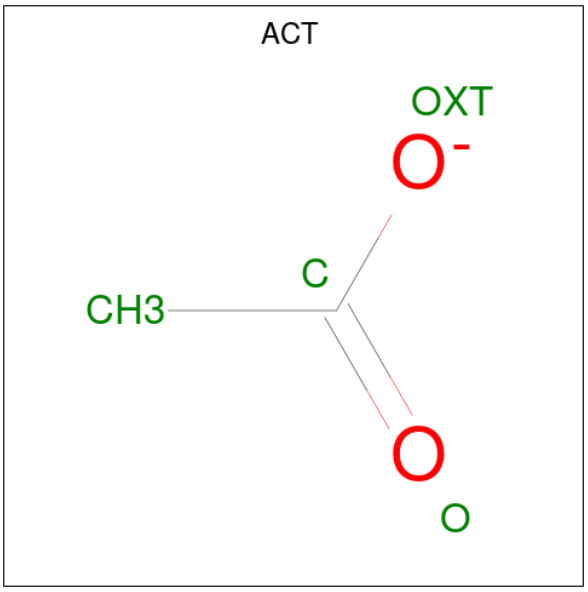
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



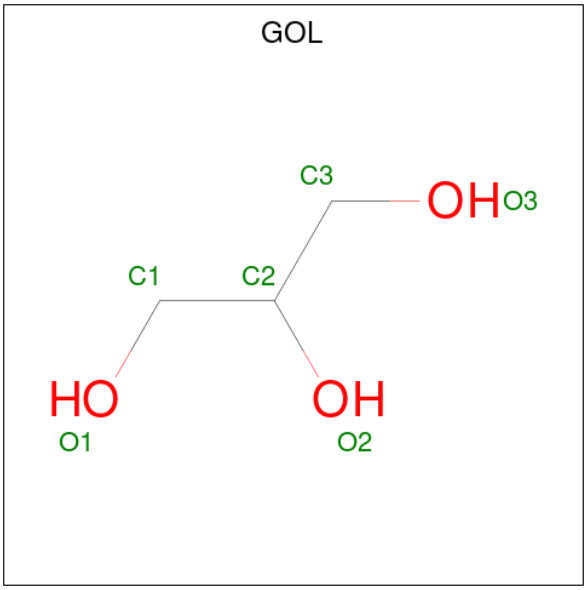
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



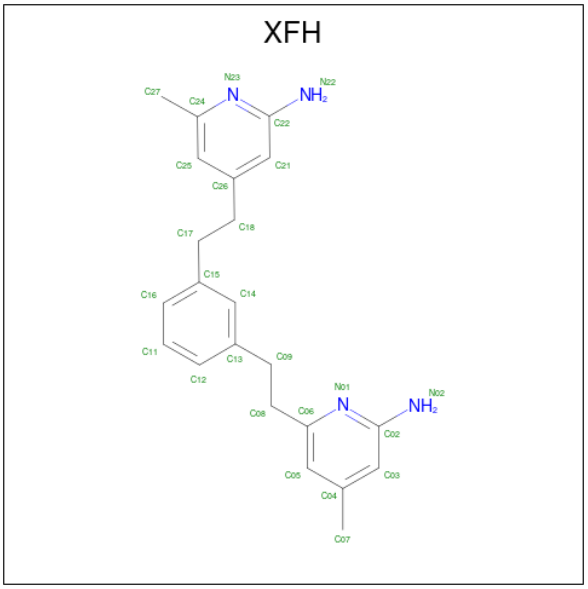
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



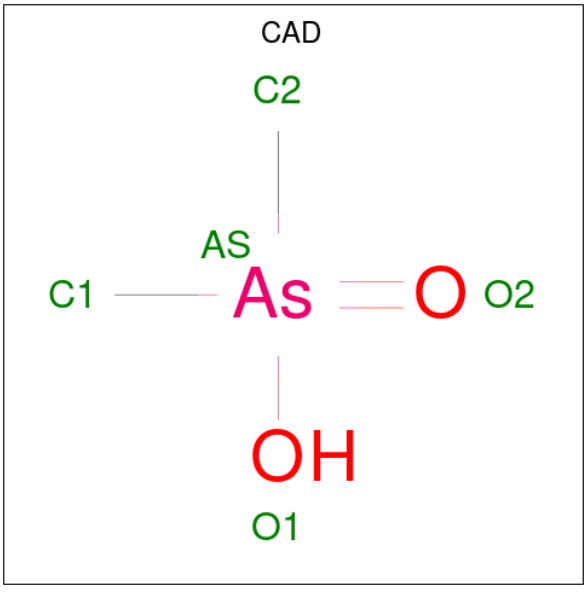
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is 6-(2-{3-[2-(2-amino-6-methylpyridin-4-yl)ethyl]phenyl}ethyl)-4-methylpyridin -2-amine (three-letter code: XFH) (formula: $C_{22}H_{26}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 26 22 4	0	0
6	B	1	Total C N 26 22 4	0	0

- Molecule 7 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total As C 3 1 2	0	0
7	B	1	Total As C 3 1 2	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is water.

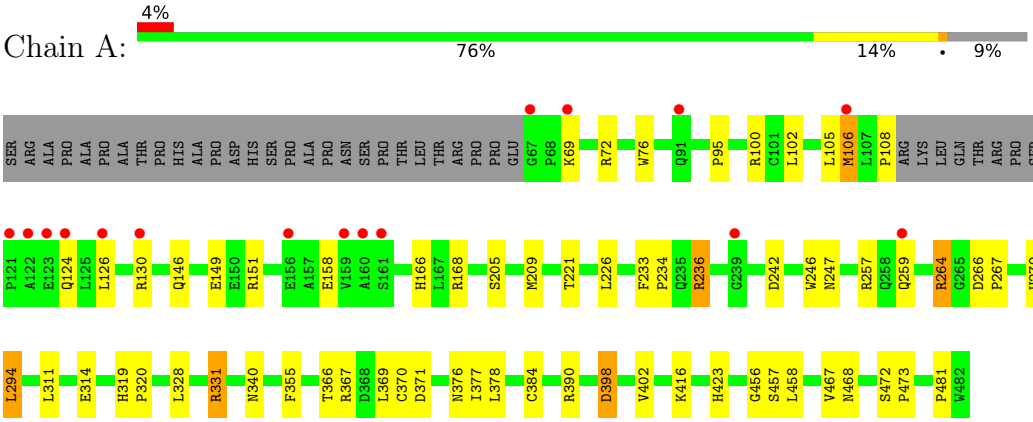
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	48	Total O 48 48	0	0
9	B	48	Total O 48 48	0	0

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.

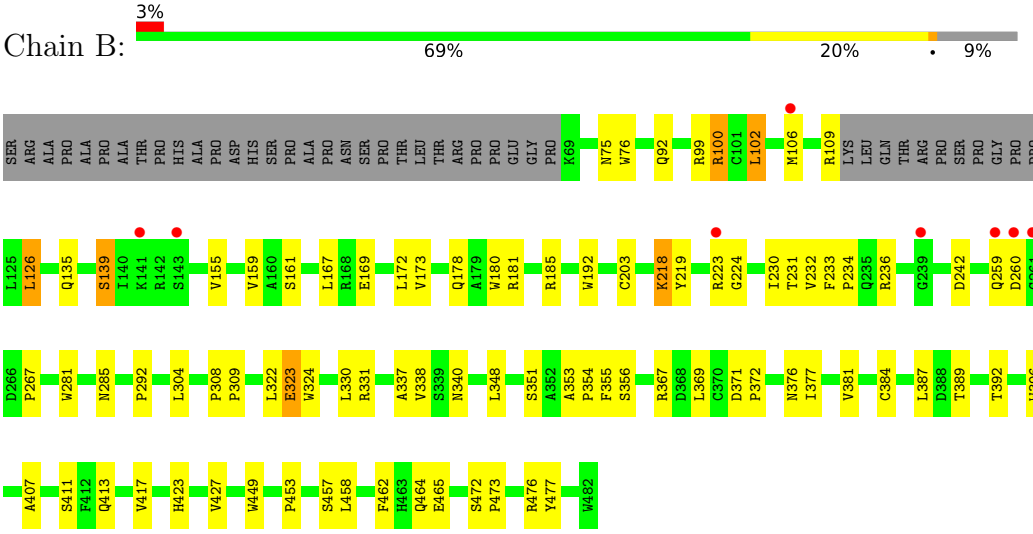
• Molecule 1: Nitric oxide synthase

Chain A:



• Molecule 1: Nitric oxide synthase

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	57.81Å 106.58Å 157.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.27 – 2.53 39.27 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.27-2.53) 97.6 (39.27-2.53)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.190 , 0.254 0.197 , 0.256	Depositor DCC
R_{free} test set	1586 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: ACT, CAD, ZN, HEM, GOL, H4B, XFH

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	0.65	0/3300	0.72	0/4494
1	B	0.68	1/3299 (0.0%)	0.72	0/4491
All	All	0.67	1/6599 (0.0%)	0.72	0/8985

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	CYS	CB-SG	-5.52	1.72	1.81

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	3210	0	3113	46	0
1	B	3210	0	3115	66	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	8	0	6	0	0
5	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	0	0
6	A	26	0	26	0	0
6	B	26	0	26	1	0
7	A	3	0	0	2	0
7	B	3	0	0	0	0
8	A	1	0	0	0	0
9	A	48	0	0	3	0
9	B	48	0	0	1	0
All	All	6715	0	6392	110	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 (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:CYS:SG	7:A:950:CAD:AS	2.52	1.28
1:A:236:ARG:HH11	1:A:236:ARG:HG3	0.87	1.03
1:A:236:ARG:HG3	1:A:236:ARG:NH1	1.64	1.00
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.45	0.97
1:A:236:ARG:HH11	1:A:236:ARG:CG	1.75	0.94
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.55	0.89
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.44	0.81
1:A:106:MET:HA	1:A:106:MET:HE2	1.65	0.79
1:A:236:ARG:HG2	1:A:242:ASP:OD1	1.85	0.76
1:A:367:ARG:NH2	1:A:371:ASP:OD2	2.22	0.72
1:B:122:ALA:O	1:B:126:LEU:HB2	1.90	0.71
1:B:106:MET:HA	1:B:106:MET:HE2	1.73	0.71
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.09	0.67
1:B:372:PRO:HA	1:B:376:ASN:ND2	2.12	0.65
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.78	0.65
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.46	0.64
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.82	0.62
1:B:218:LYS:HD3	1:B:219:TYR:N	2.15	0.61
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.35	0.61
1:B:106:MET:HA	1:B:106:MET:CE	2.33	0.58
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.85	0.58
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.04	0.57
1:A:106:MET:SD	3:A:600:H4B:H9	2.44	0.57
1:B:99:ARG:HG2	1:B:100:ARG:HD3	1.87	0.56
1:B:324:TRP:CZ3	1:B:384:CYS:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:HEM:C1C	6:B:800:XFH:H07B	2.40	0.55
1:B:75:ASN:HD22	1:B:464:GLN:NE2	2.05	0.55
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.24	0.54
1:B:324:TRP:CH2	1:B:384:CYS:HB3	2.43	0.54
1:A:467:VAL:HG13	1:B:102:LEU:CD1	2.38	0.54
1:A:398:ASP:O	1:A:402:VAL:HG23	2.08	0.54
1:A:76:TRP:CE2	1:B:106:MET:HG3	2.43	0.53
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.89	0.53
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.44	0.53
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.38	0.53
1:B:407:ALA:O	1:B:411:SER:OG	2.18	0.53
1:B:423:HIS:O	1:B:427:VAL:HG23	2.09	0.53
1:B:477:TYR:OH	2:B:500:HEM:O2D	2.20	0.53
1:B:230:ILE:HG13	1:B:355:PHE:HB3	1.92	0.52
1:A:367:ARG:HH22	5:A:880:GOL:C2	2.22	0.52
1:A:106:MET:CA	1:A:106:MET:CE	2.88	0.52
1:A:106:MET:HE2	1:A:106:MET:CA	2.38	0.52
1:A:106:MET:HA	1:A:106:MET:CE	2.38	0.52
1:B:155:VAL:O	1:B:159:VAL:HG23	2.09	0.52
1:B:106:MET:HE1	1:B:449:TRP:HE1	1.76	0.51
1:B:369:LEU:O	1:B:377:ILE:HG12	2.11	0.51
1:B:381:VAL:HG21	1:B:404:ILE:CD1	2.37	0.51
1:A:264:ARG:NH2	1:A:285:ASN:O	2.44	0.50
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.94	0.50
1:B:99:ARG:HG2	1:B:100:ARG:CD	2.42	0.49
1:B:367:ARG:NH2	1:B:371:ASP:OD2	2.45	0.49
1:A:106:MET:HG3	1:B:76:TRP:CE2	2.46	0.49
1:A:126:LEU:O	1:A:130:ARG:HG3	2.12	0.49
1:A:314:GLU:OE1	1:A:331:ARG:NH2	2.46	0.48
1:A:246:TRP:CD1	1:A:481:PRO:HG2	2.48	0.48
1:A:236:ARG:NH1	1:A:236:ARG:CG	2.46	0.48
1:B:231:THR:O	1:B:353:ALA:HA	2.13	0.48
1:B:281:TRP:CD1	1:B:292:PRO:HG3	2.49	0.48
1:B:323:GLU:H	1:B:323:GLU:HG3	1.38	0.48
2:A:500:HEM:HHC	2:A:500:HEM:CBB	2.44	0.48
1:A:366:THR:O	1:A:370:CYS:HB2	2.13	0.47
1:B:106:MET:CE	1:B:106:MET:CA	2.91	0.47
1:B:367:ARG:NE	1:B:371:ASP:OD2	2.47	0.47
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.97	0.47
1:B:224:GLY:O	1:B:417:VAL:HA	2.14	0.47
1:B:263:VAL:HG11	1:B:267:PRO:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:CYS:CB	7:A:950:CAD:AS	3.22	0.47
1:A:76:TRP:NE1	1:B:106:MET:HG3	2.29	0.47
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.96	0.47
1:B:106:MET:SD	3:B:600:H4B:H9	2.54	0.47
1:A:369:LEU:O	1:A:377:ILE:HG12	2.16	0.46
1:B:457:SER:HA	1:B:462:PHE:CG	2.50	0.46
1:A:221:THR:O	1:A:226:LEU:HD12	2.16	0.46
1:A:158:GLU:OE1	1:A:166:HIS:HD2	1.99	0.45
1:A:355:PHE:CD1	2:A:500:HEM:CAC	2.99	0.45
1:B:396:TRP:CZ3	1:B:397:LYS:HG3	2.51	0.45
1:A:151:ARG:HD3	1:A:168:ARG:NH2	2.32	0.45
1:B:260:ASP:C	1:B:262:SER:H	2.19	0.45
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.82	0.45
1:A:106:MET:HG2	1:B:465:GLU:OE2	2.18	0.44
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.99	0.44
1:A:205:SER:O	1:A:209:MET:HG3	2.17	0.44
1:A:95:PRO:HB3	1:A:108:PRO:HB3	2.00	0.44
1:A:457:SER:HB3	1:B:453:PRO:HB3	1.99	0.44
1:B:377:ILE:O	1:B:381:VAL:HG23	2.18	0.44
1:A:472:SER:HA	1:A:473:PRO:C	2.38	0.44
1:B:285:ASN:OD1	1:B:285:ASN:C	2.56	0.43
1:B:476:ARG:HH11	1:B:476:ARG:HG2	1.83	0.43
1:B:169:GLU:O	1:B:173:VAL:HG23	2.18	0.43
1:B:337:ALA:CB	1:B:356:SER:HB3	2.48	0.43
1:A:378:LEU:HB2	9:A:1004:HOH:O	2.17	0.43
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.39	0.43
1:B:106:MET:HA	1:B:185:ARG:HH22	1.84	0.43
1:B:387:LEU:HD13	1:B:396:TRP:HA	2.00	0.42
1:B:338:VAL:O	1:B:354:PRO:HA	2.19	0.42
1:A:376:ASN:ND2	9:A:1004:HOH:O	2.46	0.42
1:A:423:HIS:HB2	1:B:392:THR:HB	2.02	0.41
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.50	0.41
1:B:308:PRO:HA	1:B:309:PRO:HD3	1.93	0.41
1:B:218:LYS:HD3	1:B:219:TYR:CA	2.50	0.41
1:B:472:SER:HA	1:B:473:PRO:C	2.41	0.41
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.56	0.41
1:B:135:GLN:O	1:B:139:SER:HB3	2.20	0.41
1:A:106:MET:HG2	1:A:106:MET:H	1.54	0.41
1:B:178:GLN:NE2	1:B:181:ARG:HH11	2.15	0.41
1:B:453:PRO:HG3	9:B:1079:HOH:O	2.20	0.41
2:A:500:HEM:HBB2	2:A:500:HEM:CHC	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLY:O	1:B:267:PRO:HD3	2.21	0.40
1:A:266:ASP:HA	1:A:267:PRO:HD3	1.92	0.40
1:A:279:HIS:NE2	9:A:1021:HOH:O	2.37	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	400/444 (90%)	384 (96%)	15 (4%)	1 (0%)	41 59
1	B	399/444 (90%)	375 (94%)	24 (6%)	0	100 100
All	All	799/888 (90%)	759 (95%)	39 (5%)	1 (0%)	51 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	343/377 (91%)	320 (93%)	23 (7%)	16 29
1	B	343/377 (91%)	324 (94%)	19 (6%)	21 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	686/754 (91%)	644 (94%)	42 (6%)	18 34

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	100	ARG
1	A	102	LEU
1	A	106	MET
1	A	124	GLN
1	A	146	GLN
1	A	149	GLU
1	A	236	ARG
1	A	247	ASN
1	A	259	GLN
1	A	264	ARG
1	A	293	LEU
1	A	294	LEU
1	A	311	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	390	ARG
1	A	398	ASP
1	A	416	LYS
1	A	458	LEU
1	A	468	ASN
1	B	92	GLN
1	B	100	ARG
1	B	102	LEU
1	B	109	ARG
1	B	126	LEU
1	B	139	SER
1	B	161	SER
1	B	218	LYS
1	B	223	ARG
1	B	259	GLN
1	B	264	ARG
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG

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Mol	Chain	Res	Type
1	B	340	ASN
1	B	389	THR
1	B	398	ASP
1	B	413	GLN
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	166	HIS
1	A	258	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	259	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN
1	B	464	GLN

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 (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\#\|Z\| > 2$
7	CAD	A	950	-	0,2,4	-	-	0,1,6	-	-
6	XFH	A	800	-	28,28,28	0.74	0	38,38,38	1.26	5 (13%)
3	H4B	B	600	-	16,18,18	0.62	0	11,26,26	2.81	6 (54%)
3	H4B	A	600	-	16,18,18	1.02	0	11,26,26	2.76	5 (45%)
7	CAD	B	950	-	0,2,4	-	-	0,1,6	-	-
4	ACT	A	850	-	3,3,3	0.88	0	3,3,3	0.40	0
2	HEM	B	500	1	41,50,50	1.94	8 (19%)	45,82,82	1.38	5 (11%)
5	GOL	B	880	-	5,5,5	0.31	0	5,5,5	0.84	0
4	ACT	A	860	-	3,3,3	0.79	0	3,3,3	0.63	0
6	XFH	B	800	-	28,28,28	0.66	0	38,38,38	1.62	5 (13%)
2	HEM	A	500	1	41,50,50	1.93	7 (17%)	45,82,82	2.00	8 (17%)
5	GOL	A	880	-	5,5,5	0.38	0	5,5,5	0.29	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
6	XFH	A	800	-	-	4/10/10/10	0/3/3/3
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
3	H4B	A	600	-	-	2/8/17/17	0/2/2/2
5	GOL	B	880	-	-	4/4/4/4	-
2	HEM	B	500	1	-	2/12/54/54	-
6	XFH	B	800	-	-	1/10/10/10	0/3/3/3
2	HEM	A	500	1	-	0/12/54/54	-
5	GOL	A	880	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	7.47	1.52	1.36
2	A	500	HEM	C3D-C2D	6.75	1.51	1.36
2	A	500	HEM	C3C-C2C	-4.07	1.34	1.40
2	A	500	HEM	C3C-CAC	4.03	1.56	1.47
2	B	500	HEM	C3C-CAC	3.93	1.55	1.47
2	B	500	HEM	C3C-C2C	-3.86	1.35	1.40
2	A	500	HEM	FE-ND	3.81	2.15	1.96
2	B	500	HEM	CAB-C3B	2.69	1.54	1.47
2	A	500	HEM	CAB-C3B	2.56	1.54	1.47
2	A	500	HEM	CMA-C3A	2.55	1.56	1.51
2	A	500	HEM	C3B-C2B	-2.36	1.32	1.37
2	B	500	HEM	C3B-C2B	-2.26	1.32	1.37
2	B	500	HEM	FE-NB	2.20	2.07	1.96
2	B	500	HEM	CMD-C2D	2.08	1.55	1.50
2	B	500	HEM	O1D-CGD	2.06	1.29	1.22

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CBA-CAA-C2A	-7.50	99.81	112.62
6	B	800	XFH	C02-N01-C06	6.24	122.83	118.10
2	A	500	HEM	C4D-ND-C1D	5.94	111.21	105.07
3	B	600	H4B	C4-C4A-N5	5.53	123.76	119.12
3	A	600	H4B	C8A-C4A-C4	5.10	119.10	114.57
2	B	500	HEM	C4D-ND-C1D	4.73	109.96	105.07
2	A	500	HEM	C4C-CHD-C1D	3.90	127.71	122.56
3	B	600	H4B	C8A-C4A-C4	3.82	117.97	114.57
3	A	600	H4B	N1-C2-N3	-3.73	119.57	125.42
6	B	800	XFH	C05-C06-N01	-3.51	119.17	122.90
2	B	500	HEM	CBA-CAA-C2A	-3.49	106.67	112.62
2	A	500	HEM	CAD-C3D-C4D	3.45	130.69	124.66
3	A	600	H4B	C4-C4A-N5	3.42	121.99	119.12
3	B	600	H4B	N1-C2-N3	-3.39	120.10	125.42
3	B	600	H4B	C2-N1-C8A	3.19	121.70	114.54
3	A	600	H4B	C2-N1-C8A	3.15	121.59	114.54
2	A	500	HEM	CAD-CBD-CGD	-3.03	107.08	113.60
2	B	500	HEM	C4B-CHC-C1C	2.97	126.48	122.56
3	A	600	H4B	C2-N3-C4	2.96	120.63	115.93
6	A	800	XFH	N22-C22-N23	2.92	121.10	116.49
6	A	800	XFH	C08-C06-N01	2.85	120.20	115.95
3	B	600	H4B	C2-N3-C4	2.80	120.38	115.93
6	A	800	XFH	C05-C06-N01	-2.75	119.98	122.90
2	B	500	HEM	C1D-C2D-C3D	-2.74	104.08	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	800	XFH	C02-N01-C06	2.73	120.17	118.10
6	B	800	XFH	C26-C21-C22	2.56	119.92	117.97
3	B	600	H4B	N2-C2-N1	2.50	121.14	117.25
6	B	800	XFH	N02-C02-N01	2.47	120.40	116.49
2	A	500	HEM	CMA-C3A-C4A	-2.45	124.70	128.46
2	A	500	HEM	CMD-C2D-C1D	2.34	128.60	125.04
6	A	800	XFH	C27-C24-N23	2.29	120.22	116.56
2	A	500	HEM	O1D-CGD-CBD	-2.17	116.11	123.08
2	B	500	HEM	C4C-CHD-C1D	2.15	125.39	122.56
6	B	800	XFH	C26-C25-C24	-2.09	118.93	120.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C2A-CAA-CBA-CGA
5	A	880	GOL	C1-C2-C3-O3
5	A	880	GOL	O2-C2-C3-O3
5	B	880	GOL	O1-C1-C2-C3
5	B	880	GOL	C1-C2-C3-O3
5	B	880	GOL	O1-C1-C2-O2
5	B	880	GOL	O2-C2-C3-O3
2	B	500	HEM	C4B-C3B-CAB-CBB
3	A	600	H4B	C7-C6-C9-O9
6	A	800	XFH	C17-C18-C26-C21
6	A	800	XFH	C17-C18-C26-C25
6	B	800	XFH	C06-C08-C09-C13
6	A	800	XFH	C16-C15-C17-C18
6	A	800	XFH	C14-C15-C17-C18
3	A	600	H4B	N5-C6-C9-O9

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	950	CAD	2	0
3	B	600	H4B	1	0
3	A	600	H4B	1	0
2	B	500	HEM	4	0
6	B	800	XFH	1	0
2	A	500	HEM	4	0

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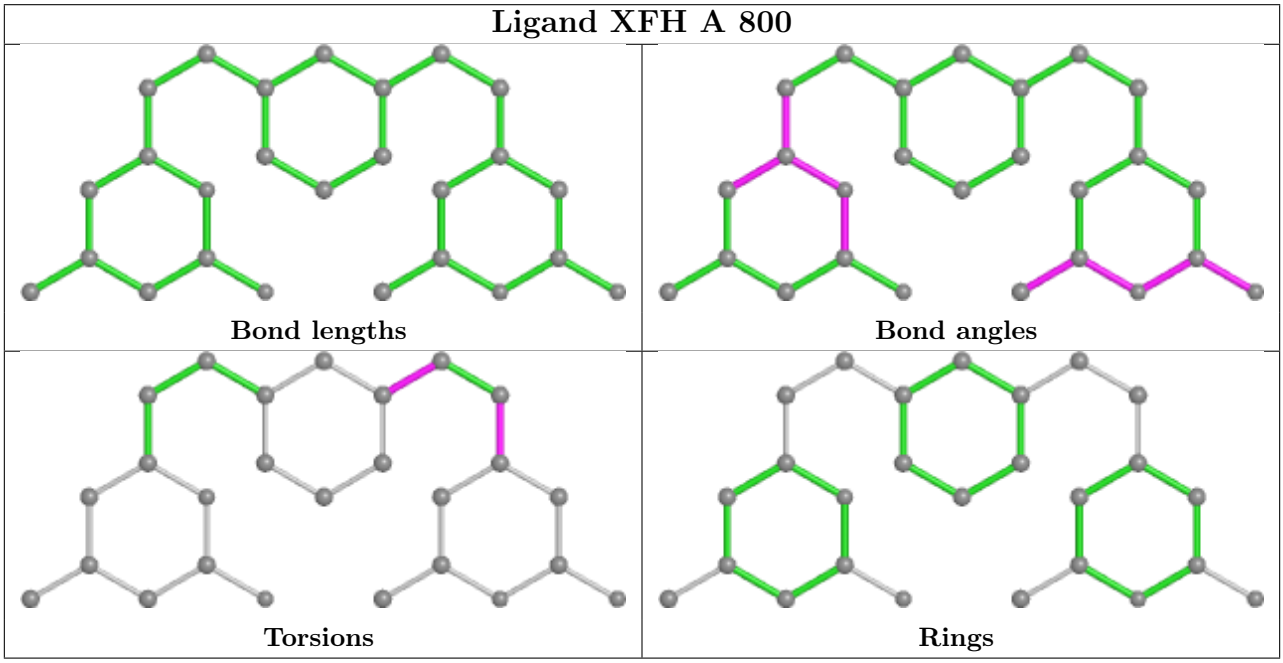
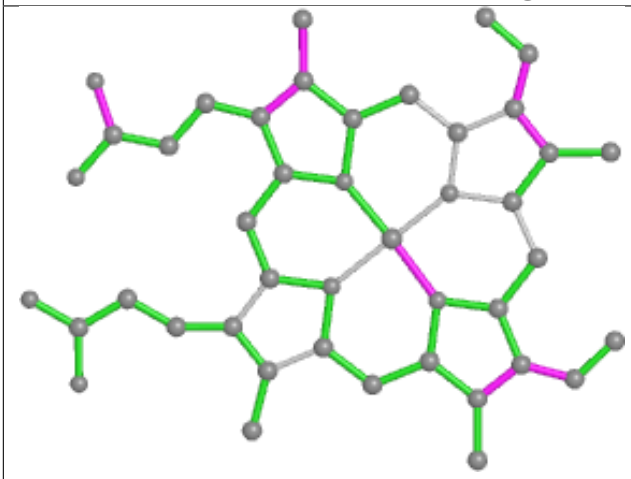
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	880	GOL	1	0

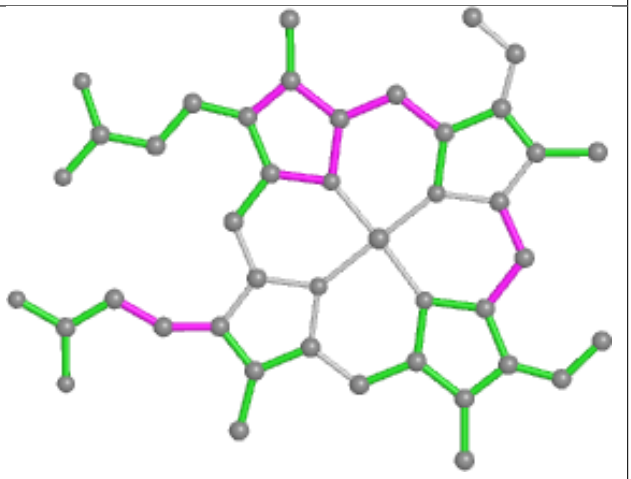
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



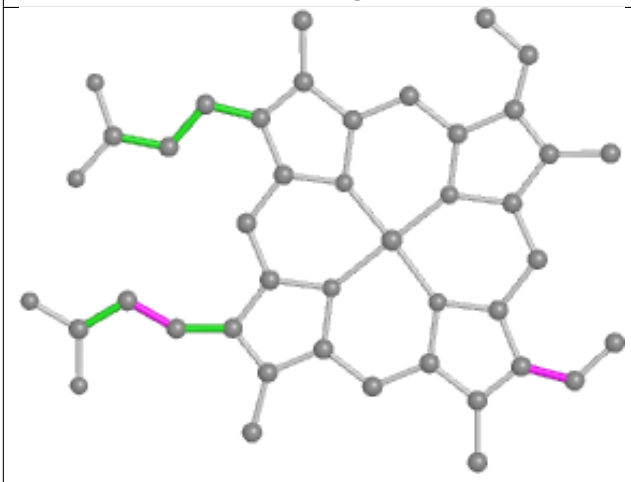
Ligand HEM B 500



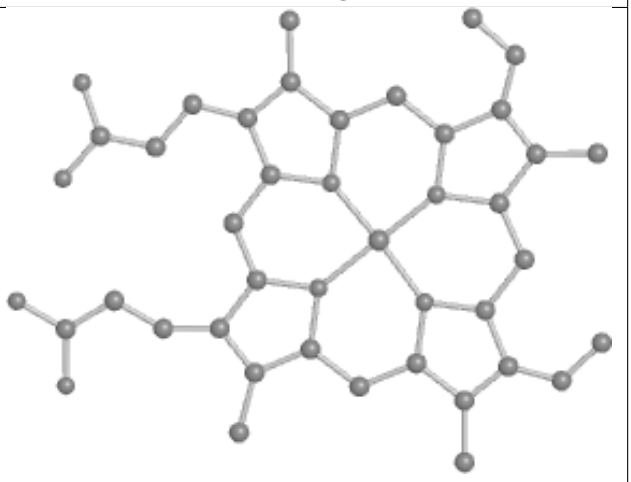
Bond lengths



Bond angles

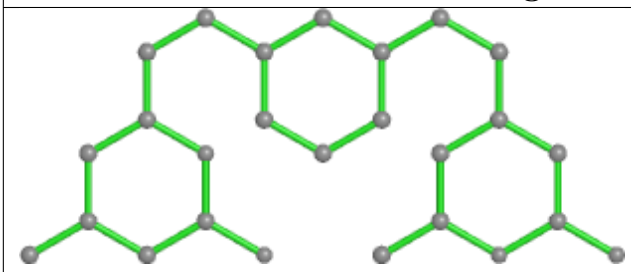


Torsions

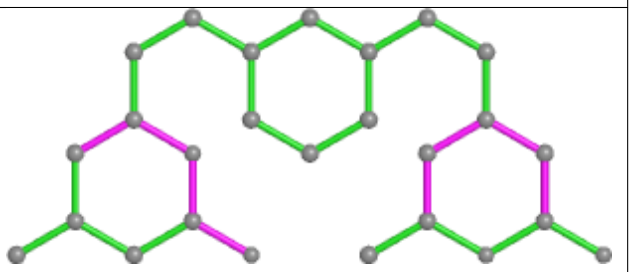


Rings

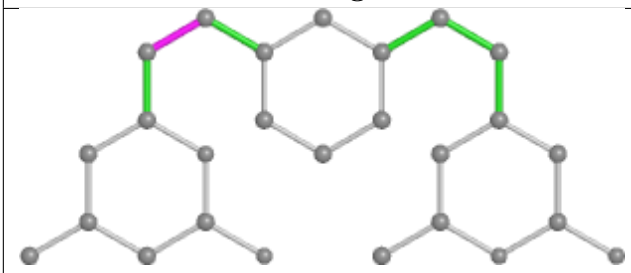
Ligand XFH B 800



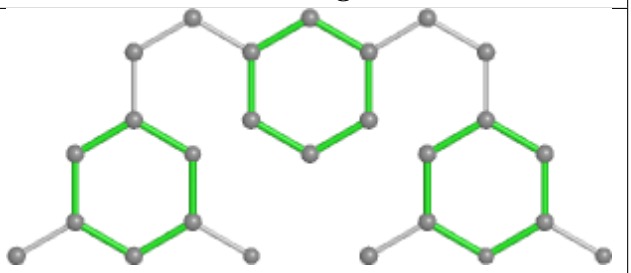
Bond lengths



Bond angles

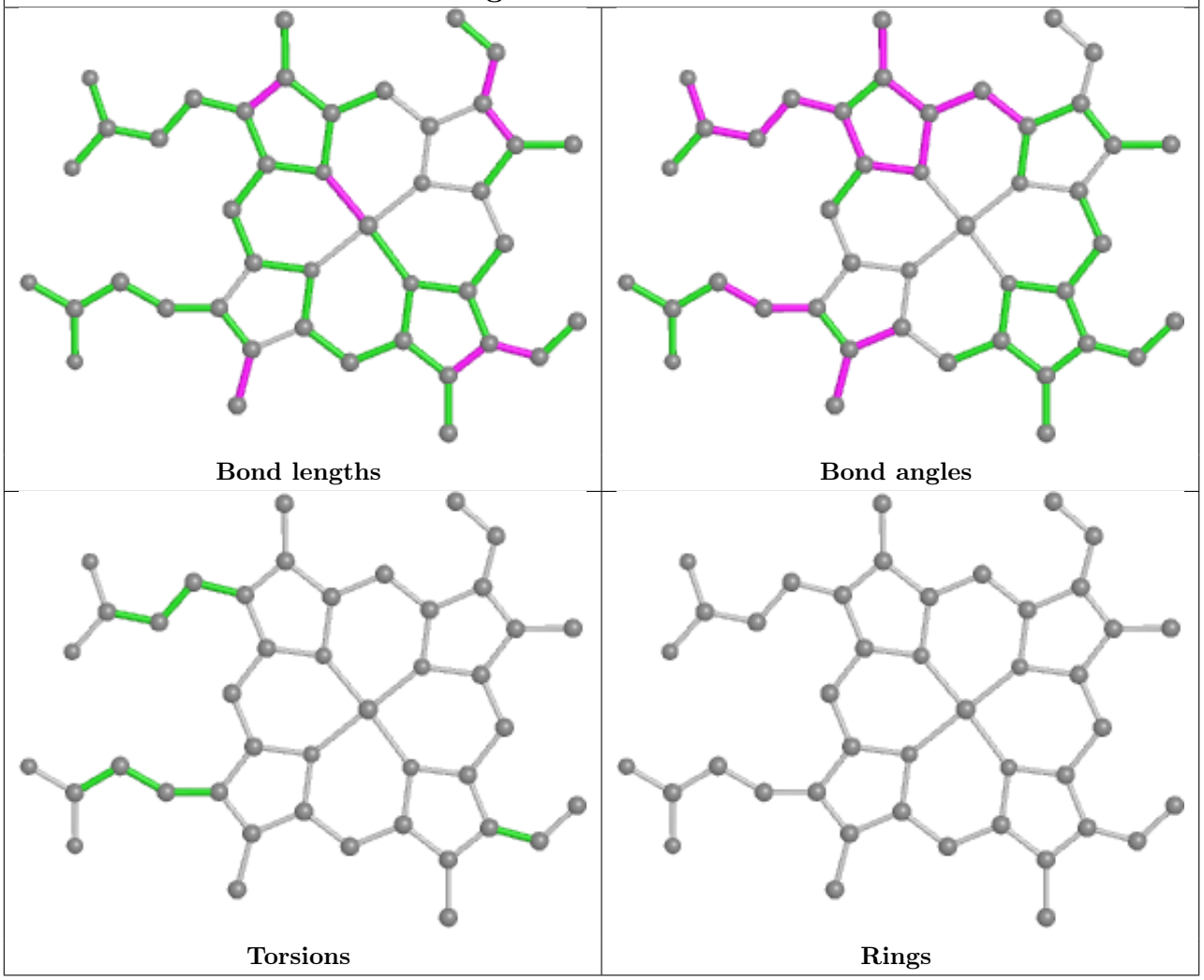


Torsions



Rings

Ligand HEM A 500



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	404/444 (90%)	0.02	16 (3%)	38	42	27, 41, 65, 84	0
1	B	403/444 (90%)	-0.08	12 (2%)	50	54	27, 42, 68, 88	0
All	All	807/888 (90%)	-0.03	28 (3%)	44	48	27, 42, 66, 88	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ALA	4.7
1	A	121	PRO	4.4
1	B	122	ALA	4.2
1	A	123	GLU	3.8
1	A	259	GLN	3.8
1	A	67	GLY	3.7
1	B	123	GLU	3.6
1	B	121	PRO	3.4
1	B	259	GLN	3.4
1	A	126	LEU	3.2
1	A	122	ALA	3.2
1	A	91	GLN	3.1
1	B	261	GLY	3.0
1	A	124	GLN	2.9
1	A	69	LYS	2.9
1	A	239	GLY	2.9
1	B	260	ASP	2.6
1	A	156	GLU	2.6
1	B	106	MET	2.3
1	A	106	MET	2.3
1	B	223	ARG	2.3
1	B	239	GLY	2.2
1	B	124	GLN	2.1
1	A	159	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	143	SER	2.1
1	A	161	SER	2.1
1	A	130	ARG	2.1
1	B	141	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)

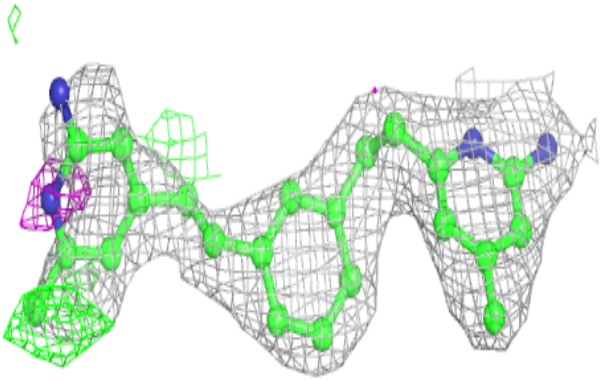
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

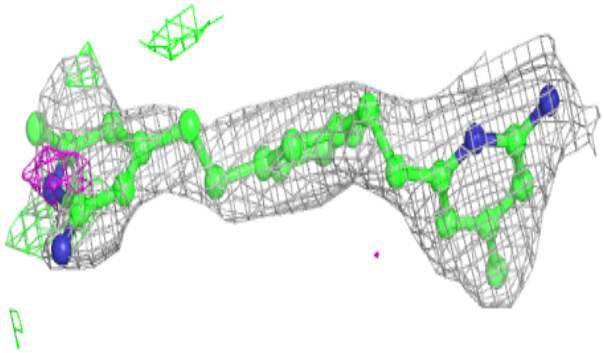
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	880	6/6	0.86	0.31	59,62,63,63	0
5	GOL	A	880	6/6	0.89	0.28	59,62,64,67	0
4	ACT	A	860	4/4	0.89	0.24	44,47,47,47	0
6	XFH	B	800	26/26	0.91	0.25	32,46,74,75	0
6	XFH	A	800	26/26	0.93	0.24	28,45,66,66	0
4	ACT	A	850	4/4	0.94	0.19	45,47,49,49	0
3	H4B	B	600	17/17	0.96	0.17	39,41,44,48	0
3	H4B	A	600	17/17	0.97	0.17	42,45,48,49	0
2	HEM	B	500	43/43	0.97	0.16	27,30,40,41	0
2	HEM	A	500	43/43	0.98	0.17	24,29,38,42	0
7	CAD	B	950	3/5	0.98	0.11	75,75,76,77	0
7	CAD	A	950	3/5	0.99	0.08	59,59,60,60	0
8	ZN	A	900	1/1	1.00	0.10	37,37,37,37	0

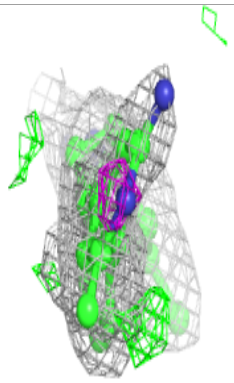
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XFH 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)

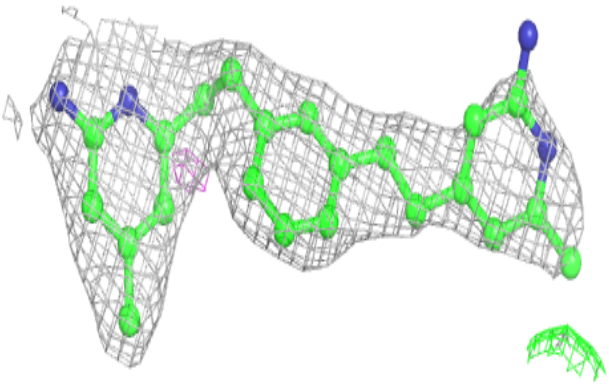


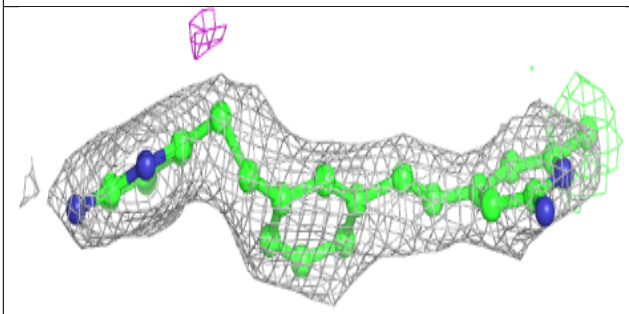


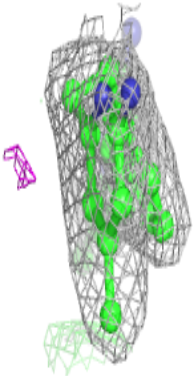


Electron density around XFH A 800:

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

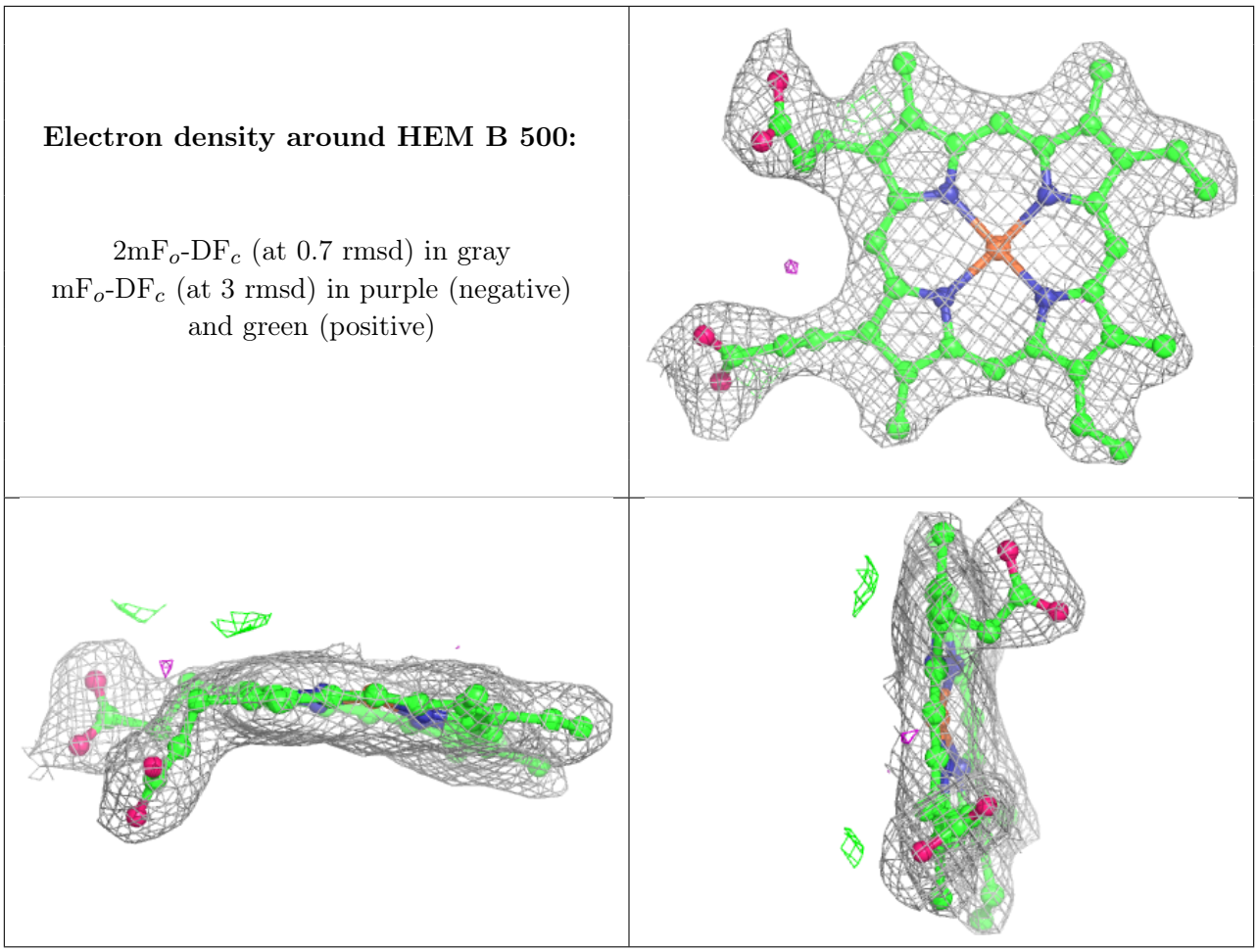






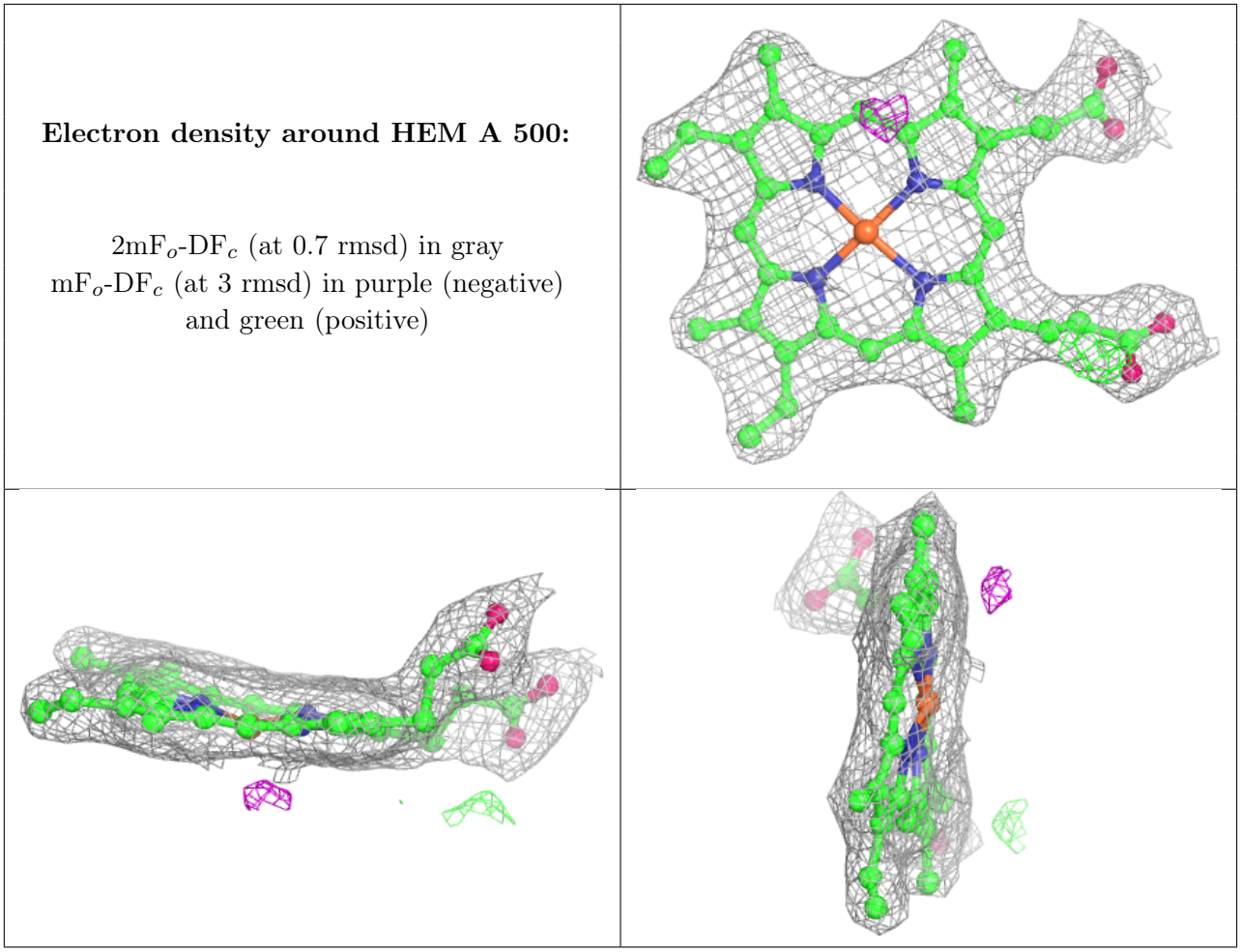
Electron density around HEM B 500:

$2mF_o$-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 500:

$2mF_o$-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.