Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 03:17 AM EST

PDB ID	:	8UFR
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 4-methyl-7-(4-methyl-2,3,4,5-tetrahydrobenzo[f][1,4]oxazepin-7-yl)quinolin-2-amine dihydrochloride
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2023-10-04
Resolution	:	1.87 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:

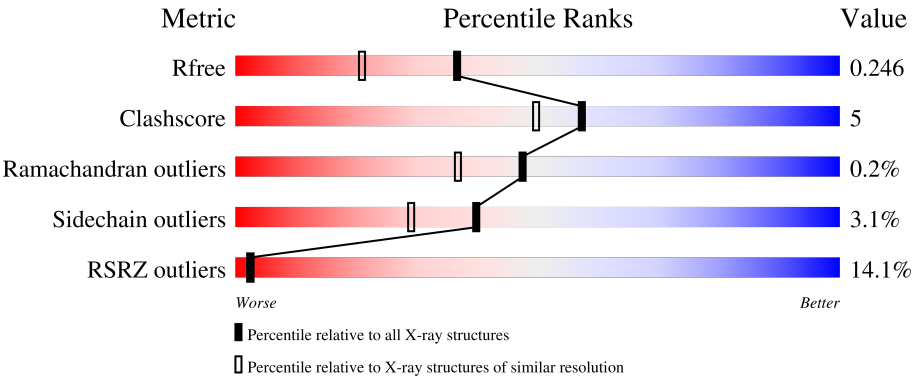
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	440	23% 76% 14% • 9%
1	B	440	8% 81% 9% • 9%
1	C	440	14% 81% 10% 9%
1	D	440	7% 83% 8% • 9%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13830 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.

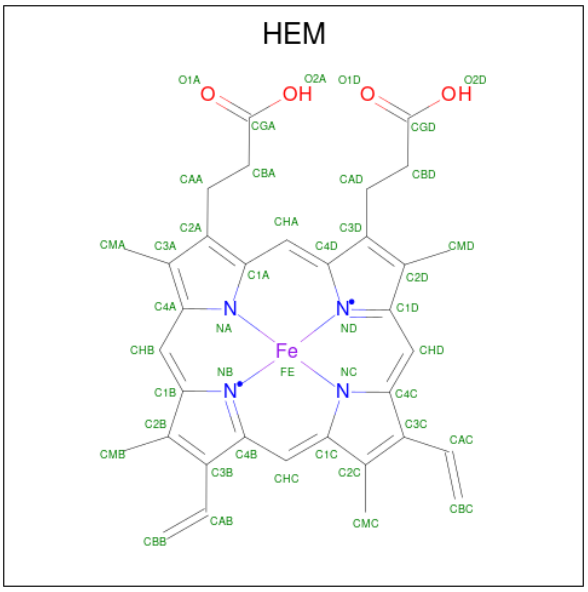
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	2	0
			3215	2047	566	586	16			
1	B	401	Total	C	N	O	S	0	3	0
			3211	2045	564	586	16			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	402	Total	C	N	O	S	0	2	0
			3215	2048	565	586	16			

There are 4 discrepancies between the modelled and reference sequences:

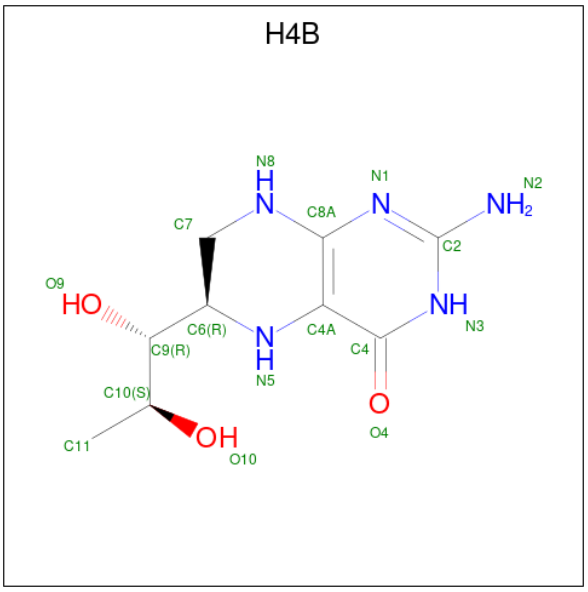
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



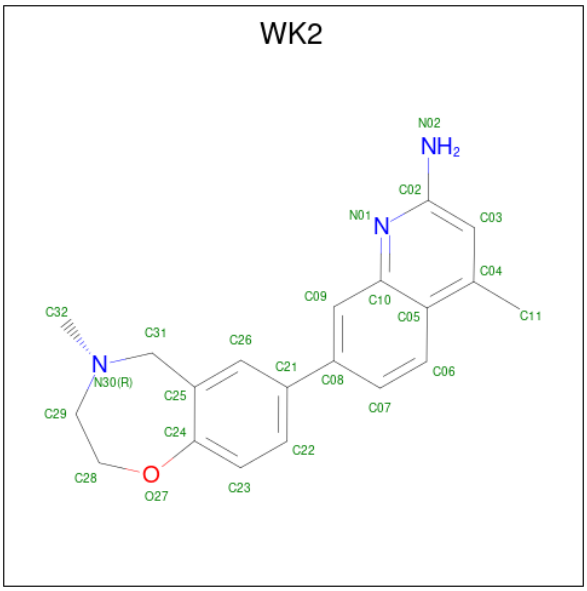
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



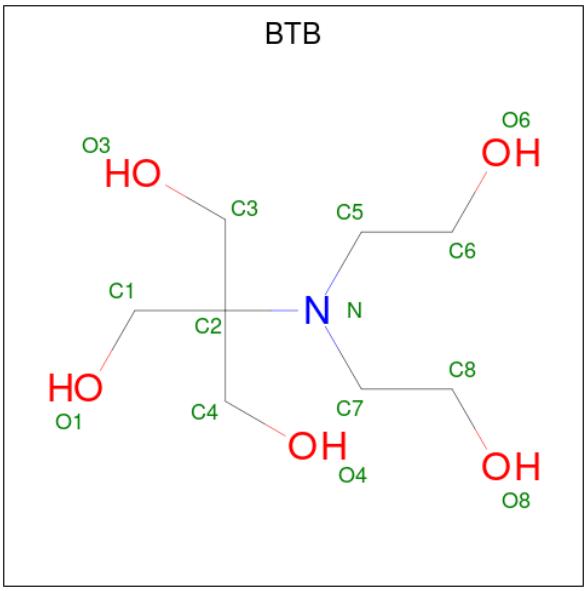
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is (7M)-4-methyl-7-(4-methyl-2,3,4,5-tetrahydro-1,4-benzoxazepin-7-yl)quinoli n-2-amine (three-letter code: WK2) (formula: $C_{20}H_{21}N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 24 20 3 1	0	0
4	B	1	Total C N O 24 20 3 1	0	0
4	C	1	Total C N O 24 20 3 1	0	0
4	D	1	Total C N O 24 20 3 1	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



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

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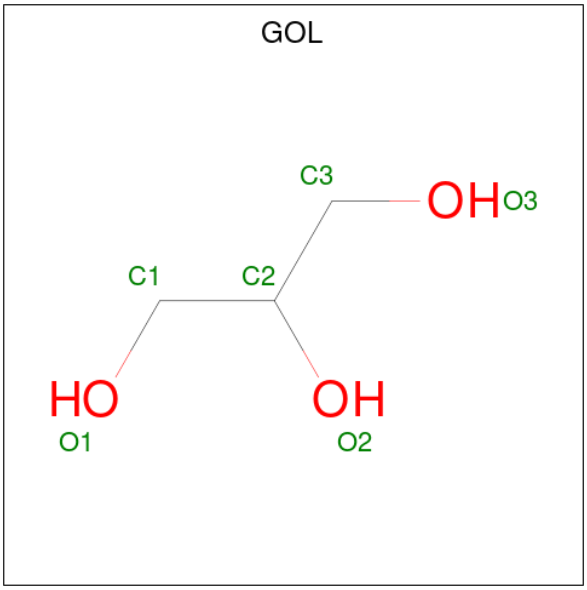
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Zn 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	B	1	Total Cl 1 1	0	0
8	C	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Gd 1 1	0	0
9	B	1	Total Gd 1 1	0	0
9	C	1	Total Gd 1 1	0	0
9	D	1	Total Gd 1 1	0	0

- Molecule 10 is water.

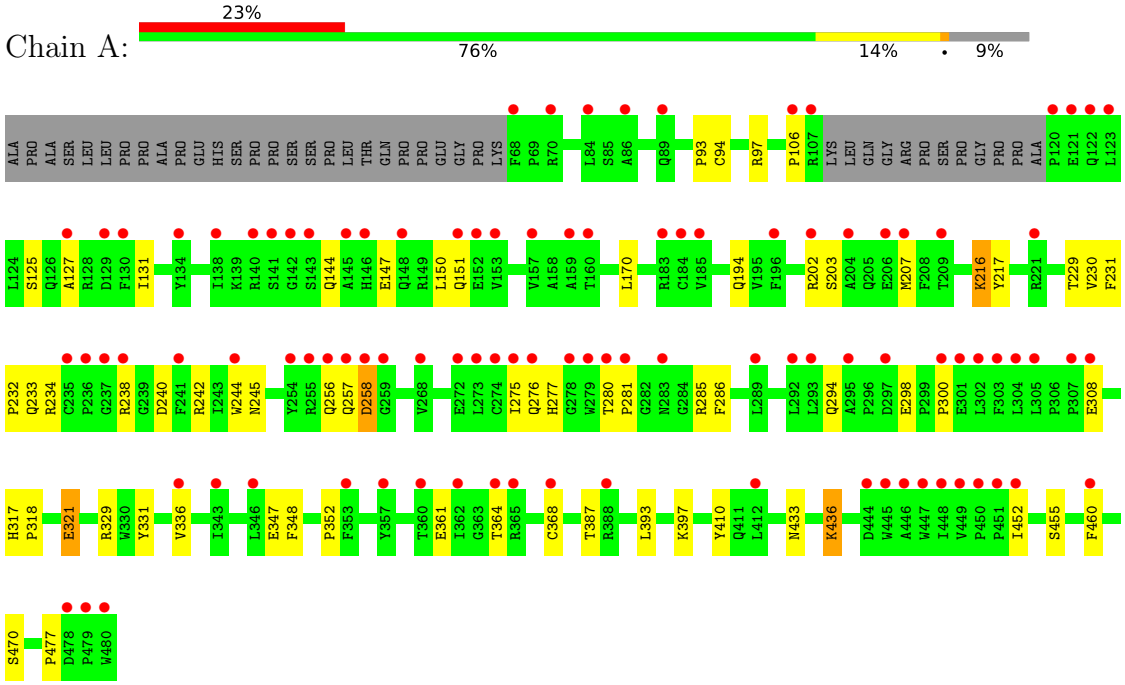
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	69	Total O 69 69	0	0
10	B	140	Total O 140 140	0	0
10	C	100	Total O 100 100	0	0
10	D	159	Total O 159 159	0	0

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.

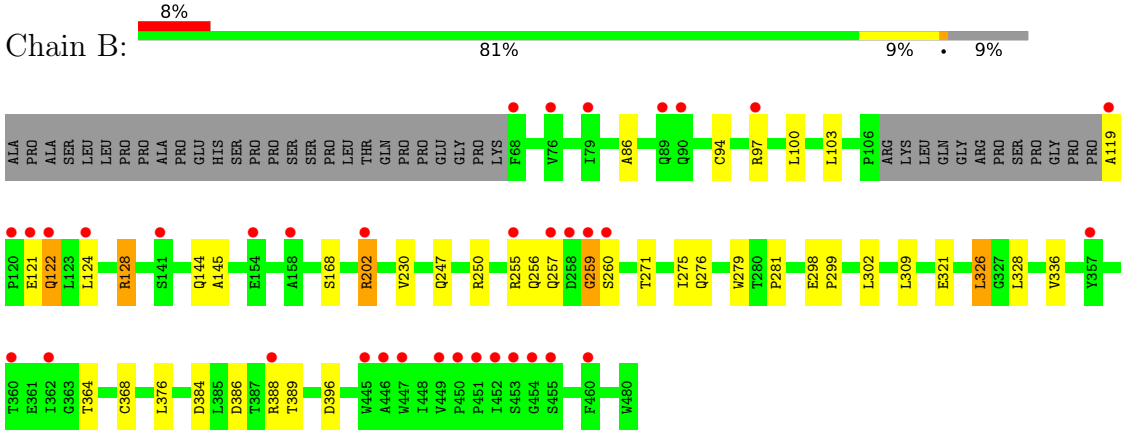
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



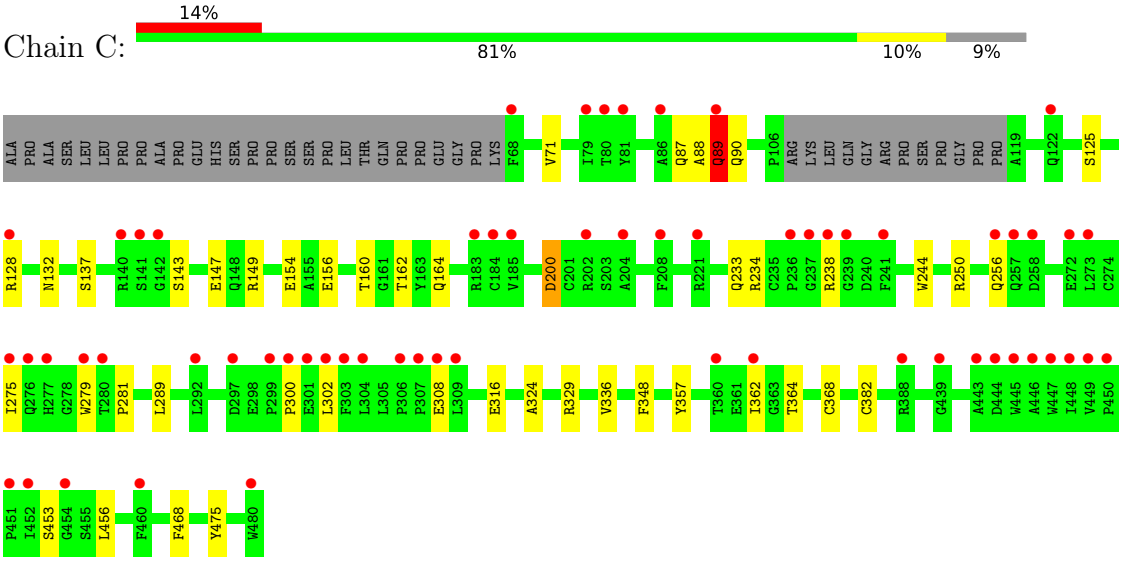
• Molecule 1: Nitric oxide synthase, endothelial

Chain B:



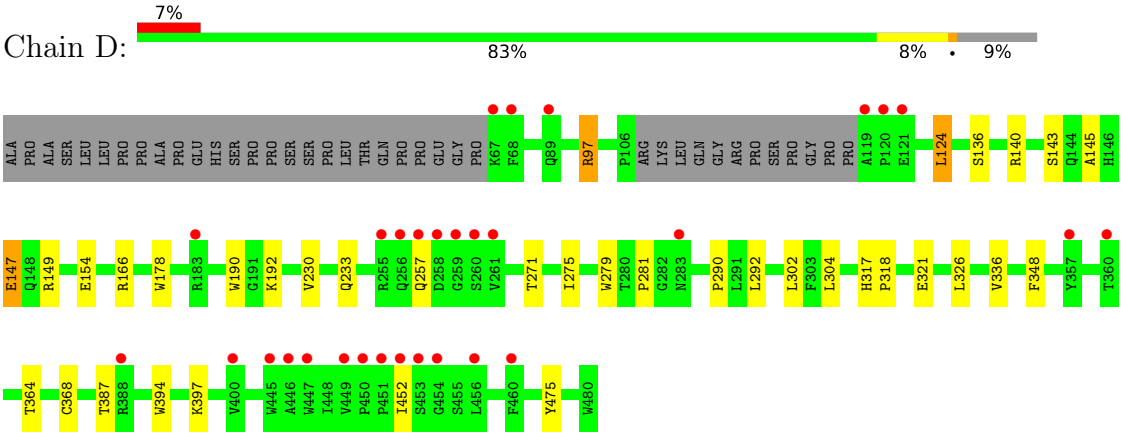
• Molecule 1: Nitric oxide synthase, endothelial

Chain C:



• Molecule 1: Nitric oxide synthase, endothelial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.49Å 152.86Å 108.94Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	39.12 – 1.87 39.13 – 1.87	Depositor EDS
% Data completeness (in resolution range)	91.5 (39.12-1.87) 91.7 (39.13-1.87)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.87Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.207 , 0.251 0.203 , 0.246	Depositor DCC
R_{free} test set	7334 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13830	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 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, HEM, GD, WK2, BTB, H4B, GOL, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.36	0/3313	0.50	0/4513
1	B	0.41	0/3312	0.55	0/4514
1	C	0.38	0/3307	0.51	0/4507
1	D	0.43	0/3313	0.57	0/4514
All	All	0.39	0/13245	0.53	0/18048

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	3215	0	3118	36	0
1	B	3211	0	3114	29	0
1	C	3209	0	3109	21	0
1	D	3215	0	3121	20	0
2	A	43	0	30	2	0
2	B	43	0	30	6	0
2	C	43	0	30	2	0
2	D	43	0	30	4	0
3	A	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	2	0
3	C	17	0	15	0	0
3	D	17	0	15	0	0
4	A	24	0	0	2	0
4	B	24	0	0	2	0
4	C	24	0	0	1	0
4	D	24	0	0	2	0
5	A	42	0	57	6	0
5	B	42	0	54	4	0
5	C	42	0	56	6	0
5	D	28	0	36	5	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	0	0
7	C	6	0	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	69	0	0	2	0
10	B	140	0	0	2	0
10	C	100	0	0	0	0
10	D	159	0	0	1	0
All	All	13830	0	12861	129	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 5.

All (129) 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:B:257:GLN:HA	1:B:259:GLY:H	1.32	0.93
1:B:119:ALA:HB1	1:B:122:GLN:HE21	1.50	0.76
2:B:501:HEM:O1A	10:B:601:HOH:O	2.02	0.76
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.68	0.74
1:A:433:ASN:HA	1:A:436:LYS:HE3	1.71	0.73
1:A:387:THR:O	5:A:505:BTB:O8	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.72	0.72
1:B:257:GLN:HA	1:B:259:GLY:N	2.05	0.71
1:C:200:ASP:OD1	1:C:200:ASP:N	2.25	0.70
1:C:160:THR:HG23	1:C:162:THR:H	1.59	0.68
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.75	0.68
1:B:336:VAL:HG21	4:B:503:WK2:C07	2.24	0.67
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.77	0.66
1:A:321:GLU:H	1:A:321:GLU:CD	1.98	0.66
1:D:397:LYS:NZ	10:D:601:HOH:O	2.29	0.66
1:D:336:VAL:HG21	4:D:503:WK2:C07	2.26	0.65
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.79	0.64
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.80	0.62
1:B:298:GLU:HG3	1:B:299:PRO:HD2	1.82	0.62
1:C:336:VAL:HG21	4:C:503:WK2:C07	2.31	0.61
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.34	0.60
5:A:506:BTB:O3	5:A:506:BTB:O1	2.14	0.60
1:D:271:THR:O	1:D:275:ILE:HG12	2.02	0.60
1:B:298:GLU:OE2	5:B:505:BTB:N	2.36	0.58
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.21	0.58
1:A:336:VAL:HG21	4:A:503:WK2:C07	2.33	0.58
1:D:143:SER:O	1:D:147:GLU:HG2	2.05	0.56
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.88	0.55
1:C:156:GLU:O	1:C:160:THR:HG22	2.06	0.55
1:C:149:ARG:NH2	1:C:164:GLN:O	2.34	0.55
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.87	0.55
1:C:128:ARG:O	1:C:132:ASN:ND2	2.39	0.55
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.42	0.55
1:D:140:ARG:HH12	1:D:145:ALA:HB3	1.71	0.55
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.90	0.53
5:D:505:BTB:O4	5:D:505:BTB:O1	2.08	0.53
1:B:298:GLU:HG2	10:B:723:HOH:O	2.08	0.53
1:C:382:CYS:HA	5:C:504:BTB:H12	1.89	0.53
5:B:505:BTB:O3	5:B:505:BTB:H51	2.08	0.52
1:A:97:ARG:NH2	1:B:86:ALA:O	2.43	0.52
1:C:250:ARG:HB2	1:C:289:LEU:HD12	1.91	0.52
1:C:475:TYR:OH	2:C:501:HEM:O2D	2.27	0.52
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.92	0.52
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.92	0.51
1:B:321:GLU:OE2	5:B:504:BTB:O4	2.28	0.51
1:A:308:GLU:H	1:A:308:GLU:CD	2.14	0.51
1:A:242:ARG:NH1	1:A:477:PRO:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.93	0.50
1:B:202:ARG:HH11	1:B:202:ARG:HB2	1.76	0.50
1:A:216:LYS:HG3	1:A:217:TYR:N	2.27	0.50
1:B:97:ARG:HH11	1:B:97:ARG:HB3	1.78	0.49
1:B:275:ILE:HG12	1:B:281:PRO:HG3	1.94	0.49
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.93	0.49
1:A:233:GLN:HG2	10:A:603:HOH:O	2.12	0.48
1:C:364:THR:O	1:C:368:CYS:HB2	2.13	0.48
1:B:384:ASP:OD1	5:C:505:BTB:H72	2.14	0.48
1:A:244:TRP:NE1	1:A:294:GLN:OE1	2.35	0.48
1:C:90:GLN:HG2	1:C:468:PHE:CE2	2.48	0.48
1:D:475:TYR:OH	2:D:501:HEM:O2D	2.25	0.47
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.49	0.47
1:A:127:ALA:O	1:A:131:ILE:HG12	2.15	0.46
1:B:386:ASP:OD1	1:B:388:ARG:HG2	2.15	0.46
2:B:501:HEM:CGA	3:B:502:H4B:HN22	2.28	0.46
2:B:501:HEM:CGA	3:B:502:H4B:HN3	2.28	0.46
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.97	0.46
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.56	0.46
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.97	0.46
1:D:364:THR:HG21	1:D:452:ILE:HG23	1.97	0.46
1:A:202:ARG:O	1:A:203:SER:HB3	2.16	0.45
5:C:506:BTB:H41	5:C:506:BTB:H51	1.55	0.45
1:C:88:ALA:HB3	1:D:97:ARG:HG3	1.98	0.45
1:A:256:GLN:HB3	1:A:258:ASP:H	1.81	0.45
1:B:144:GLN:NE2	1:B:145:ALA:H	2.14	0.45
5:A:506:BTB:H71	5:A:506:BTB:H11	1.84	0.45
5:C:505:BTB:H51	5:C:505:BTB:H11	1.37	0.44
1:B:124:LEU:HD22	1:B:128:ARG:HH12	1.82	0.44
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.52	0.44
1:B:256:GLN:HB2	1:B:260:SER:O	2.17	0.44
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.87	0.44
1:A:258:ASP:N	1:A:258:ASP:OD1	2.50	0.44
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.99	0.44
1:D:292:LEU:HD23	1:D:292:LEU:HA	1.89	0.44
1:A:331:TYR:O	1:A:410:TYR:OH	2.34	0.43
5:B:506:BTB:H11	5:B:506:BTB:H72	1.65	0.43
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.48	0.43
1:A:232:PRO:HA	10:A:603:HOH:O	2.18	0.43
5:A:506:BTB:H42	5:A:506:BTB:H72	1.84	0.43
1:A:229:THR:O	1:A:352:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:OE2	5:A:506:BTB:H41	2.19	0.43
1:B:364:THR:O	1:B:368:CYS:HB2	2.18	0.43
1:D:364:THR:O	1:D:368:CYS:HB2	2.18	0.43
5:D:505:BTB:H52	5:D:505:BTB:H81	1.64	0.43
1:A:361:GLU:OE2	4:A:503:WK2:N02	2.52	0.43
2:D:501:HEM:HBD1	4:D:503:WK2:C22	2.49	0.42
1:A:94:CYS:HB3	1:B:94:CYS:HB3	2.00	0.42
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.02	0.42
5:C:504:BTB:H12	5:C:504:BTB:H51	1.83	0.42
1:B:121:GLU:H	1:B:121:GLU:CD	2.22	0.42
1:A:275:ILE:HD11	1:A:281:PRO:HB3	2.01	0.42
5:D:504:BTB:H32	5:D:504:BTB:H51	1.44	0.42
1:A:455:SER:HA	1:A:460:PHE:CG	2.54	0.42
1:C:316[B]:GLU:HG2	1:C:324:ALA:HB2	2.02	0.42
5:D:505:BTB:H12	5:D:505:BTB:H71	1.76	0.42
5:C:505:BTB:H41	5:C:505:BTB:O8	2.20	0.42
1:A:286:PHE:HB2	1:A:329:ARG:HH11	1.85	0.41
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.55	0.41
5:A:504:BTB:H72	5:A:504:BTB:H41	1.62	0.41
1:C:143:SER:O	1:C:147:GLU:HG2	2.20	0.41
1:C:275:ILE:HG12	1:C:281:PRO:HG3	2.01	0.41
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.55	0.41
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.55	0.41
1:A:207:MET:HA	1:A:231:PHE:CE1	2.56	0.41
1:C:89:GLN:H	1:C:89:GLN:HG2	1.54	0.41
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.88	0.41
1:A:147:GLU:O	1:A:151:GLN:NE2	2.51	0.41
1:A:364:THR:O	1:A:368:CYS:HB2	2.21	0.41
1:C:244:TRP:CZ2	1:C:300:PRO:HG3	2.56	0.41
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.55	0.41
1:D:387:THR:HA	1:D:394:TRP:CD1	2.56	0.41
1:A:170:LEU:HD11	1:A:230:VAL:HG11	2.03	0.41
1:A:277:HIS:NE2	1:A:300:PRO:HG2	2.35	0.41
1:B:255:ARG:O	1:B:256:GLN:HG3	2.21	0.41
1:A:194:GLN:HG2	1:A:217:TYR:CZ	2.56	0.40
2:A:501:HEM:CGA	3:A:502:H4B:HN22	2.34	0.40
1:D:124:LEU:HD11	1:D:154:GLU:HG3	2.04	0.40
1:B:271:THR:O	1:B:275:ILE:HG13	2.21	0.40
2:B:501:HEM:HBA2	4:B:503:WK2:C09	2.52	0.40
1:A:93:PRO:HB3	1:A:106:PRO:HB3	2.03	0.40
1:A:393:LEU:O	1:A:397:LYS:HG3	2.20	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	399/440 (91%)	373 (94%)	25 (6%)	1 (0%)	41	30
1	B	400/440 (91%)	390 (98%)	9 (2%)	1 (0%)	41	30
1	C	399/440 (91%)	389 (98%)	9 (2%)	1 (0%)	41	30
1	D	400/440 (91%)	392 (98%)	8 (2%)	0	100	100
All	All	1598/1760 (91%)	1544 (97%)	51 (3%)	3 (0%)	47	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
1	A	144	GLN
1	B	259	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	343/373 (92%)	330 (96%)	13 (4%)	33	21
1	B	343/373 (92%)	333 (97%)	10 (3%)	42	32
1	C	342/373 (92%)	330 (96%)	12 (4%)	36	24
1	D	343/373 (92%)	335 (98%)	8 (2%)	50	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1371/1492 (92%)	1328 (97%)	43 (3%)	40 29

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	SER
1	A	216	LYS
1	A	238	ARG
1	A	240	ASP
1	A	245	ASN
1	A	257	GLN
1	A	258	ASP
1	A	276	GLN
1	A	280	THR
1	A	285	ARG
1	A	321	GLU
1	A	436	LYS
1	A	470	SER
1	B	122	GLN
1	B	128	ARG
1	B	168[A]	SER
1	B	168[B]	SER
1	B	202	ARG
1	B	230	VAL
1	B	276	GLN
1	B	326	LEU
1	B	389	THR
1	B	396	ASP
1	C	71	VAL
1	C	87	GLN
1	C	89	GLN
1	C	125	SER
1	C	137	SER
1	C	154	GLU
1	C	200	ASP
1	C	234	ARG
1	C	238	ARG
1	C	256	GLN
1	C	308	GLU
1	C	329	ARG
1	D	97	ARG
1	D	124	LEU

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Mol	Chain	Res	Type
1	D	136	SER
1	D	147	GLU
1	D	192	LYS
1	D	230	VAL
1	D	257	GLN
1	D	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	B	122	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

Of 35 ligands modelled in this entry, 10 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	WK2	C	503	-	27,27,27	1.02	1 (3%)	34,39,39	2.28	13 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	501	1	41,50,50	1.52	5 (12%)	45,82,82	1.71	11 (24%)
3	H4B	A	502	-	16,18,18	1.07	0	11,26,26	2.96	6 (54%)
3	H4B	C	502	-	16,18,18	0.93	0	11,26,26	2.60	6 (54%)
3	H4B	D	502	-	16,18,18	0.77	0	11,26,26	2.81	6 (54%)
2	HEM	C	501	1	41,50,50	1.53	5 (12%)	45,82,82	1.75	12 (26%)
3	H4B	B	502	-	16,18,18	1.06	1 (6%)	11,26,26	2.88	5 (45%)
7	GOL	C	508	-	5,5,5	0.42	0	5,5,5	0.45	0
5	BTB	D	505	-	13,13,13	0.41	0	7,16,16	0.82	0
5	BTB	A	504	9	13,13,13	0.39	0	7,16,16	0.61	0
7	GOL	A	508	-	5,5,5	0.39	0	5,5,5	0.35	0
2	HEM	B	501	1	41,50,50	1.52	8 (19%)	45,82,82	1.88	14 (31%)
5	BTB	B	504	9	13,13,13	0.55	0	7,16,16	0.86	0
4	WK2	D	503	-	27,27,27	0.99	0	34,39,39	2.52	12 (35%)
5	BTB	D	504	9	13,13,13	0.40	0	7,16,16	0.83	0
4	WK2	A	503	-	27,27,27	1.07	2 (7%)	34,39,39	2.54	10 (29%)
5	BTB	B	505	-	13,13,13	0.51	0	7,16,16	0.80	0
5	BTB	A	506	-	13,13,13	0.39	0	7,16,16	0.28	0
2	HEM	D	501	1	41,50,50	1.45	4 (9%)	45,82,82	1.87	14 (31%)
5	BTB	B	506	-	13,13,13	0.38	0	7,16,16	0.31	0
4	WK2	B	503	-	27,27,27	0.97	0	34,39,39	2.07	9 (26%)
5	BTB	C	505	-	13,13,13	0.59	0	7,16,16	0.94	0
5	BTB	A	505	-	13,13,13	0.43	0	7,16,16	0.86	0
5	BTB	C	504	9	13,13,13	0.42	0	7,16,16	1.09	1 (14%)
5	BTB	C	506	-	13,13,13	0.38	0	7,16,16	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	WK2	C	503	-	-	0/4/14/14	0/3/4/4
2	HEM	A	501	1	-	4/12/54/54	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	2/12/54/54	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
7	GOL	C	508	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	D	505	-	-	13/21/21/21	-
5	BTB	A	504	9	-	4/21/21/21	-
7	GOL	A	508	-	-	2/4/4/4	-
2	HEM	B	501	1	-	3/12/54/54	-
5	BTB	B	504	9	-	0/21/21/21	-
4	WK2	D	503	-	-	0/4/14/14	0/3/4/4
5	BTB	D	504	9	-	9/21/21/21	-
4	WK2	A	503	-	-	0/4/14/14	0/3/4/4
5	BTB	B	505	-	-	4/21/21/21	-
5	BTB	A	506	-	-	6/21/21/21	-
2	HEM	D	501	1	-	2/12/54/54	-
5	BTB	B	506	-	-	2/21/21/21	-
4	WK2	B	503	-	-	0/4/14/14	0/3/4/4
5	BTB	C	505	-	-	12/21/21/21	-
5	BTB	A	505	-	-	13/21/21/21	-
5	BTB	C	504	9	-	2/21/21/21	-
5	BTB	C	506	-	-	4/21/21/21	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-3.82	1.35	1.40
2	B	501	HEM	C3C-CAC	3.78	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.67	1.35	1.40
2	C	501	HEM	C3C-CAC	3.66	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.54	1.35	1.40
2	D	501	HEM	C3C-CAC	3.53	1.55	1.47
2	A	501	HEM	C3C-CAC	3.49	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.25	1.35	1.40
2	C	501	HEM	CAB-C3B	3.20	1.56	1.47
2	C	501	HEM	FE-NB	3.18	2.12	1.96
2	A	501	HEM	CAB-C3B	3.09	1.55	1.47
2	D	501	HEM	FE-NB	3.06	2.12	1.96
2	B	501	HEM	CAB-C3B	2.91	1.55	1.47
2	A	501	HEM	FE-NB	2.84	2.10	1.96
2	D	501	HEM	CAB-C3B	2.83	1.55	1.47
2	B	501	HEM	FE-NB	2.79	2.10	1.96
2	B	501	HEM	CMB-C2B	2.47	1.56	1.50
2	A	501	HEM	FE-ND	2.42	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	WK2	C02-N01	2.40	1.36	1.33
4	A	503	WK2	C31-C25	2.17	1.54	1.51
2	C	501	HEM	CMB-C2B	2.12	1.55	1.50
2	B	501	HEM	FE-ND	2.12	2.07	1.96
2	B	501	HEM	C2C-C1C	2.11	1.47	1.42
2	B	501	HEM	O2A-CGA	-2.07	1.23	1.30
4	A	503	WK2	C26-C25	2.04	1.43	1.39
3	B	502	H4B	C2-N2	2.03	1.38	1.33

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	WK2	C28-C29-N30	8.54	125.33	113.41
4	D	503	WK2	C28-C29-N30	8.07	124.67	113.41
3	A	502	H4B	C8A-C4A-C4	6.89	120.69	114.57
4	D	503	WK2	C32-N30-C31	-6.54	99.71	111.07
4	A	503	WK2	C32-N30-C31	-6.21	100.29	111.07
3	C	502	H4B	C8A-C4A-C4	5.58	119.52	114.57
3	B	502	H4B	C8A-C4A-C4	5.46	119.42	114.57
4	C	503	WK2	C28-C29-N30	5.44	121.00	113.41
4	B	503	WK2	C32-N30-C31	-5.30	101.88	111.07
4	B	503	WK2	C28-C29-N30	5.20	120.67	113.41
2	C	501	HEM	C4B-CHC-C1C	5.16	129.37	122.56
4	C	503	WK2	C05-C10-N01	-4.85	117.67	122.81
3	D	502	H4B	C8A-C4A-C4	4.74	118.78	114.57
4	C	503	WK2	C04-C05-C10	4.72	120.56	118.01
4	C	503	WK2	C32-N30-C31	-4.53	103.21	111.07
2	D	501	HEM	C4C-CHD-C1D	4.40	128.36	122.56
4	A	503	WK2	C05-C10-N01	-4.38	118.17	122.81
3	B	502	H4B	N1-C2-N3	-4.23	118.78	125.42
2	B	501	HEM	C4D-ND-C1D	4.18	109.39	105.07
4	A	503	WK2	C04-C05-C10	4.06	120.21	118.01
4	D	503	WK2	C04-C05-C10	3.98	120.17	118.01
3	D	502	H4B	C4-C4A-N5	3.97	122.46	119.12
3	B	502	H4B	C2-N3-C4	3.89	122.11	115.93
3	A	502	H4B	C2-N3-C4	3.84	122.03	115.93
4	D	503	WK2	C05-C10-N01	-3.83	118.75	122.81
4	B	503	WK2	C05-C10-N01	-3.75	118.83	122.81
2	A	501	HEM	C4B-CHC-C1C	3.74	127.50	122.56
3	D	502	H4B	C2-N3-C4	3.72	121.84	115.93
2	D	501	HEM	C4B-CHC-C1C	3.68	127.42	122.56
2	B	501	HEM	C4B-CHC-C1C	3.68	127.42	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	CMA-C3A-C4A	-3.65	122.86	128.46
4	B	503	WK2	C04-C05-C10	3.61	119.96	118.01
2	B	501	HEM	CMC-C2C-C3C	3.55	131.32	124.68
3	D	502	H4B	N1-C2-N3	-3.50	119.93	125.42
3	A	502	H4B	N1-C2-N3	-3.49	119.95	125.42
2	D	501	HEM	CMC-C2C-C3C	3.46	131.15	124.68
4	A	503	WK2	C32-N30-C29	-3.46	102.60	110.30
4	A	503	WK2	C07-C08-C21	-3.44	115.40	121.36
4	D	503	WK2	C07-C08-C21	-3.42	115.44	121.36
2	B	501	HEM	C1B-NB-C4B	3.35	108.54	105.07
2	C	501	HEM	CAD-CBD-CGD	-3.34	106.42	113.60
2	A	501	HEM	C1B-NB-C4B	3.31	108.49	105.07
3	C	502	H4B	N1-C2-N3	-3.21	120.38	125.42
2	A	501	HEM	C3B-C2B-C1B	3.21	108.87	106.49
2	D	501	HEM	CHC-C4B-C3B	3.16	129.41	124.57
2	D	501	HEM	CAD-CBD-CGD	-3.15	106.81	113.60
2	B	501	HEM	C3D-C4D-ND	-3.11	106.70	110.17
4	C	503	WK2	C07-C08-C21	-3.10	115.98	121.36
3	C	502	H4B	C2-N3-C4	3.10	120.85	115.93
3	B	502	H4B	C2-N1-C8A	3.09	121.47	114.54
2	A	501	HEM	C4D-ND-C1D	3.07	108.24	105.07
2	C	501	HEM	C3D-C4D-ND	-3.06	106.75	110.17
4	B	503	WK2	C31-C25-C26	-3.05	115.25	119.17
4	D	503	WK2	C28-O27-C24	3.04	120.26	116.03
2	D	501	HEM	C3D-C4D-ND	-3.02	106.80	110.17
2	D	501	HEM	C4D-ND-C1D	2.99	108.16	105.07
2	C	501	HEM	C1B-NB-C4B	2.97	108.14	105.07
2	C	501	HEM	C4D-ND-C1D	2.92	108.09	105.07
2	B	501	HEM	CAD-CBD-CGD	-2.88	107.40	113.60
2	B	501	HEM	CHC-C4B-C3B	2.87	128.96	124.57
4	A	503	WK2	N02-C02-N01	2.86	120.63	118.26
4	C	503	WK2	C26-C21-C08	2.86	125.59	120.86
2	B	501	HEM	CBA-CAA-C2A	-2.86	107.75	112.62
4	B	503	WK2	C31-C25-C24	2.81	125.27	119.92
4	D	503	WK2	C31-C25-C24	2.74	125.15	119.92
2	B	501	HEM	C4C-CHD-C1D	2.74	126.17	122.56
2	B	501	HEM	C2D-C1D-ND	-2.72	106.63	109.88
2	D	501	HEM	CBA-CAA-C2A	-2.70	108.01	112.62
4	D	503	WK2	C08-C09-C10	-2.69	119.09	121.44
3	D	502	H4B	C2-N1-C8A	2.67	120.52	114.54
2	B	501	HEM	CHA-C4D-ND	2.67	127.68	124.38
3	B	502	H4B	N2-C2-N1	2.66	121.40	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	H4B	N2-C2-N3	2.66	121.38	117.25
2	C	501	HEM	C3B-C2B-C1B	2.65	108.45	106.49
3	C	502	H4B	C2-N1-C8A	2.65	120.47	114.54
2	A	501	HEM	C4C-CHD-C1D	2.59	125.98	122.56
3	A	502	H4B	C2-N1-C8A	2.57	120.31	114.54
3	A	502	H4B	N2-C2-N3	2.56	121.24	117.25
4	D	503	WK2	C32-N30-C29	-2.55	104.63	110.30
4	C	503	WK2	C22-C21-C08	-2.53	116.97	121.36
4	C	503	WK2	C31-C25-C24	2.52	124.72	119.92
4	A	503	WK2	C28-O27-C24	2.51	119.52	116.03
4	C	503	WK2	N02-C02-N01	2.50	120.33	118.26
4	D	503	WK2	C31-C25-C26	-2.48	115.99	119.17
4	C	503	WK2	C09-C08-C21	2.48	126.70	121.05
2	D	501	HEM	CMA-C3A-C4A	-2.43	124.73	128.46
4	C	503	WK2	C32-N30-C29	-2.42	104.92	110.30
2	B	501	HEM	CAA-CBA-CGA	-2.40	107.03	113.76
2	C	501	HEM	CMA-C3A-C4A	-2.40	124.78	128.46
4	C	503	WK2	C31-C25-C26	-2.39	116.11	119.17
2	B	501	HEM	CMA-C3A-C4A	-2.38	124.81	128.46
4	A	503	WK2	C08-C09-C10	-2.36	119.37	121.44
2	C	501	HEM	CHA-C4D-ND	2.36	127.30	124.38
4	C	503	WK2	C03-C04-C05	2.35	120.10	117.78
4	B	503	WK2	C07-C08-C21	-2.29	117.39	121.36
2	D	501	HEM	C3B-C2B-C1B	2.27	108.17	106.49
2	D	501	HEM	CHC-C4B-NB	-2.24	121.99	124.43
2	D	501	HEM	C1B-NB-C4B	2.24	107.39	105.07
4	D	503	WK2	C26-C21-C08	2.22	124.54	120.86
2	A	501	HEM	CMC-C2C-C3C	2.22	128.84	124.68
2	C	501	HEM	CBA-CAA-C2A	-2.20	108.87	112.62
2	D	501	HEM	O2A-CGA-CBA	2.19	121.07	114.03
4	B	503	WK2	C26-C21-C08	2.19	124.48	120.86
3	A	502	H4B	C4A-C4-N3	-2.18	117.81	124.01
4	D	503	WK2	C09-C08-C21	2.18	126.02	121.05
4	A	503	WK2	C03-C04-C05	2.17	119.92	117.78
2	A	501	HEM	CHC-C4B-C3B	2.17	127.89	124.57
2	A	501	HEM	CAA-CBA-CGA	-2.14	107.75	113.76
3	C	502	H4B	C4A-N5-C6	-2.14	115.34	121.16
4	B	503	WK2	C03-C04-C05	2.12	119.87	117.78
5	C	504	BTB	O3-C3-C2	2.11	117.23	111.44
2	B	501	HEM	C3B-C2B-C1B	2.11	108.05	106.49
2	C	501	HEM	CAD-C3D-C2D	-2.09	123.99	127.88
2	D	501	HEM	C4D-C3D-C2D	2.09	109.93	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	CMA-C3A-C2A	2.07	128.84	124.94
3	C	502	H4B	N2-C2-N3	2.03	120.41	117.25
2	C	501	HEM	CHC-C4B-C3B	2.03	127.67	124.57
2	A	501	HEM	C3D-C4D-ND	-2.03	107.91	110.17
2	C	501	HEM	C4A-C3A-C2A	2.00	108.39	107.00

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C3-O3
5	A	505	BTB	C4-C2-C3-O3
5	A	505	BTB	N-C2-C3-O3
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	506	BTB	O1-C1-C2-C3
5	A	506	BTB	O1-C1-C2-N
5	A	506	BTB	C1-C2-C3-O3
5	A	506	BTB	C4-C2-C3-O3
5	A	506	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	506	BTB	C3-C2-C4-O4
5	C	504	BTB	C4-C2-C3-O3
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	C	505	BTB	N-C5-C6-O6
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C5
5	D	505	BTB	C4-C2-N-C7
5	D	505	BTB	C8-C7-N-C5
7	C	508	GOL	O1-C1-C2-O2
7	C	508	GOL	O1-C1-C2-C3
2	A	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C2A-CAA-CBA-CGA
7	A	508	GOL	O1-C1-C2-C3
5	A	505	BTB	N-C5-C6-O6
2	B	501	HEM	C4B-C3B-CAB-CBB
7	A	508	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C7-C8-O8
5	A	504	BTB	N-C5-C6-O6
2	D	501	HEM	C2A-CAA-CBA-CGA
5	C	505	BTB	N-C7-C8-O8
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
3	D	502	H4B	N5-C6-C9-O9
5	A	506	BTB	O1-C1-C2-C4
5	C	504	BTB	C1-C2-C4-O4
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C7
5	B	505	BTB	N-C2-C4-O4
5	C	505	BTB	O1-C1-C2-N

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Mol	Chain	Res	Type	Atoms
5	C	505	BTB	N-C2-C4-O4
5	C	506	BTB	C1-C2-N-C7
5	C	506	BTB	C3-C2-N-C5
5	C	506	BTB	C3-C2-N-C7
5	C	506	BTB	C4-C2-N-C5
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	C1-C2-N-C5
5	D	504	BTB	C3-C2-N-C5
2	D	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O2A
5	D	504	BTB	N-C7-C8-O8
3	B	502	H4B	N5-C6-C9-O9
5	B	506	BTB	C1-C2-C4-O4
5	C	505	BTB	O1-C1-C2-C3
5	C	505	BTB	C4-C2-C3-O3

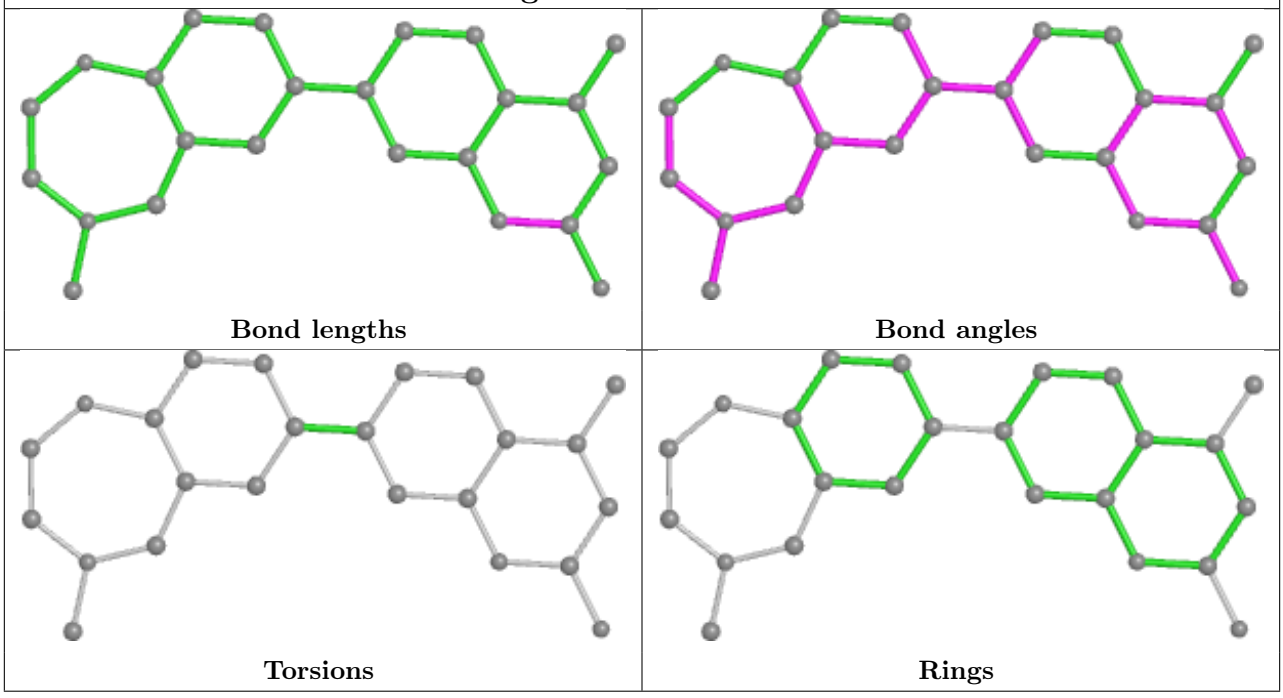
There are no ring outliers.

21 monomers are involved in 40 short contacts:

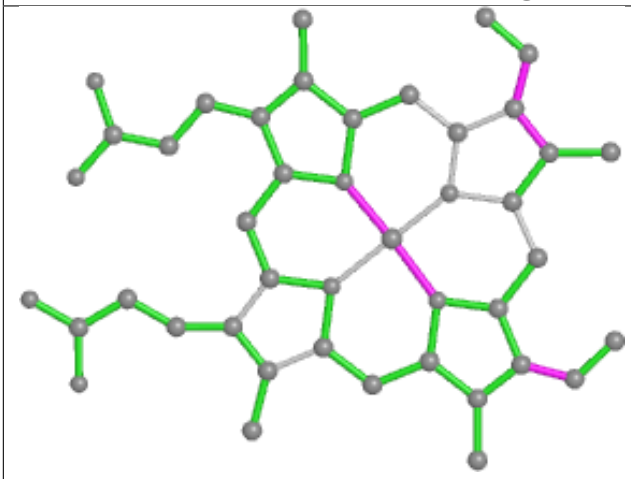
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	WK2	1	0
2	A	501	HEM	2	0
3	A	502	H4B	1	0
2	C	501	HEM	2	0
3	B	502	H4B	2	0
5	D	505	BTB	3	0
5	A	504	BTB	1	0
2	B	501	HEM	6	0
5	B	504	BTB	1	0
4	D	503	WK2	2	0
5	D	504	BTB	2	0
4	A	503	WK2	2	0
5	B	505	BTB	2	0
5	A	506	BTB	4	0
2	D	501	HEM	4	0
5	B	506	BTB	1	0
4	B	503	WK2	2	0
5	C	505	BTB	3	0
5	A	505	BTB	1	0
5	C	504	BTB	2	0
5	C	506	BTB	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.

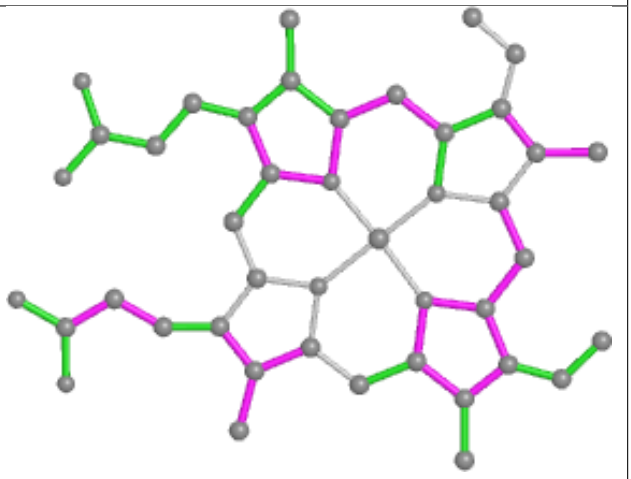
Ligand WK2 C 503



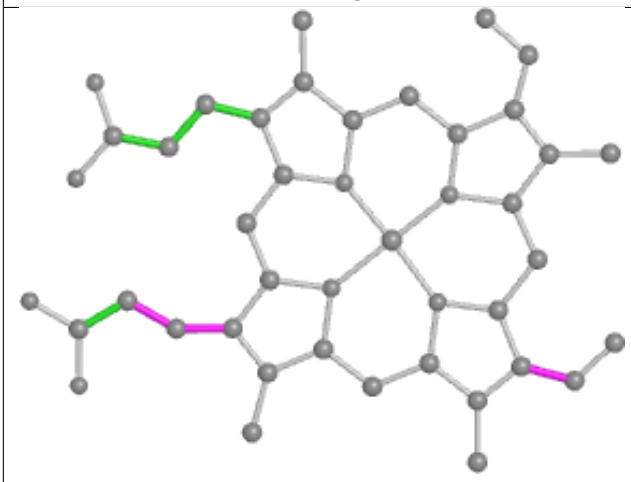
Ligand HEM A 501



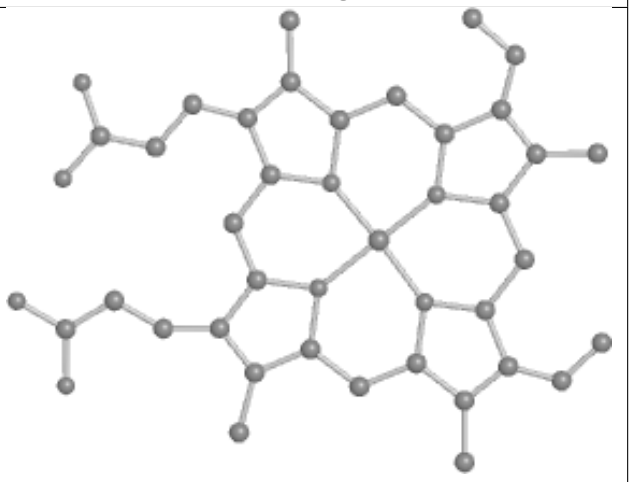
Bond lengths



Bond angles

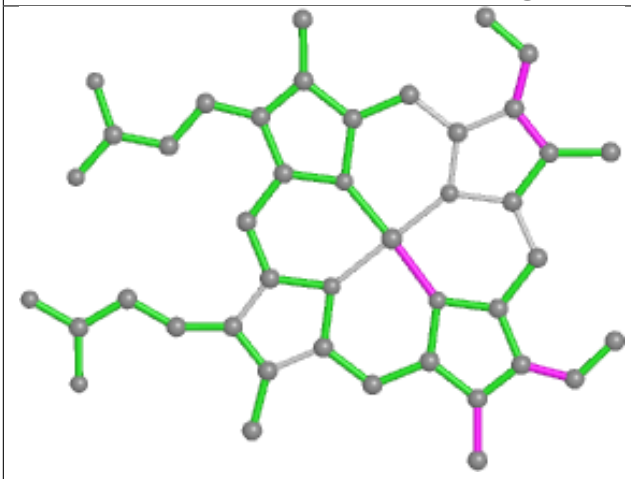


Torsions

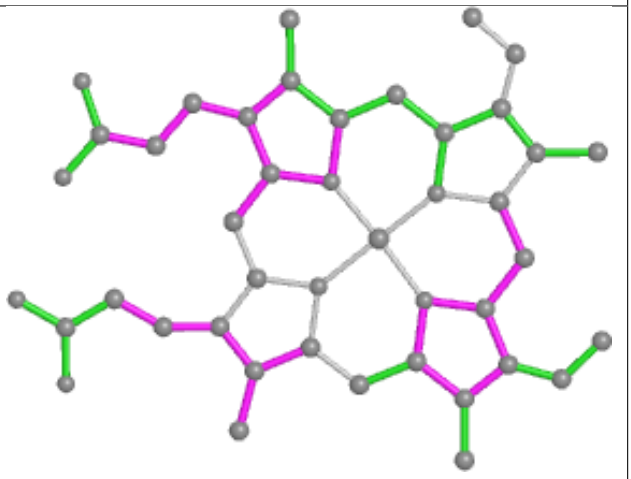


Rings

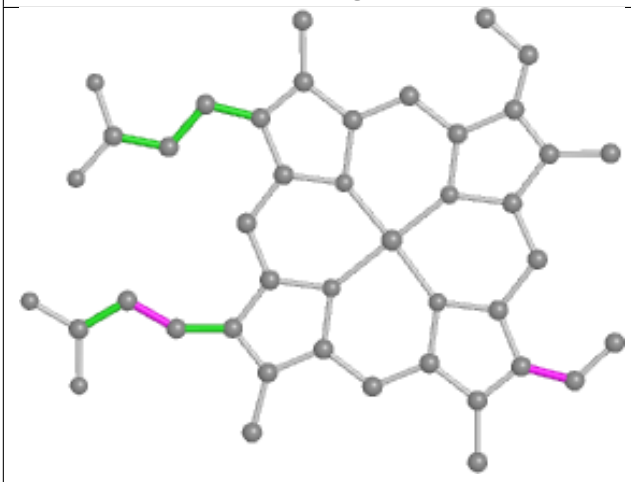
Ligand HEM C 501



Bond lengths



Bond angles



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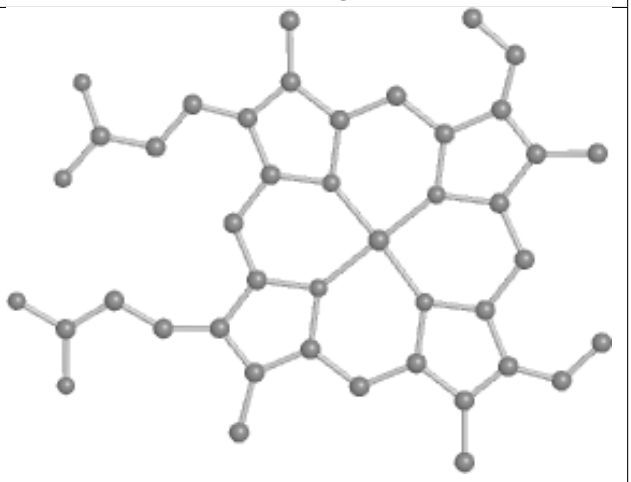
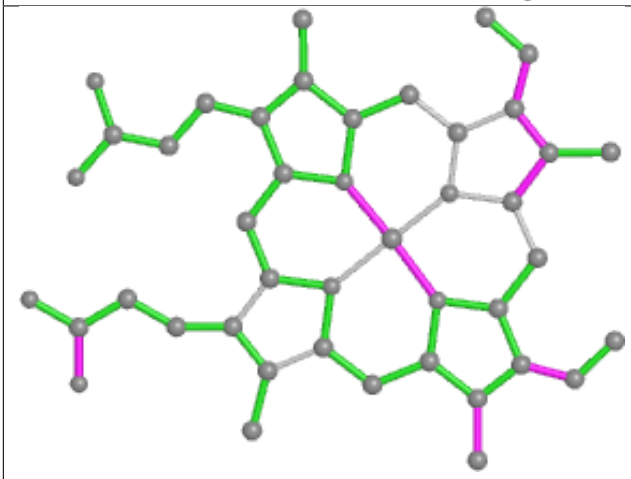
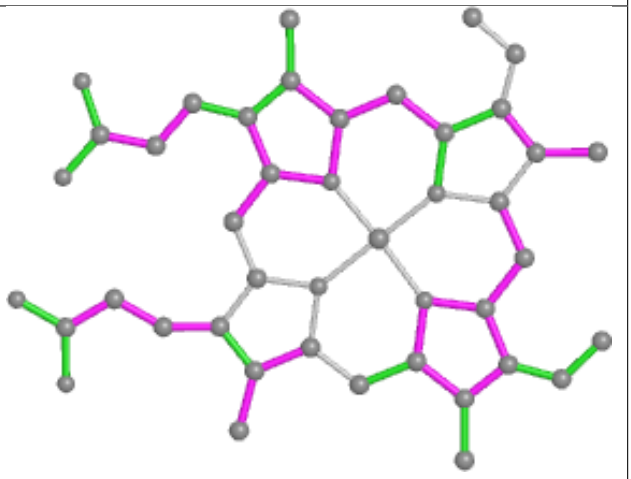


Rings

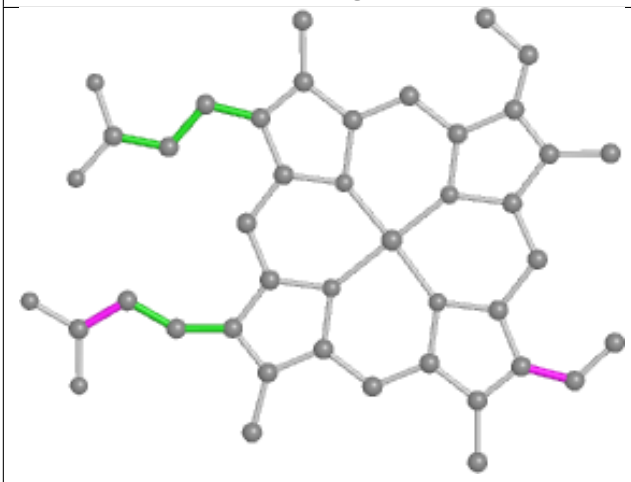
Ligand HEM B 501



Bond lengths



Bond angles



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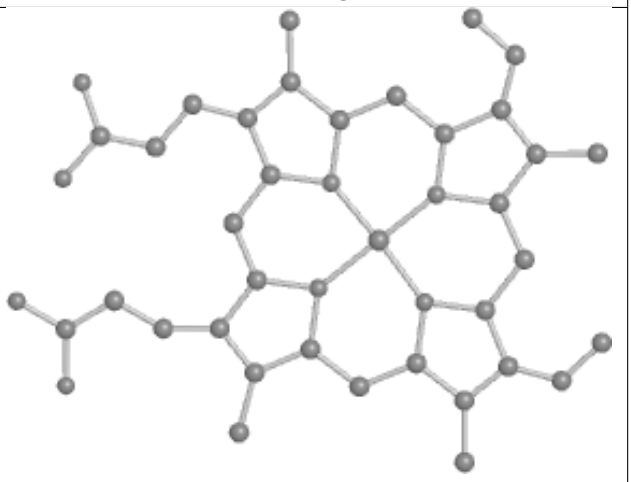
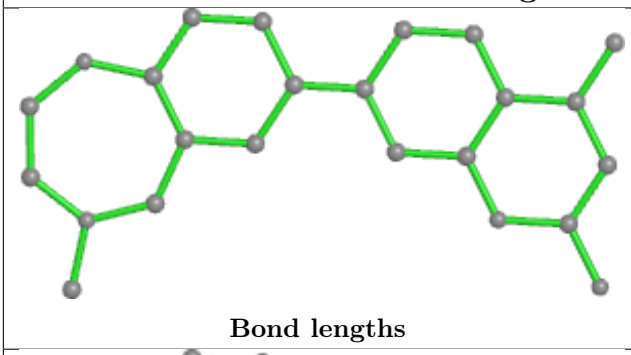
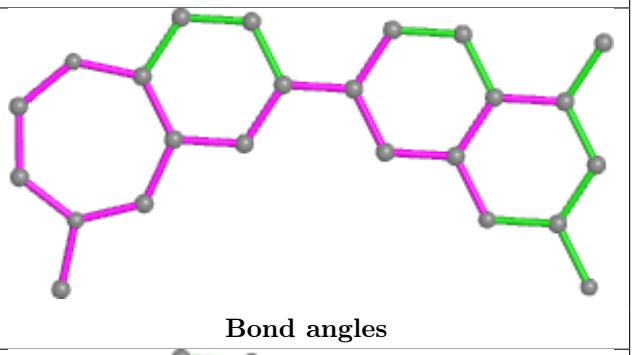


Rings

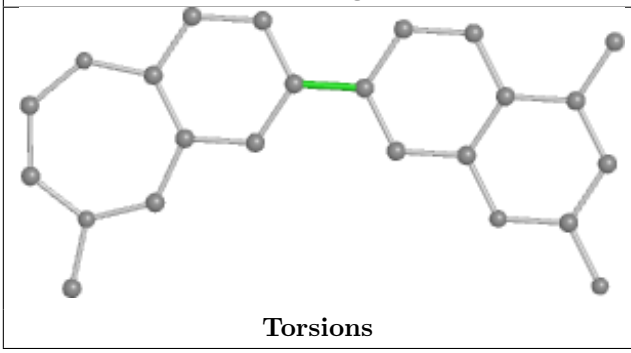
Ligand WK2 D 503



Bond lengths



Bond angles



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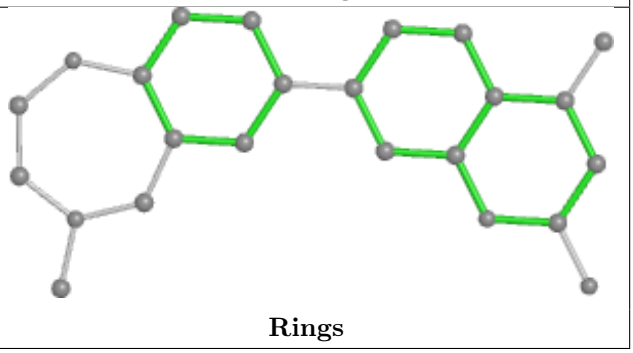
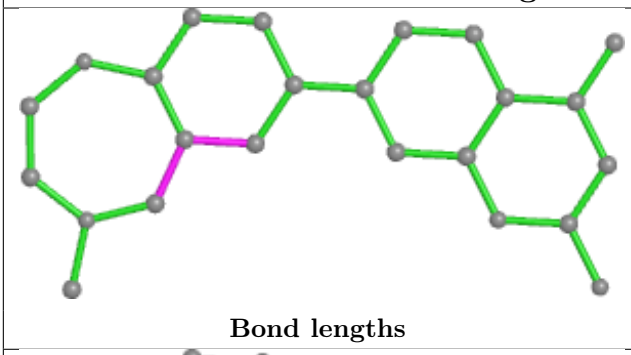
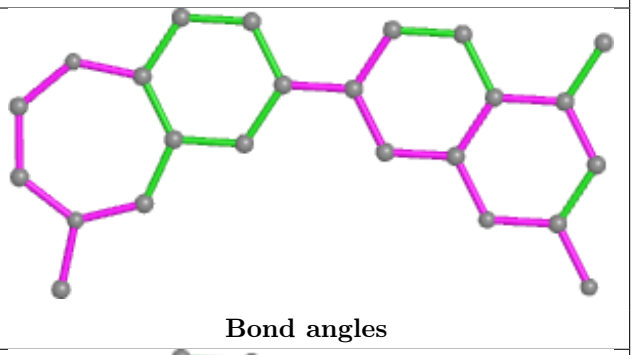


Rings

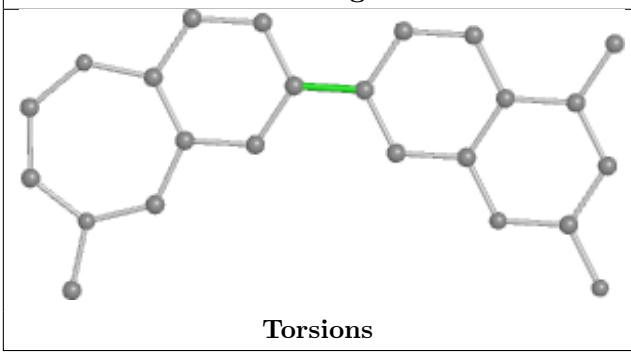
Ligand WK2 A 503



Bond lengths



Bond angles



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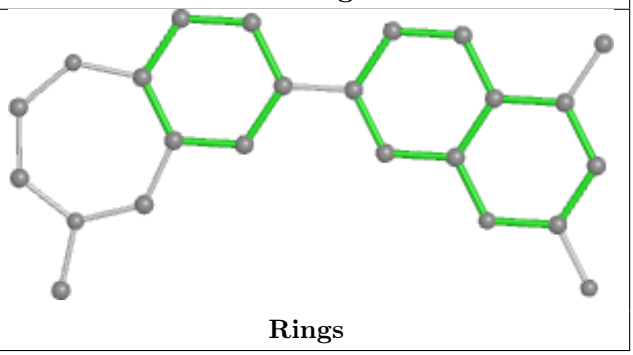
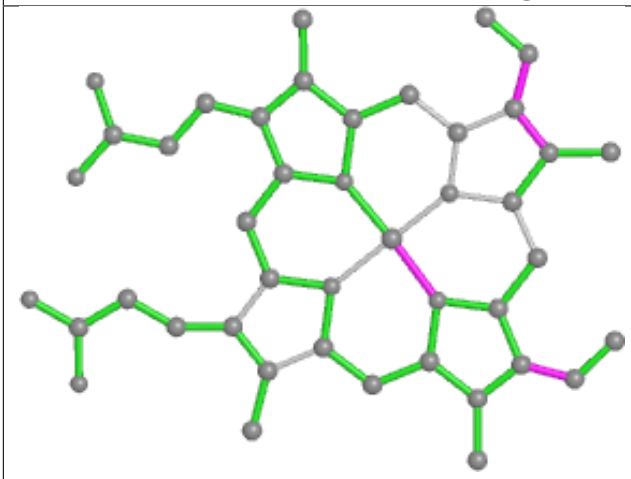


Rings

Ligand HEM D 501



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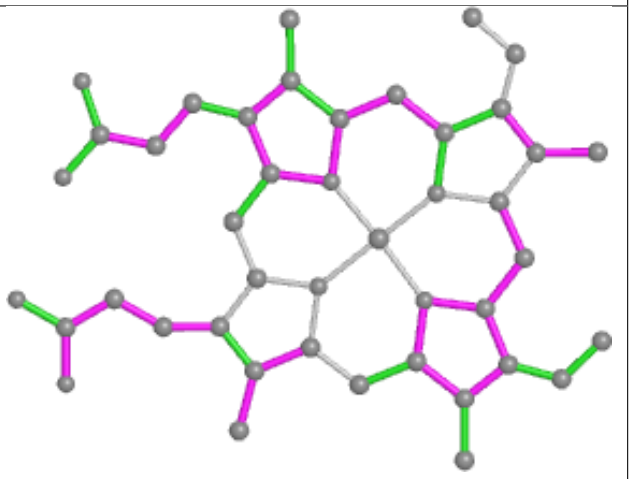
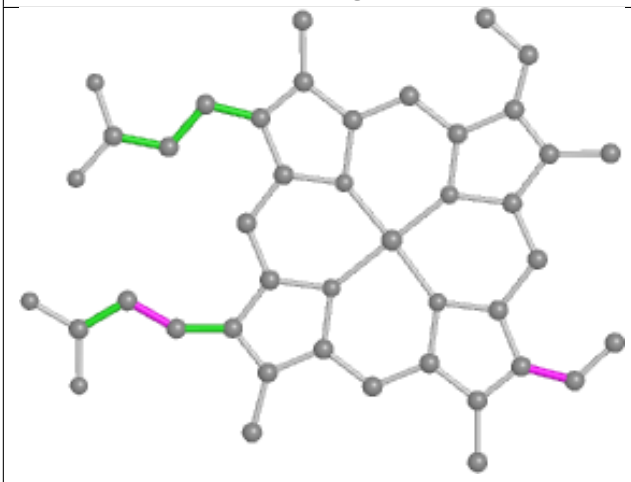
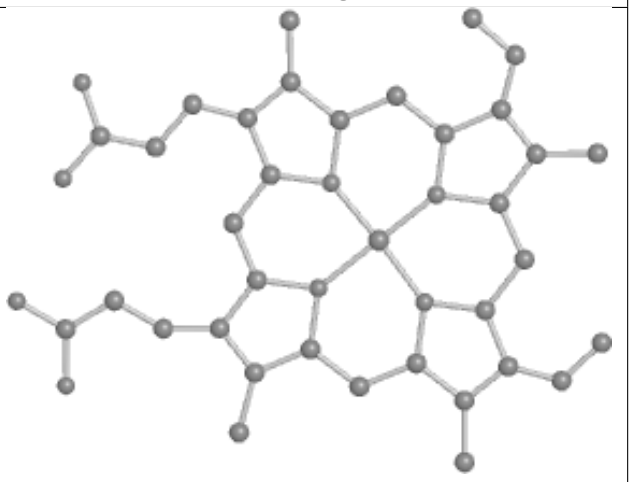


Bond angles

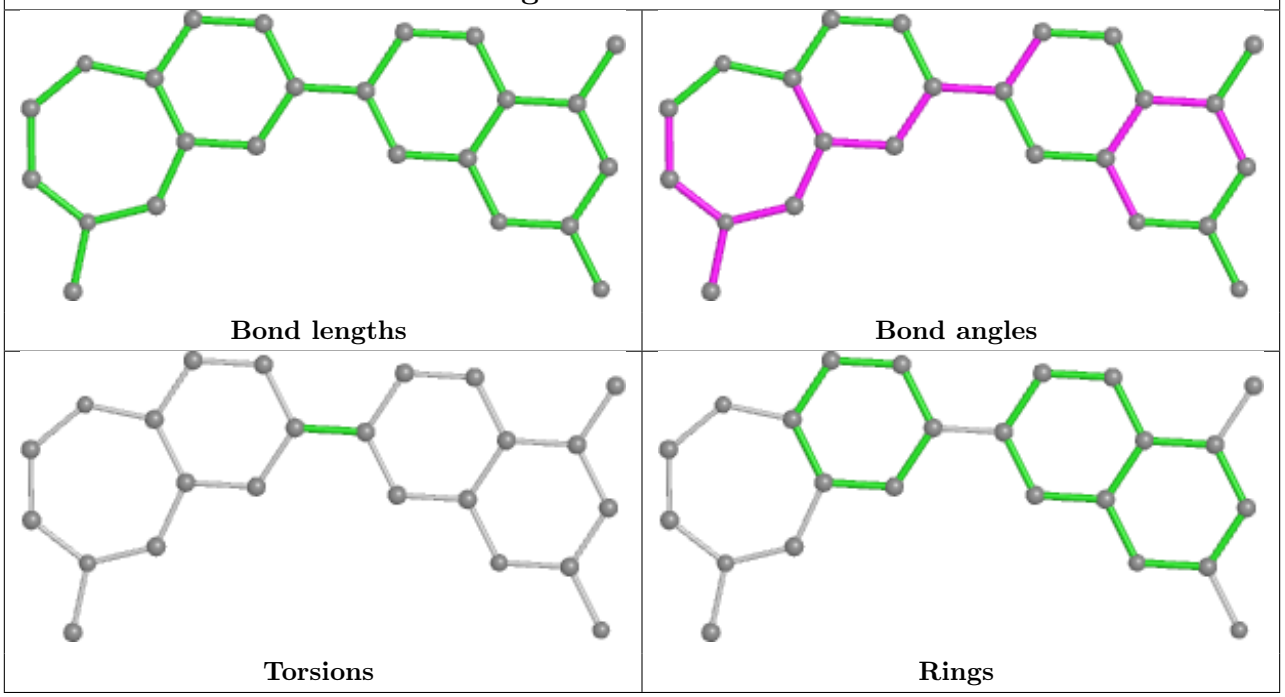


Torsions



Rings

Ligand WK2 B 503



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	401/440 (91%)	1.33	100 (24%) 0 0	32, 67, 125, 152	0
1	B	401/440 (91%)	0.43	35 (8%) 10 11	29, 47, 77, 96	0
1	C	401/440 (91%)	0.91	62 (15%) 2 2	32, 58, 97, 120	0
1	D	402/440 (91%)	0.36	30 (7%) 14 15	28, 46, 74, 96	0
All	All	1605/1760 (91%)	0.76	227 (14%) 2 2	28, 54, 103, 152	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	9.9
1	A	153	VAL	7.8
1	A	259	GLY	7.2
1	A	280	THR	6.2
1	A	480	TRP	6.1
1	A	142	GLY	6.1
1	A	447	TRP	6.0
1	A	256	GLN	5.9
1	A	145	ALA	5.9
1	A	141	SER	5.7
1	A	275	ILE	5.7
1	B	257	GLN	5.5
1	A	293	LEU	5.5
1	A	107	ARG	5.3
1	C	236	PRO	5.2
1	B	259	GLY	5.2
1	A	448	ILE	5.2
1	C	280	THR	5.1
1	A	273	LEU	5.1
1	C	238	ARG	5.0
1	A	281	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	258	ASP	5.0
1	C	448	ILE	5.0
1	A	300	PRO	4.9
1	A	302	LEU	4.9
1	A	268	VAL	4.9
1	C	480	TRP	4.8
1	C	304	LEU	4.8
1	A	446	ALA	4.7
1	A	304	LEU	4.6
1	C	142	GLY	4.6
1	C	447	TRP	4.5
1	D	258	ASP	4.3
1	B	452	ILE	4.3
1	D	257	GLN	4.3
1	C	258	ASP	4.3
1	A	244	TRP	4.3
1	A	238	ARG	4.2
1	D	89	GLN	4.2
1	C	68	PHE	4.2
1	C	257	GLN	4.2
1	B	460	PHE	4.2
1	D	67	LYS	4.2
1	A	297	ASP	4.2
1	C	275	ILE	4.2
1	C	450	PRO	4.2
1	A	451	PRO	4.1
1	B	260	SER	4.1
1	D	260	SER	4.1
1	C	445	TRP	4.1
1	D	446	ALA	4.1
1	B	122	GLN	4.1
1	D	261	VAL	4.1
1	A	258	ASP	4.1
1	C	204	ALA	4.1
1	B	68	PHE	4.0
1	A	254	TYR	4.0
1	A	184	CYS	4.0
1	A	452	ILE	4.0
1	B	119	ALA	4.0
1	C	446	ALA	4.0
1	D	259	GLY	3.9
1	A	445	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	3.9
1	A	122	GLN	3.9
1	D	452	ILE	3.9
1	B	446	ALA	3.8
1	A	412	LEU	3.8
1	C	451	PRO	3.8
1	A	237	GLY	3.8
1	D	256	GLN	3.8
1	B	388	ARG	3.8
1	A	185	VAL	3.7
1	A	301	GLU	3.7
1	A	450	PRO	3.7
1	A	449	VAL	3.6
1	A	89	GLN	3.6
1	C	184	CYS	3.6
1	A	86	ALA	3.6
1	C	297	ASP	3.6
1	A	272	GLU	3.6
1	C	449	VAL	3.6
1	D	255	ARG	3.5
1	C	300	PRO	3.5
1	C	221	ARG	3.5
1	A	279	TRP	3.4
1	B	141[A]	SER	3.4
1	A	257	GLN	3.4
1	A	295	ALA	3.3
1	A	127	ALA	3.3
1	D	451	PRO	3.3
1	A	255	ARG	3.3
1	C	452	ILE	3.3
1	C	237	GLY	3.3
1	C	292	LEU	3.3
1	C	140	ARG	3.2
1	C	307	PRO	3.2
1	A	143	SER	3.2
1	B	449	VAL	3.2
1	B	454	GLY	3.2
1	D	121	GLU	3.2
1	D	445	TRP	3.1
1	D	119	ALA	3.1
1	A	207	MET	3.1
1	D	460	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	346	LEU	3.1
1	C	302	LEU	3.1
1	A	360	THR	3.1
1	A	183	ARG	3.1
1	A	138	ILE	3.1
1	C	388	ARG	3.1
1	B	89	GLN	3.0
1	A	303	PHE	3.0
1	A	276	GLN	3.0
1	A	305	LEU	3.0
1	C	360	THR	3.0
1	A	151	GLN	2.9
1	D	68	PHE	2.9
1	A	206	GLU	2.9
1	B	450	PRO	2.9
1	A	160	THR	2.9
1	A	146	HIS	2.9
1	C	299	PRO	2.9
1	C	306	PRO	2.9
1	A	68	PHE	2.9
1	A	130	PHE	2.9
1	D	360	THR	2.8
1	A	479	PRO	2.8
1	A	121	GLU	2.8
1	B	79	ILE	2.8
1	C	208	PHE	2.8
1	A	336	VAL	2.8
1	A	307	PRO	2.8
1	B	445	TRP	2.8
1	A	274	CYS	2.8
1	A	148	GLN	2.8
1	D	454	GLY	2.7
1	C	277	HIS	2.7
1	C	301	GLU	2.7
1	C	303	PHE	2.7
1	A	357	TYR	2.7
1	C	239	GLY	2.7
1	D	450	PRO	2.7
1	C	89	GLN	2.7
1	A	283	ASN	2.7
1	A	478	ASP	2.7
1	C	81	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	2.7
1	B	451	PRO	2.6
1	C	276	GLN	2.6
1	D	400	VAL	2.6
1	D	449	VAL	2.6
1	B	453	SER	2.6
1	A	152	GLU	2.6
1	C	272	GLU	2.6
1	B	90	GLN	2.6
1	B	124	LEU	2.6
1	B	97	ARG	2.6
1	A	221	ARG	2.5
1	C	79	ILE	2.5
1	B	121	GLU	2.5
1	C	141	SER	2.5
1	A	368	CYS	2.5
1	B	357	TYR	2.5
1	C	454	GLY	2.5
1	D	447	TRP	2.5
1	A	140	ARG	2.5
1	A	353	PHE	2.5
1	A	460	PHE	2.5
1	C	309	LEU	2.5
1	A	365	ARG	2.5
1	D	120	PRO	2.5
1	A	292	LEU	2.5
1	C	460	PHE	2.5
1	B	360	THR	2.5
1	D	456	LEU	2.5
1	A	202	ARG	2.4
1	D	388	ARG	2.4
1	A	308	GLU	2.4
1	A	444	ASP	2.4
1	C	273	LEU	2.3
1	A	362	ILE	2.3
1	C	183	ARG	2.3
1	C	185	VAL	2.3
1	C	86	ALA	2.3
1	C	439	GLY	2.3
1	A	364	THR	2.3
1	B	255	ARG	2.3
1	D	357	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	120	PRO	2.2
1	A	343	ILE	2.2
1	A	134	TYR	2.2
1	B	202	ARG	2.2
1	C	202	ARG	2.2
1	C	241	PHE	2.2
1	A	241	PHE	2.2
1	B	158	ALA	2.2
1	A	129	ASP	2.2
1	C	444	ASP	2.2
1	A	84	LEU	2.2
1	A	159	ALA	2.2
1	D	183	ARG	2.2
1	A	157	VAL	2.2
1	D	453	SER	2.1
1	C	362	ILE	2.1
1	B	455	SER	2.1
1	B	447	TRP	2.1
1	A	289	LEU	2.1
1	A	106	PRO	2.1
1	C	256	GLN	2.1
1	C	308	GLU	2.1
1	A	235	CYS	2.1
1	D	283	ASN	2.1
1	A	236	PRO	2.1
1	A	278	GLY	2.1
1	A	209	THR	2.1
1	C	80	THR	2.1
1	A	196	PHE	2.1
1	B	76	VAL	2.1
1	C	443	ALA	2.1
1	A	70	ARG	2.0
1	C	279	TRP	2.0
1	C	122	GLN	2.0
1	B	362	ILE	2.0
1	A	388	ARG	2.0
1	C	128	ARG	2.0
1	B	154	GLU	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	BTB	A	506	14/14	0.68	0.31	95,108,111,111	0
5	BTB	B	506	14/14	0.72	0.36	82,104,108,113	0
5	BTB	C	506	14/14	0.73	0.22	84,96,103,106	0
5	BTB	D	504	14/14	0.77	0.21	20,66,86,94	0
5	BTB	D	505	14/14	0.81	0.16	69,75,95,100	0
5	BTB	B	505	14/14	0.85	0.23	39,68,76,85	0
5	BTB	B	504	14/14	0.86	0.16	32,60,88,99	0
7	GOL	A	508	6/6	0.86	0.14	64,80,93,98	0
3	H4B	A	502	17/17	0.88	0.24	53,69,78,79	0
4	WK2	C	503	24/24	0.88	0.32	42,73,105,109	0
4	WK2	A	503	24/24	0.89	0.33	41,83,112,115	0
5	BTB	C	505	14/14	0.89	0.19	33,75,87,89	0
4	WK2	B	503	24/24	0.90	0.17	29,50,97,98	0
3	H4B	C	502	17/17	0.90	0.23	41,61,77,77	0
5	BTB	A	505	14/14	0.90	0.13	67,79,87,95	0
3	H4B	D	502	17/17	0.91	0.19	39,51,70,71	0
3	H4B	B	502	17/17	0.91	0.18	37,52,62,64	0
7	GOL	C	508	6/6	0.92	0.16	48,61,68,71	0
5	BTB	A	504	14/14	0.93	0.27	45,82,91,98	0
4	WK2	D	503	24/24	0.93	0.14	31,52,89,93	0
5	BTB	C	504	14/14	0.93	0.24	31,63,86,86	0
8	CL	A	509	1/1	0.93	0.16	63,63,63,63	0
9	GD	C	510	1/1	0.93	0.06	100,100,100,100	0
2	HEM	A	501	43/43	0.94	0.22	41,59,89,103	0
8	CL	C	509	1/1	0.95	0.19	56,56,56,56	0
8	CL	D	506	1/1	0.96	0.11	51,51,51,51	0
2	HEM	C	501	43/43	0.97	0.20	32,46,88,95	0
2	HEM	D	501	43/43	0.97	0.11	21,31,60,72	0
9	GD	A	510	1/1	0.97	0.05	99,99,99,99	0
2	HEM	B	501	43/43	0.97	0.13	25,33,64,83	0
9	GD	D	507	1/1	0.97	0.11	50,50,50,50	0
8	CL	B	507	1/1	0.98	0.12	52,52,52,52	0

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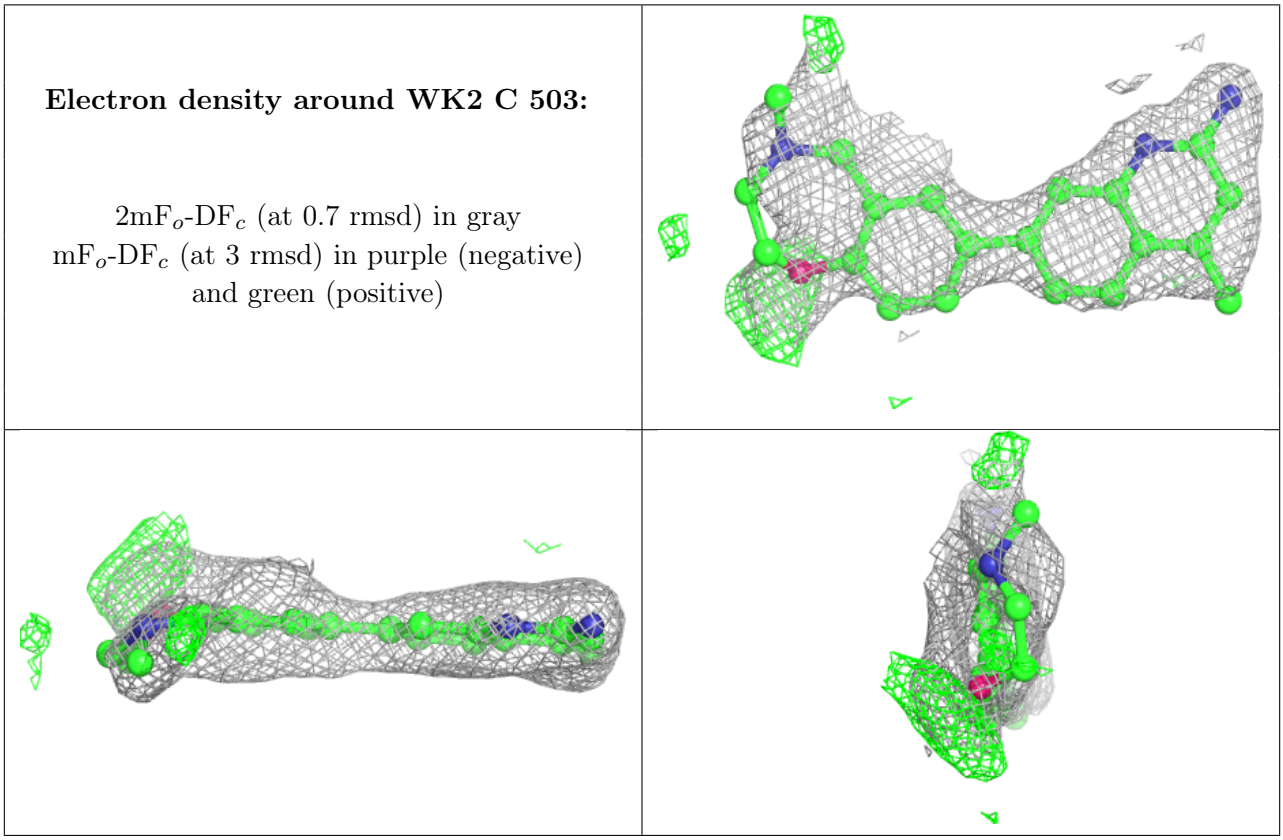
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GD	B	508	1/1	0.98	0.12	50,50,50,50	0
6	ZN	A	507	1/1	0.99	0.07	45,45,45,45	0
6	ZN	C	507	1/1	1.00	0.09	38,38,38,38	0

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.

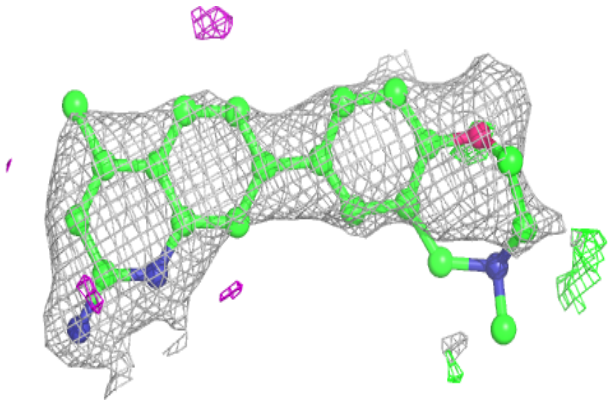
Electron density around WK2 C 503:

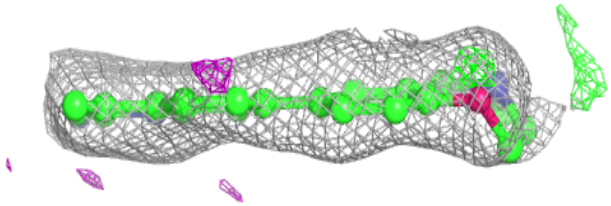
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

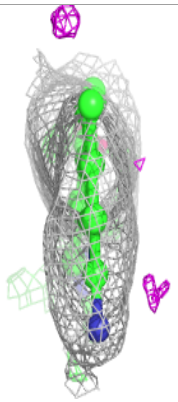


Electron density around WK2 A 503:

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

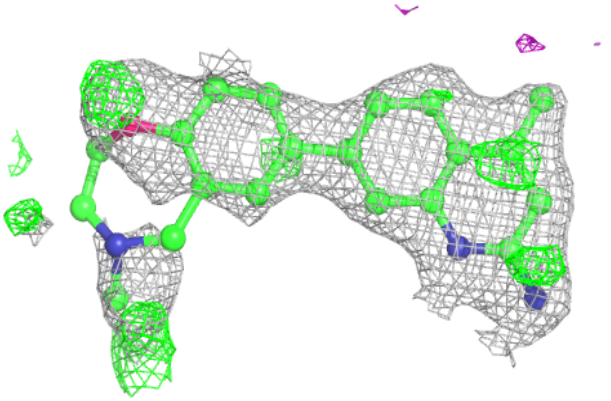


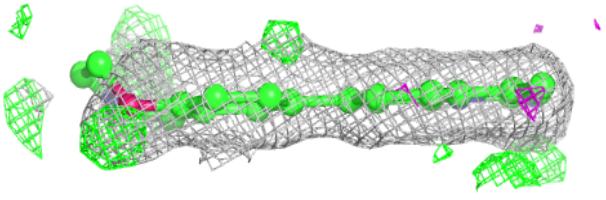


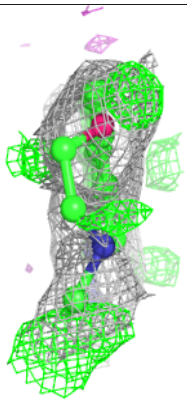


Electron density around WK2 B 503:

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

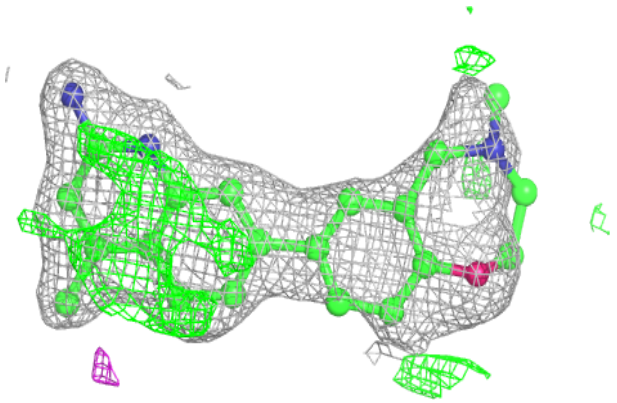


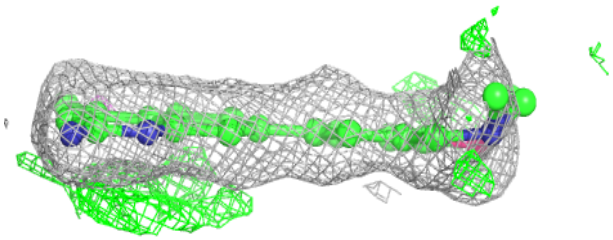


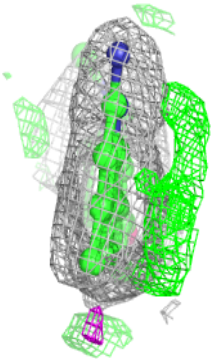


Electron density around WK2 D 503:

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

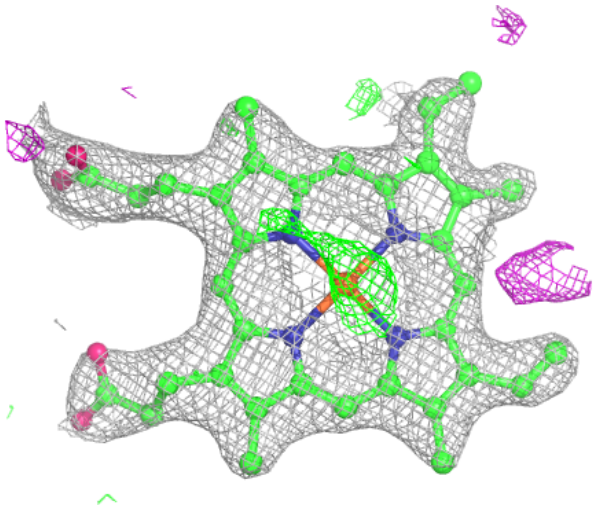


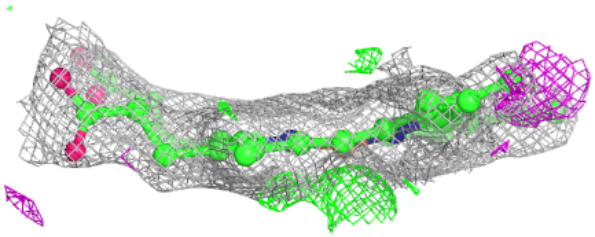


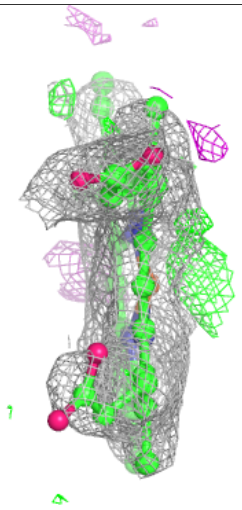


Electron density around HEM A 501:

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

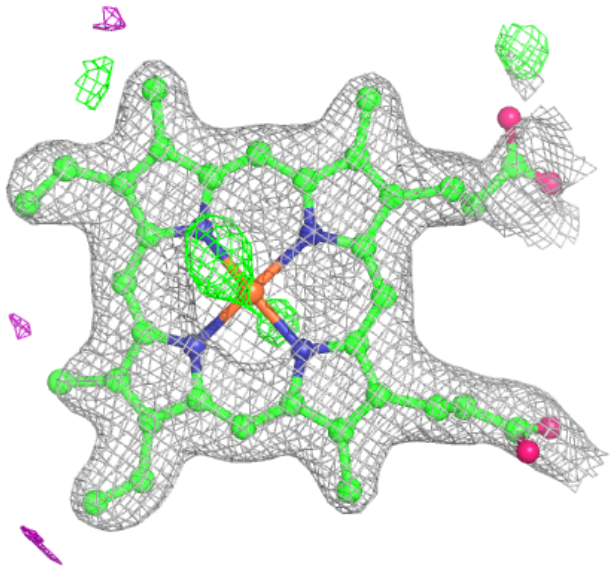


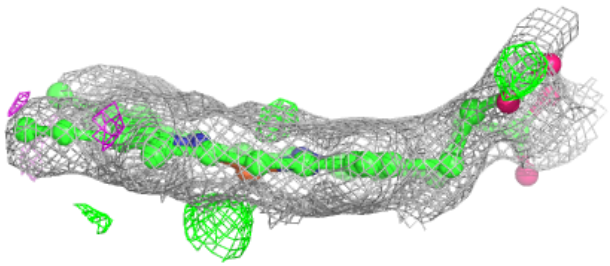


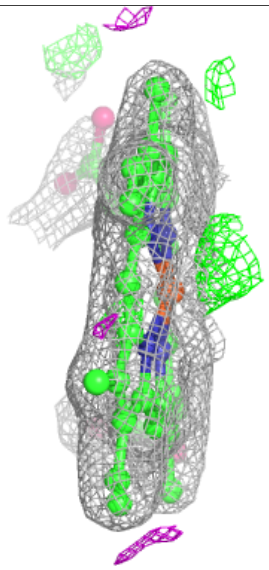


Electron density around HEM C 501:

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

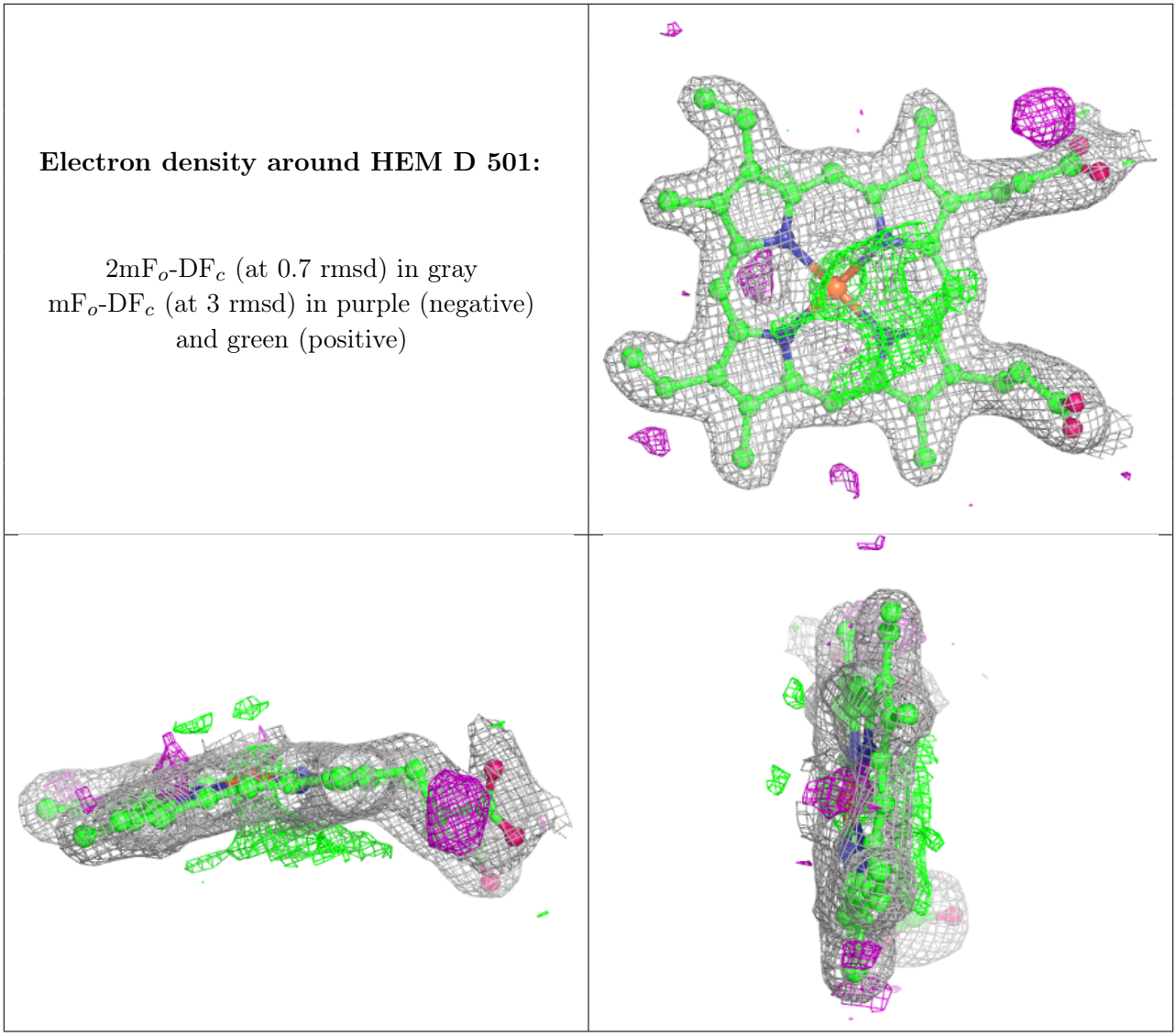






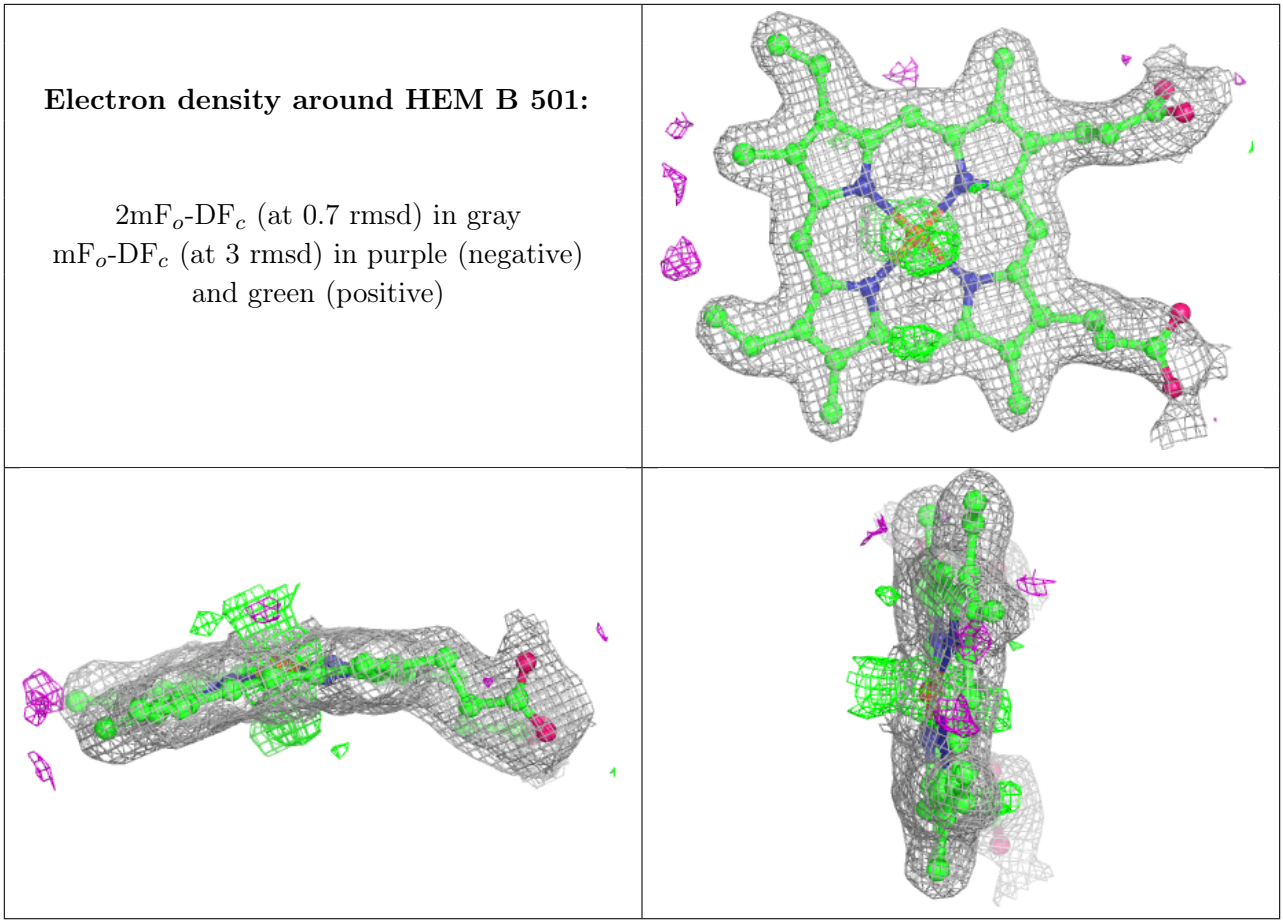
Electron density around HEM D 501:

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



Electron density around HEM B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.