Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 07:47 PM BST

PDB ID	:	4B7H
Title	:	Structure of a highdose liganded bacterial catalase
Authors	:	Gumiero, A.; Walsh, M.
Deposited on	:	2012-08-20
Resolution	:	1.39 Å(reported)

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

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

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

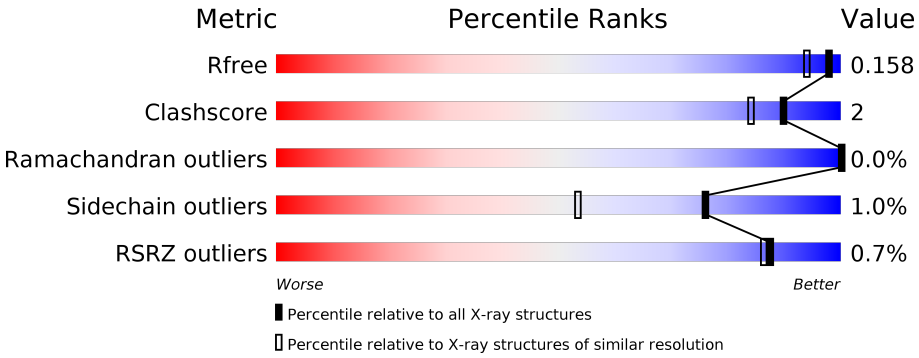
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 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 1.39 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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

Mol	Chain	Length	Quality of chain
1	A	515	95%
1	B	515	96%
1	C	515	94% 6%
1	D	515	96%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18897 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.

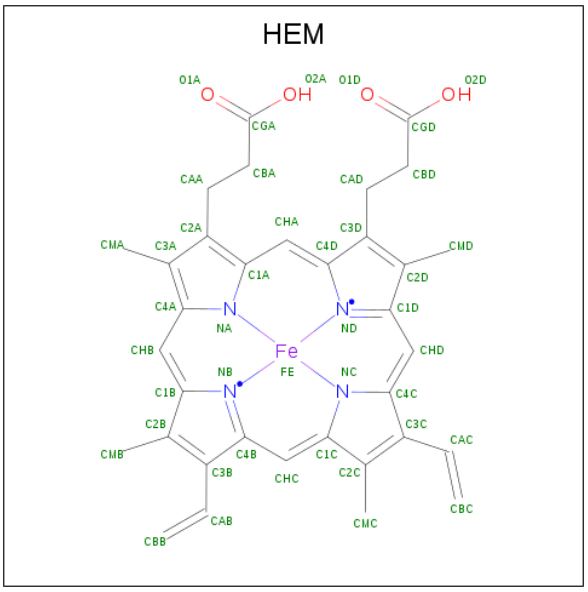
- Molecule 1 is a protein called CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	10	0
			4206	2643	737	817	9			
1	B	514	Total	C	N	O	S	0	6	0
			4176	2624	735	808	9			
1	C	514	Total	C	N	O	S	0	9	0
			4196	2636	743	808	9			
1	D	514	Total	C	N	O	S	0	6	0
			4176	2624	738	805	9			

There are 4 discrepancies between the modelled and reference sequences:

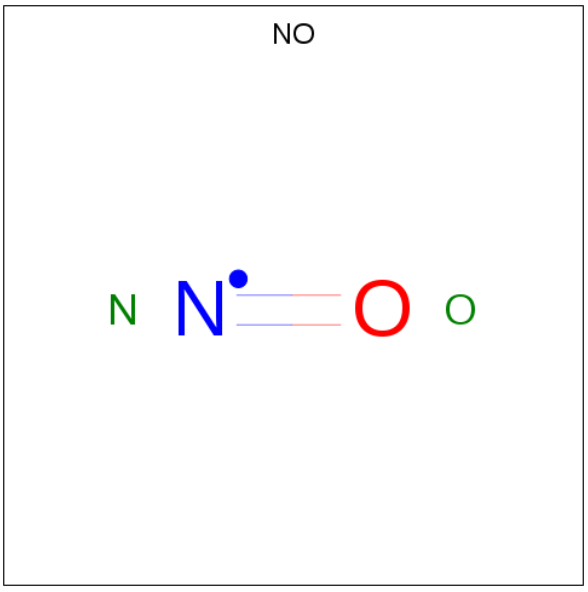
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ILE	LEU	conflict	UNP Q6M8A6
B	327	ILE	LEU	conflict	UNP Q6M8A6
C	327	ILE	LEU	conflict	UNP Q6M8A6
D	327	ILE	LEU	conflict	UNP Q6M8A6

- 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 NITRIC OXIDE (three-letter code: NO) (formula: NO).

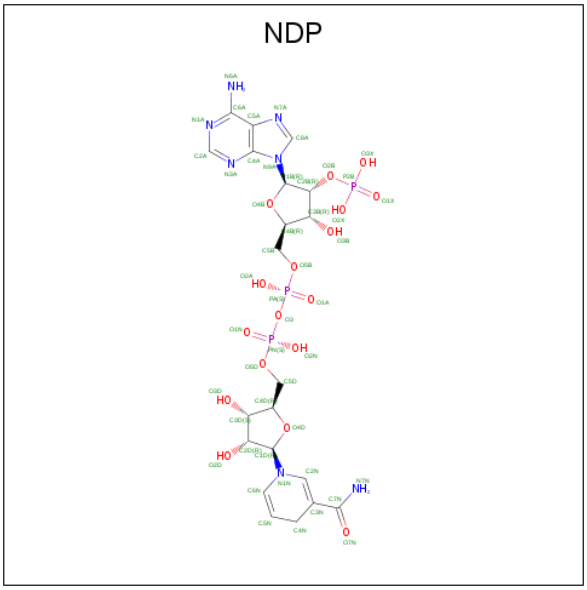


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 2 1 1	0	0
3	B	1	Total N O 2 1 1	0	0
3	C	1	Total N O 2 1 1	0	0
3	D	1	Total N O 2 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 48 21 7 17 3	0	0
5	B	1	Total C N O P 48 21 7 17 3	0	0
5	C	1	Total C N O P 48 21 7 17 3	0	0

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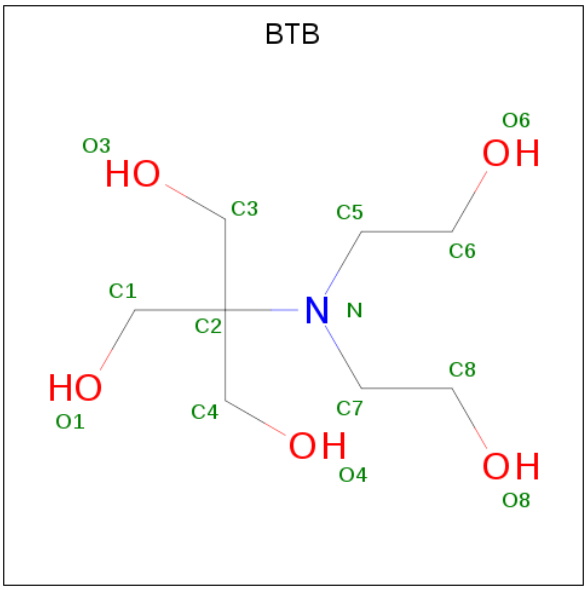
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



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

- Molecule 7 is water.

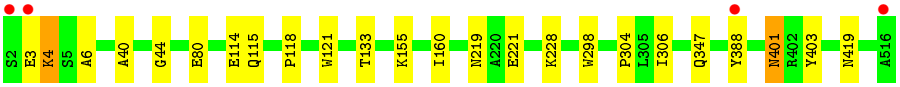
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	552	Total	O	0	0
			552	552		
7	B	433	Total	O	0	0
			433	433		
7	C	389	Total	O	0	0
			389	389		
7	D	339	Total	O	0	0
			339	339		

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: CATALASE

Chain A:

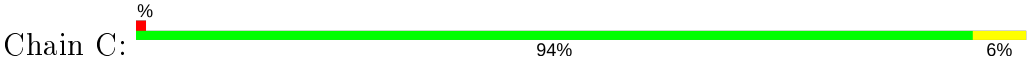


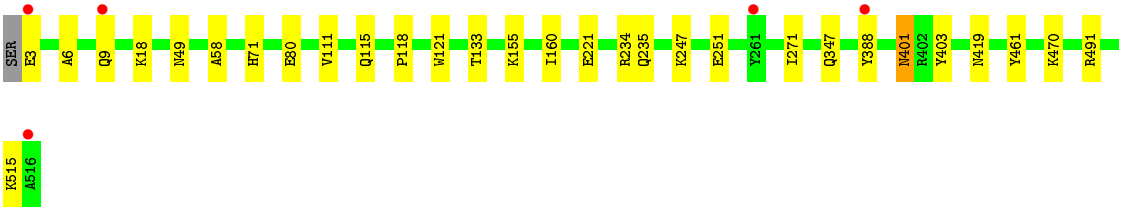
- Molecule 1: CATALASE

Chain B:

- Molecule 1: CATALASE

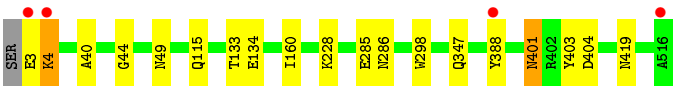
Chain C:





- Molecule 1: CATALASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	151.60Å 151.60Å 156.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.33 – 1.39 78.44 – 1.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (67.33-1.39) 99.9 (78.44-1.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 1.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.130 , 0.157 0.131 , 0.158	Depositor DCC
R_{free} test set	20518 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	11.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	18897	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NO, BTB, NDP, CL

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	0.40	2/4346 (0.0%)	0.57	0/5903
1	B	0.42	3/4304 (0.1%)	0.57	0/5847
1	C	0.39	2/4330 (0.0%)	0.56	1/5881 (0.0%)
1	D	0.41	3/4304 (0.1%)	0.56	0/5846
All	All	0.40	10/17284 (0.1%)	0.56	1/23477 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	419	ASN	C-N	-12.09	1.06	1.34
1	D	419	ASN	C-N	-11.25	1.08	1.34
1	A	419	ASN	C-N	-10.78	1.09	1.34
1	C	419	ASN	C-N	-9.53	1.12	1.34
1	B	435	PRO	C-N	6.84	1.49	1.34
1	B	160	ILE	C-N	6.46	1.48	1.34
1	C	160	ILE	C-N	6.05	1.48	1.34
1	D	160	ILE	C-N	5.73	1.47	1.34
1	D	285	GLU	C-N	-5.56	1.21	1.34
1	A	160	ILE	C-N	5.30	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	58	ALA	C-N-CA	-5.08	108.99	121.70

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	4206	0	3945	14	0
1	B	4176	0	3914	14	0
1	C	4196	0	3949	23	0
1	D	4176	0	3922	16	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	48	0	26	0	0
5	B	48	0	26	0	0
5	C	48	0	26	0	0
5	D	48	0	26	0	0
6	B	28	0	38	0	0
6	C	14	0	19	0	0
6	D	14	0	19	3	0
7	A	552	0	0	3	0
7	B	433	0	0	5	0
7	C	389	0	0	2	0
7	D	339	0	0	4	0
All	All	18897	0	16030	58	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 2.

All (58) 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:401:ASN:HD22	1:B:403:TYR:H	1.19	0.86
1:A:401:ASN:HD22	1:A:403:TYR:H	1.21	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ASN:HD22	1:C:403:TYR:H	1.21	0.86
1:D:401:ASN:HD22	1:D:403:TYR:H	1.21	0.85
1:B:115[A]:GLN:O	7:B:2097:HOH:O	2.02	0.77
1:B:235:GLN:HE22	1:B:271:ILE:H	1.31	0.77
1:C:235:GLN:HE22	1:C:271:ILE:H	1.32	0.76
1:B:115[A]:GLN:NE2	7:B:2039:HOH:O	2.21	0.73
1:A:219:ASN:OD1	1:A:221[A]:GLU:HG2	1.91	0.70
7:A:2086:HOH:O	1:C:115[B]:GLN:NE2	2.27	0.68
1:B:115[B]:GLN:NE2	7:B:2041:HOH:O	2.10	0.67
1:D:115[A]:GLN:O	7:D:2091:HOH:O	2.14	0.66
1:C:491[A]:ARG:HG3	7:C:2374:HOH:O	2.02	0.60
7:B:2355:HOH:O	1:C:491[A]:ARG:NH2	2.37	0.57
1:A:4:LYS:H	1:A:4:LYS:NZ	2.03	0.56
1:A:115[A]:GLN:O	7:A:2144:HOH:O	2.18	0.55
1:C:247:LYS:NZ	1:C:251:GLU:OE2	2.36	0.55
7:B:2048:HOH:O	1:D:115[B]:GLN:NE2	2.42	0.53
1:C:235:GLN:NE2	1:C:271:ILE:H	2.06	0.52
1:B:115[B]:GLN:O	1:D:115[B]:GLN:O	2.31	0.49
1:B:401:ASN:ND2	1:B:403:TYR:H	2.01	0.48
1:C:461:TYR:O	1:C:470:LYS:HE2	2.14	0.47
1:C:388[A]:TYR:HB2	1:D:388[A]:TYR:CZ	2.51	0.46
1:A:388[B]:TYR:HB2	1:B:388[B]:TYR:CZ	2.50	0.46
1:D:134:GLU:HG3	7:D:2078:HOH:O	2.16	0.46
1:A:6:ALA:HB3	1:A:80:GLU:HG2	1.98	0.46
1:C:6:ALA:HB3	1:C:80:GLU:HG2	1.97	0.46
1:B:6:ALA:HB3	1:B:80:GLU:HG2	1.98	0.45
1:C:388[A]:TYR:OH	6:D:1519:BTB:H81	2.16	0.45
1:D:4:LYS:H	1:D:4:LYS:HG3	1.38	0.45
1:D:40:ALA:O	1:D:44:GLY:HA3	2.17	0.44
6:D:1519:BTB:H72	6:D:1519:BTB:H41	1.66	0.44
1:B:228:LYS:HE2	1:B:298:TRP:CE2	2.53	0.44
1:D:134:GLU:HG3	7:D:2108:HOH:O	2.18	0.44
1:C:118:PRO:HD2	1:C:121:TRP:CE2	2.53	0.44
1:C:388[B]:TYR:CZ	1:D:388[B]:TYR:HB2	2.53	0.44
1:C:115[A]:GLN:O	7:C:2109:HOH:O	2.21	0.43
1:D:228:LYS:HE2	1:D:298:TRP:CE2	2.53	0.43
1:A:304:PRO:O	1:A:306:ILE:HD12	2.17	0.43
1:B:235:GLN:NE2	1:B:271:ILE:H	2.07	0.43
1:D:286:ASN:OD1	7:D:2199:HOH:O	2.20	0.43
1:C:401:ASN:ND2	1:C:403:TYR:H	2.02	0.43
1:B:114:GLU:HB3	1:D:115[B]:GLN:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLN:HA	1:B:49:ASN:HD21	1.84	0.42
1:C:347:GLN:CB	1:D:49:ASN:HD21	2.32	0.42
1:C:18:LYS:HZ1	1:D:404:ASP:HB2	1.83	0.42
1:A:115[B]:GLN:O	1:C:115[B]:GLN:O	2.38	0.42
1:C:234:ARG:HG3	1:C:271:ILE:HG22	2.02	0.42
6:D:1519:BTB:H51	6:D:1519:BTB:H12	1.47	0.42
1:A:118:PRO:HD2	1:A:121:TRP:CE2	2.55	0.41
1:A:40:ALA:O	1:A:44:GLY:HA3	2.20	0.41
1:A:4:LYS:H	1:A:4:LYS:HZ2	1.67	0.41
7:A:2148:HOH:O	1:C:118:PRO:HD3	2.21	0.41
1:A:228:LYS:HE2	1:A:298:TRP:CE2	2.56	0.41
1:B:147:THR:HG23	1:B:190:GLN:HE21	1.84	0.41
1:A:114:GLU:HB3	1:C:115[B]:GLN:HG3	2.02	0.41
1:C:49:ASN:HD21	1:D:347:GLN:CB	2.34	0.41
1:C:71:HIS:CE1	1:C:111:VAL:HG22	2.56	0.41

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	523/515 (102%)	503 (96%)	19 (4%)	1 (0%)	47	21
1	B	518/515 (101%)	501 (97%)	17 (3%)	0	100	100
1	C	521/515 (101%)	504 (97%)	17 (3%)	0	100	100
1	D	518/515 (101%)	499 (96%)	19 (4%)	0	100	100
All	All	2080/2060 (101%)	2007 (96%)	72 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU

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	445/436 (102%)	441 (99%)	4 (1%)	78	58
1	B	440/436 (101%)	437 (99%)	3 (1%)	84	66
1	C	443/436 (102%)	436 (98%)	7 (2%)	62	33
1	D	440/436 (101%)	436 (99%)	4 (1%)	78	58
All	All	1768/1744 (101%)	1750 (99%)	18 (1%)	76	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	133	THR
1	A	155	LYS
1	A	401	ASN
1	B	133	THR
1	B	155	LYS
1	B	401	ASN
1	C	3	GLU
1	C	9	GLN
1	C	133	THR
1	C	155	LYS
1	C	221	GLU
1	C	401	ASN
1	C	515	LYS
1	D	3	GLU
1	D	4	LYS
1	D	133	THR
1	D	401	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	46	ASN
1	A	49	ASN
1	A	61	ASN
1	A	300	GLN
1	A	316	ASN
1	A	401	ASN
1	A	498	ASN
1	B	22	ASN
1	B	46	ASN
1	B	49	ASN
1	B	61	ASN
1	B	97	GLN
1	B	190	GLN
1	B	235	GLN
1	B	316	ASN
1	B	401	ASN
1	B	436	HIS
1	B	498	ASN
1	C	22	ASN
1	C	46	ASN
1	C	49	ASN
1	C	61	ASN
1	C	97	GLN
1	C	190	GLN
1	C	235	GLN
1	C	286	ASN
1	C	316	ASN
1	C	401	ASN
1	C	498	ASN
1	D	22	ASN
1	D	46	ASN
1	D	49	ASN
1	D	61	ASN
1	D	97	GLN
1	D	316	ASN
1	D	401	ASN
1	D	498	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	HEM	D	1517	1,3	27,50,50	1.90	5 (18%)	17,82,82	1.99	7 (41%)
2	HEM	A	1517	1,3	27,50,50	1.93	5 (18%)	17,82,82	1.92	6 (35%)
6	BTB	B	1520	-	13,13,13	1.34	3 (23%)	7,16,16	0.79	0
5	NDP	D	1518	-	45,52,52	1.52	4 (8%)	53,80,80	1.18	3 (5%)
3	NO	B	1522	2	0,1,1	0.00	-	-		
6	BTB	C	1518	-	13,13,13	1.26	2 (15%)	7,16,16	0.54	0
6	BTB	D	1519	-	13,13,13	1.26	2 (15%)	7,16,16	0.41	0
3	NO	C	1520	2	0,1,1	0.00	-	-		
5	NDP	C	1519	-	45,52,52	1.52	4 (8%)	53,80,80	1.18	3 (5%)
2	HEM	B	1517	1,3	27,50,50	1.95	6 (22%)	17,82,82	1.84	7 (41%)
5	NDP	A	1520	-	45,52,52	1.51	4 (8%)	53,80,80	1.13	3 (5%)
2	HEM	C	1517	1,3	27,50,50	1.96	7 (25%)	17,82,82	1.63	4 (23%)
3	NO	A	1518	2	0,1,1	0.00	-	-		
6	BTB	B	1521	-	13,13,13	1.29	3 (23%)	7,16,16	0.62	0
3	NO	D	1520	2	0,1,1	0.00	-	-		
5	NDP	B	1518	-	45,52,52	1.51	4 (8%)	53,80,80	1.15	2 (3%)

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
2	HEM	D	1517	1,3	-	0/6/54/54	-
2	HEM	A	1517	1,3	-	0/6/54/54	-
6	BTB	B	1520	-	-	3/21/21/21	-
5	NDP	D	1518	-	-	6/30/77/77	0/5/5/5
6	BTB	C	1518	-	-	4/21/21/21	-
6	BTB	D	1519	-	-	1/21/21/21	-
5	NDP	C	1519	-	-	7/30/77/77	0/5/5/5
2	HEM	B	1517	1,3	-	0/6/54/54	-
5	NDP	A	1520	-	-	6/30/77/77	0/5/5/5
2	HEM	C	1517	1,3	-	0/6/54/54	-
6	BTB	B	1521	-	-	3/21/21/21	-
5	NDP	B	1518	-	-	6/30/77/77	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1518	NDP	O7N-C7N	6.66	1.40	1.24
5	A	1520	NDP	O7N-C7N	6.66	1.40	1.24
5	C	1519	NDP	O7N-C7N	6.63	1.40	1.24
5	D	1518	NDP	O7N-C7N	6.60	1.40	1.24
2	B	1517	HEM	C3D-C2D	4.64	1.51	1.37
2	D	1517	HEM	C3D-C2D	4.58	1.51	1.37
2	A	1517	HEM	C3D-C2D	4.46	1.50	1.37
2	C	1517	HEM	C3D-C2D	4.41	1.50	1.37
5	D	1518	NDP	C2A-N3A	4.10	1.38	1.32
5	B	1518	NDP	C2A-N3A	4.05	1.38	1.32
5	A	1520	NDP	C2A-N3A	3.99	1.38	1.32
2	B	1517	HEM	C3C-C2C	-3.95	1.34	1.40
5	C	1519	NDP	C2A-N3A	3.94	1.38	1.32
2	A	1517	HEM	C3C-C2C	-3.93	1.34	1.40
2	C	1517	HEM	C3B-C2B	-3.89	1.35	1.40
5	A	1520	NDP	C6N-C5N	3.76	1.40	1.33
2	C	1517	HEM	C3C-C2C	-3.75	1.35	1.40
5	B	1518	NDP	C6N-C5N	3.74	1.40	1.33
5	C	1519	NDP	C6N-C5N	3.72	1.40	1.33
5	D	1518	NDP	C6N-C5N	3.66	1.39	1.33
2	B	1517	HEM	C3B-C2B	-3.66	1.35	1.40
2	A	1517	HEM	C3C-CAC	3.63	1.55	1.47
2	D	1517	HEM	C3B-C2B	-3.63	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1517	HEM	C3B-C2B	-3.59	1.35	1.40
2	D	1517	HEM	C3C-CAC	3.55	1.55	1.47
2	C	1517	HEM	C3B-CAB	3.54	1.55	1.47
2	C	1517	HEM	C3C-CAC	3.51	1.55	1.47
2	B	1517	HEM	C3B-CAB	3.51	1.55	1.47
2	D	1517	HEM	C3C-C2C	-3.42	1.35	1.40
2	B	1517	HEM	C3C-CAC	3.32	1.54	1.47
2	A	1517	HEM	C3B-CAB	3.22	1.54	1.47
2	D	1517	HEM	C3B-CAB	3.12	1.54	1.47
5	C	1519	NDP	C2A-N1A	2.70	1.38	1.33
5	D	1518	NDP	C2A-N1A	2.60	1.38	1.33
5	B	1518	NDP	C2A-N1A	2.57	1.38	1.33
6	C	1518	BTB	C1-C2	-2.52	1.50	1.53
6	D	1519	BTB	C1-C2	-2.51	1.50	1.53
5	A	1520	NDP	C2A-N1A	2.47	1.38	1.33
6	B	1520	BTB	C4-C2	-2.37	1.50	1.53
6	B	1520	BTB	C1-C2	-2.36	1.50	1.53
6	B	1520	BTB	C3-C2	-2.31	1.50	1.53
6	B	1521	BTB	C4-C2	-2.28	1.50	1.53
6	B	1521	BTB	C3-C2	-2.22	1.50	1.53
6	B	1521	BTB	C1-C2	-2.13	1.50	1.53
6	D	1519	BTB	C3-C2	-2.11	1.50	1.53
6	C	1518	BTB	C4-C2	-2.10	1.50	1.53
2	B	1517	HEM	CAA-C2A	2.07	1.55	1.52
2	C	1517	HEM	C1D-ND	2.05	1.40	1.36
2	C	1517	HEM	CAA-C2A	2.04	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1519	NDP	N3A-C2A-N1A	-5.47	120.12	128.68
5	D	1518	NDP	N3A-C2A-N1A	-5.44	120.17	128.68
5	A	1520	NDP	N3A-C2A-N1A	-5.43	120.19	128.68
5	B	1518	NDP	N3A-C2A-N1A	-5.40	120.23	128.68
2	D	1517	HEM	CAD-CBD-CGD	-4.32	105.42	112.67
2	A	1517	HEM	CAD-CBD-CGD	-4.20	105.62	112.67
2	B	1517	HEM	CAD-CBD-CGD	-3.88	106.16	112.67
2	C	1517	HEM	CAD-CBD-CGD	-3.66	106.53	112.67
2	A	1517	HEM	CMA-C3A-C4A	-3.45	123.15	128.46
2	D	1517	HEM	CMA-C3A-C4A	-3.30	123.39	128.46
2	B	1517	HEM	CMA-C3A-C4A	-3.06	123.76	128.46
2	D	1517	HEM	CBD-CAD-C3D	-2.95	107.04	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1517	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
2	B	1517	HEM	C1D-C2D-C3D	-2.52	105.24	107.00
2	D	1517	HEM	CMB-C2B-C3B	2.35	129.07	124.68
2	D	1517	HEM	CMC-C2C-C3C	2.30	128.98	124.68
2	A	1517	HEM	CMB-C2B-C3B	2.27	128.92	124.68
2	A	1517	HEM	CBD-CAD-C3D	-2.23	108.37	112.48
2	C	1517	HEM	C1D-C2D-C3D	-2.23	105.44	107.00
5	A	1520	NDP	PN-O3-PA	-2.23	125.18	132.83
5	C	1519	NDP	PN-O3-PA	-2.22	125.19	132.83
2	B	1517	HEM	CBD-CAD-C3D	-2.20	108.42	112.48
2	A	1517	HEM	C1D-C2D-C3D	-2.19	105.47	107.00
5	D	1518	NDP	PN-O3-PA	-2.18	125.35	132.83
2	D	1517	HEM	C4A-C3A-C2A	2.18	108.51	107.00
5	C	1519	NDP	C3D-C2D-C1D	2.15	105.52	101.43
2	B	1517	HEM	CMC-C2C-C3C	2.13	128.67	124.68
5	D	1518	NDP	C3D-C2D-C1D	2.13	105.47	101.43
2	D	1517	HEM	CBA-CAA-C2A	-2.12	108.58	112.49
2	B	1517	HEM	C4A-C3A-C2A	2.08	108.44	107.00
2	C	1517	HEM	CBA-CAA-C2A	-2.06	108.68	112.49
5	B	1518	NDP	C3D-C2D-C1D	2.06	105.33	101.43
5	A	1520	NDP	C3D-C2D-C1D	2.04	105.31	101.43
2	B	1517	HEM	CMB-C2B-C3B	2.04	128.50	124.68
2	A	1517	HEM	C4A-C3A-C2A	2.03	108.41	107.00

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1520	BTB	C1-C2-C3-O3
6	B	1520	BTB	C4-C2-C3-O3
6	B	1520	BTB	N-C2-C3-O3
6	C	1518	BTB	C1-C2-C4-O4
6	C	1518	BTB	C3-C2-C4-O4
6	C	1518	BTB	N-C2-C4-O4
6	B	1521	BTB	C1-C2-C3-O3
6	B	1521	BTB	C4-C2-C3-O3
6	B	1521	BTB	N-C2-C3-O3
5	B	1518	NDP	C5D-O5D-PN-O3
6	D	1519	BTB	N-C7-C8-O8
6	C	1518	BTB	N-C5-C6-O6
5	D	1518	NDP	C5D-O5D-PN-O3
5	C	1519	NDP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
5	A	1520	NDP	C5D-O5D-PN-O3
5	D	1518	NDP	PA-O3-PN-O1N
5	A	1520	NDP	PA-O3-PN-O1N
5	C	1519	NDP	O4D-C1D-N1N-C6N
5	B	1518	NDP	O4D-C1D-N1N-C6N
5	D	1518	NDP	O4D-C1D-N1N-C6N
5	D	1518	NDP	C2D-C1D-N1N-C6N
5	C	1519	NDP	C2D-C1D-N1N-C6N
5	A	1520	NDP	O4D-C1D-N1N-C6N
5	C	1519	NDP	PA-O3-PN-O2N
5	A	1520	NDP	C2D-C1D-N1N-C6N
5	B	1518	NDP	C2D-C1D-N1N-C6N
5	B	1518	NDP	O4B-C4B-C5B-O5B
5	B	1518	NDP	PA-O3-PN-O1N
5	D	1518	NDP	O4B-C4B-C5B-O5B
5	A	1520	NDP	O4B-C4B-C5B-O5B
5	C	1519	NDP	O4B-C4B-C5B-O5B
5	D	1518	NDP	PA-O3-PN-O2N
5	C	1519	NDP	PA-O3-PN-O1N
5	A	1520	NDP	PA-O3-PN-O2N
5	B	1518	NDP	PA-O3-PN-O2N
5	C	1519	NDP	C5D-O5D-PN-O1N

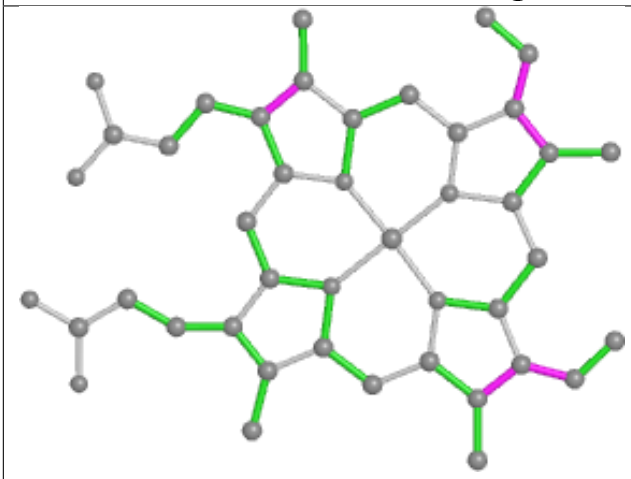
There are no ring outliers.

1 monomer is involved in 3 short contacts:

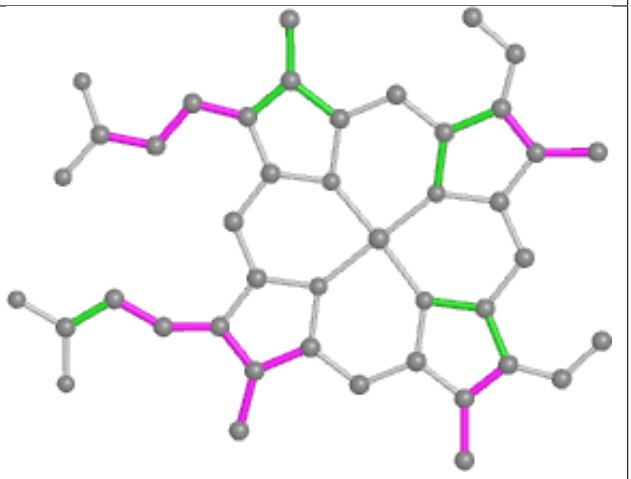
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1519	BTB	3	0

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.

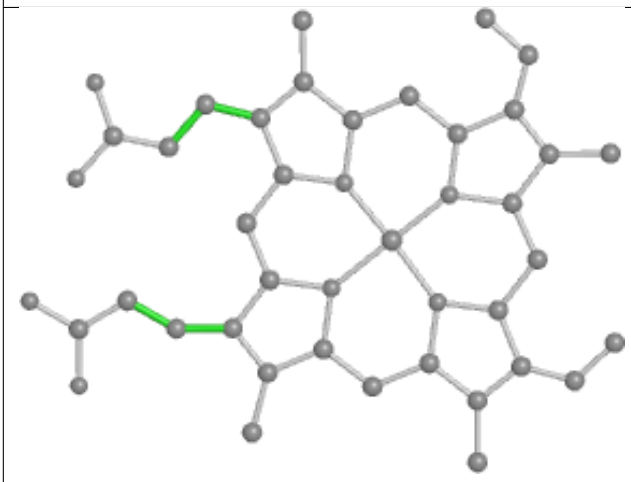
Ligand HEM D 1517



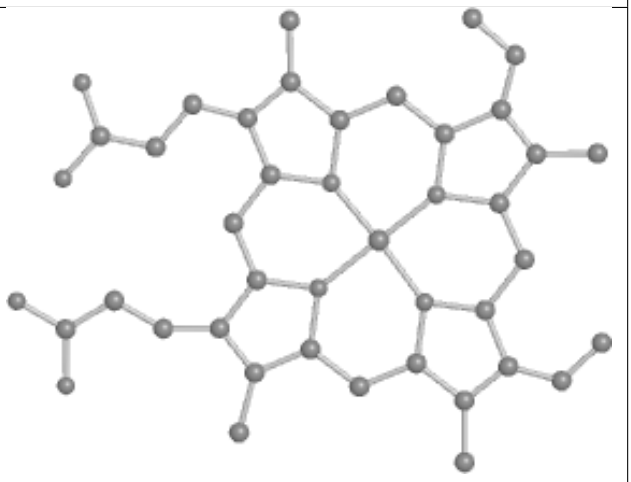
Bond lengths



Bond angles

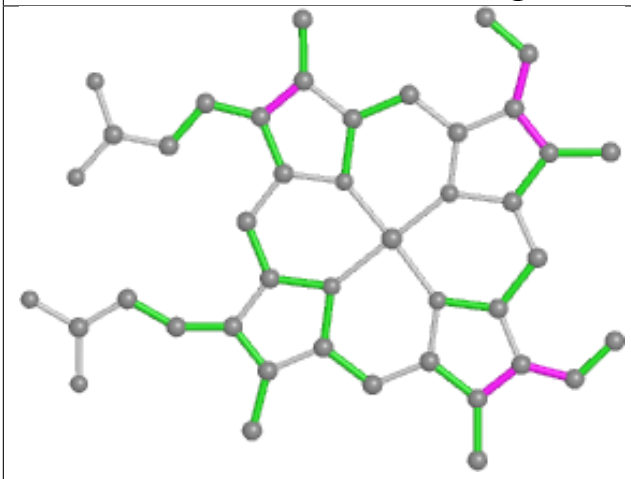


Torsions

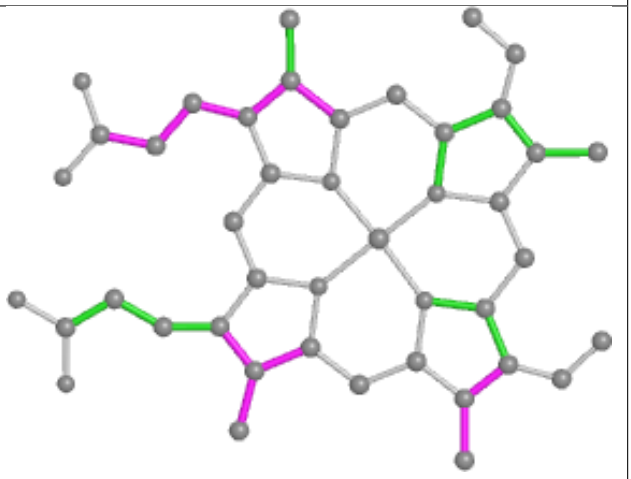


Rings

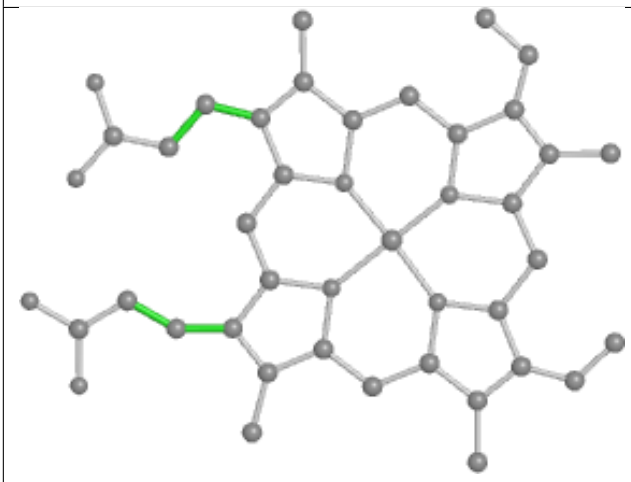
Ligand HEM A 1517



Bond lengths



Bond angles



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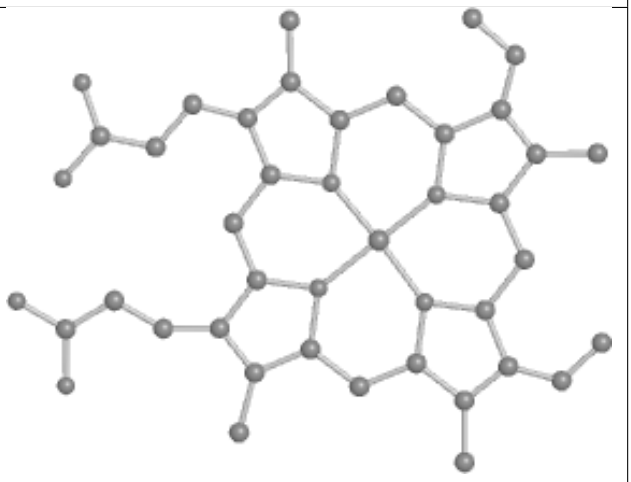
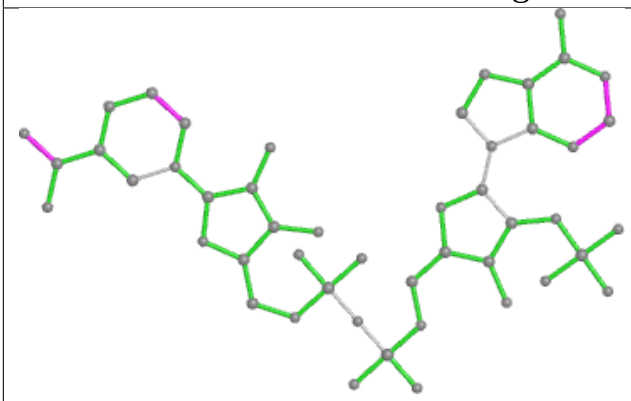
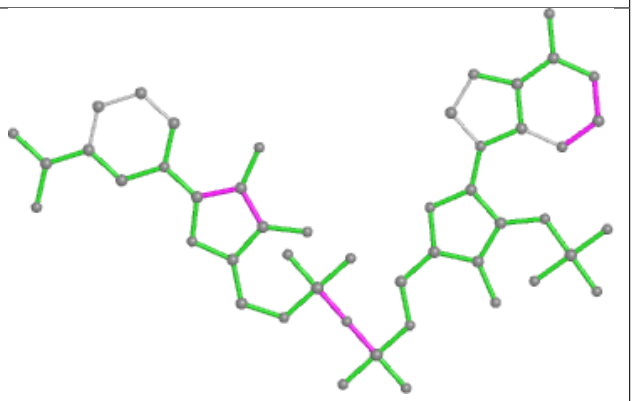


Rings

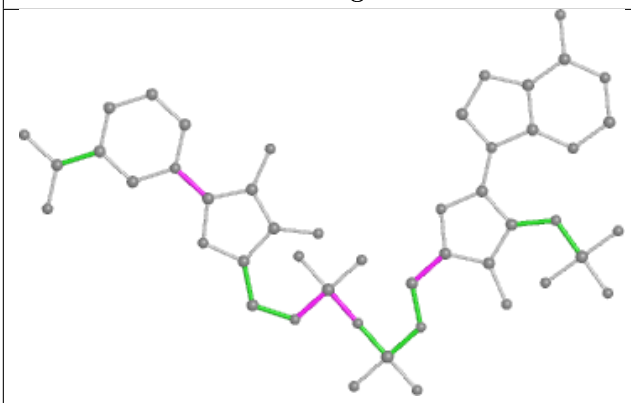
Ligand NDP D 1518



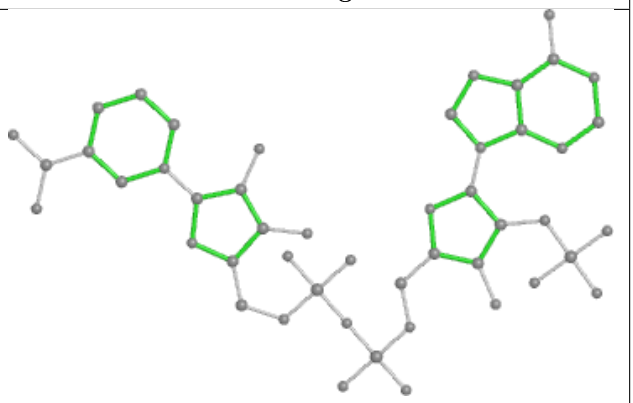
Bond lengths



Bond angles

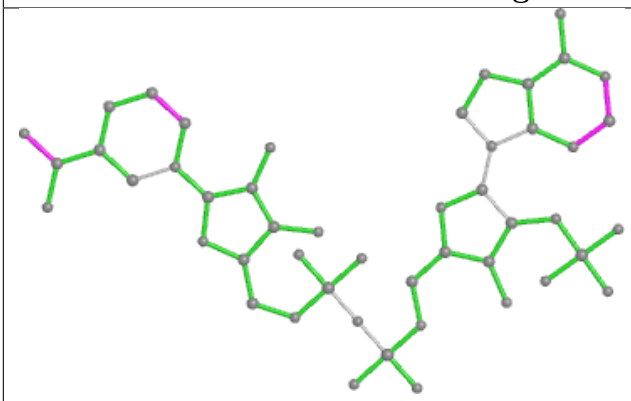


Torsions

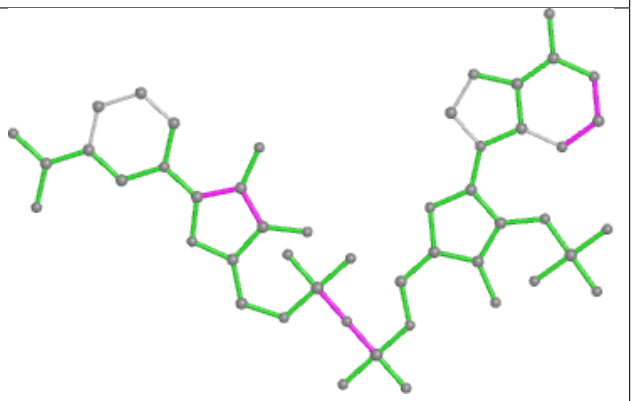


Rings

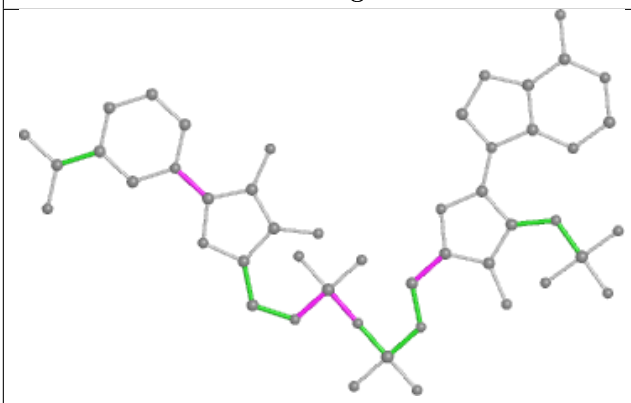
Ligand NDP C 1519



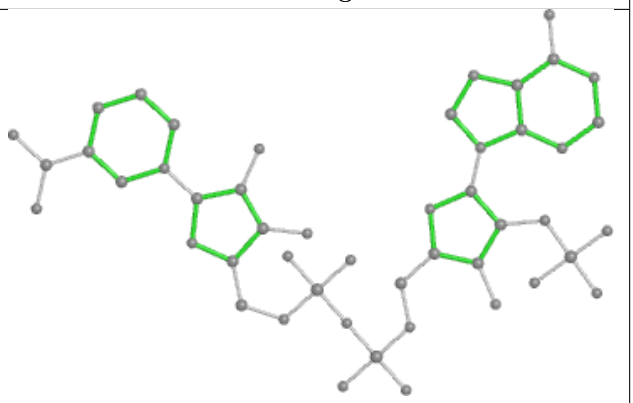
Bond lengths



Bond angles

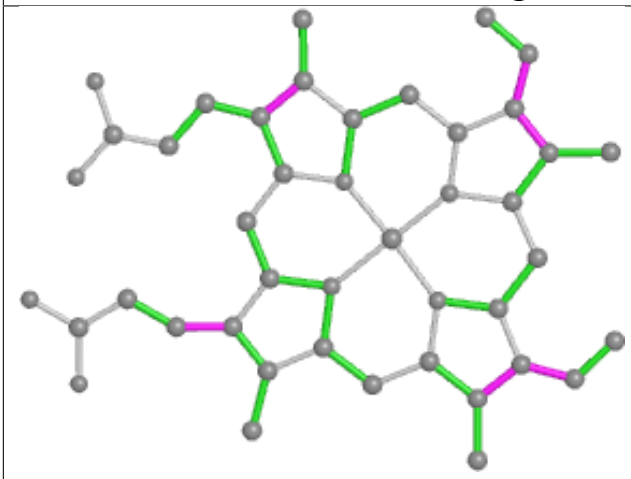


Torsions

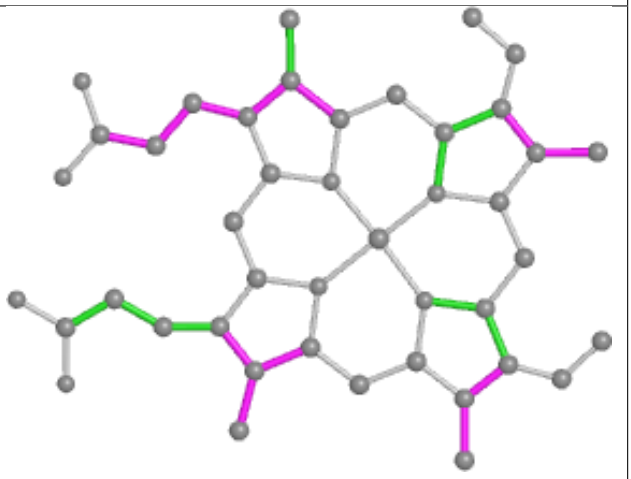


Rings

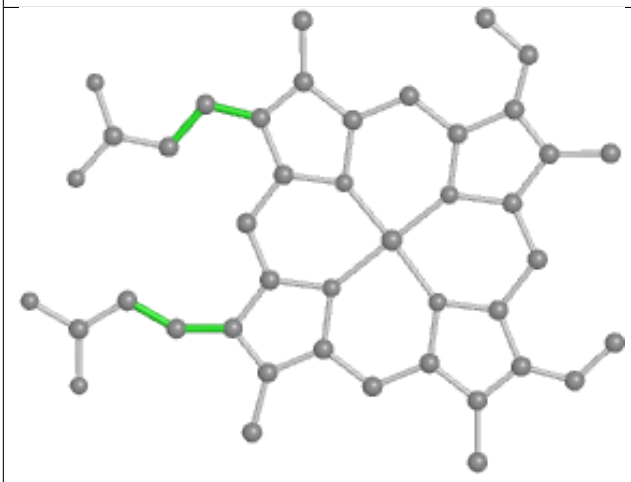
Ligand HEM B 1517



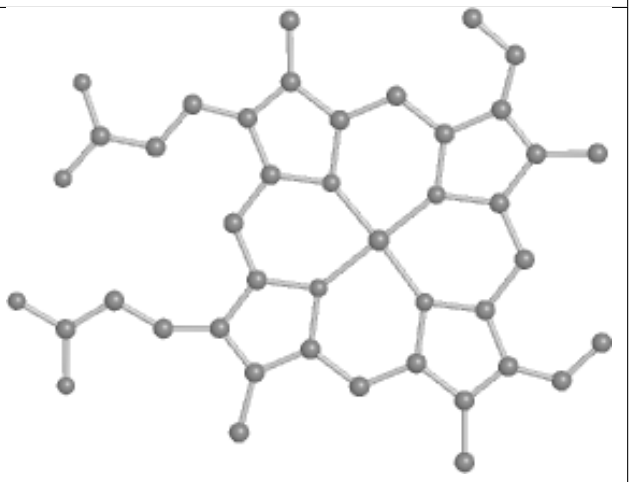
Bond lengths



Bond angles

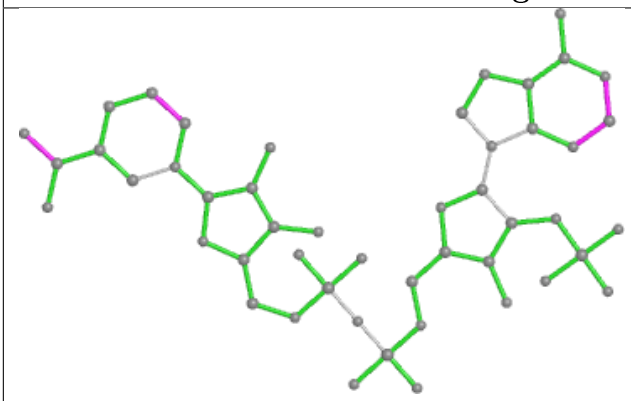


Torsions

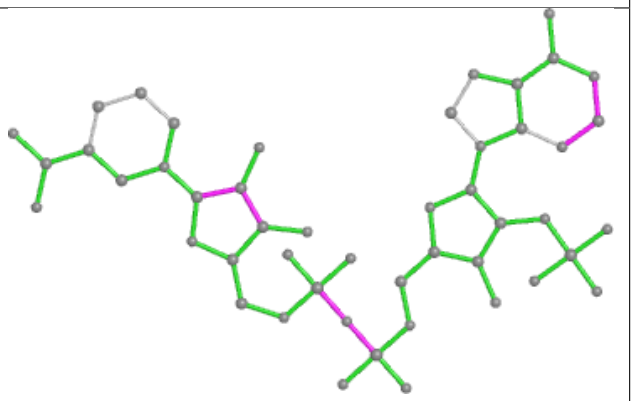


Rings

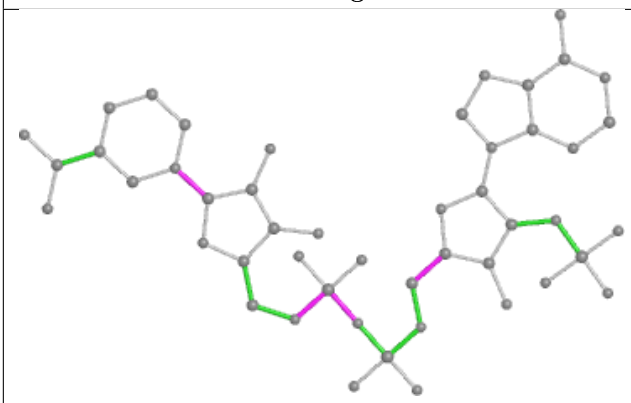
Ligand NDP A 1520



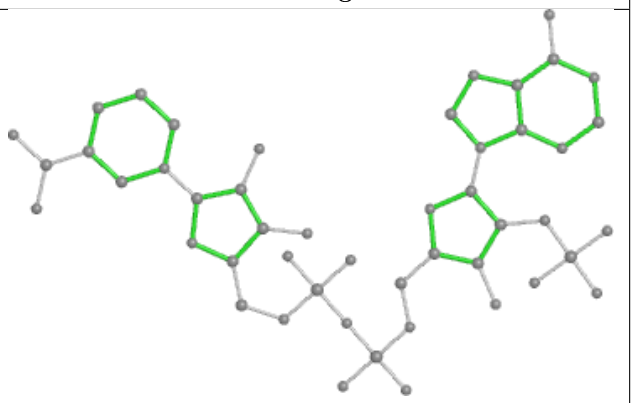
Bond lengths



Bond angles

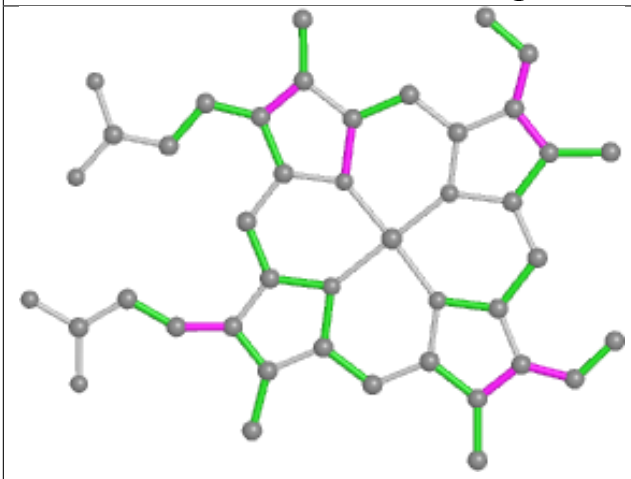


Torsions

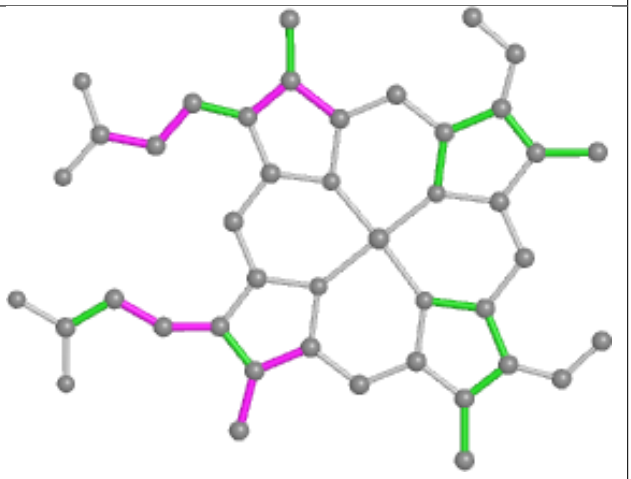


Rings

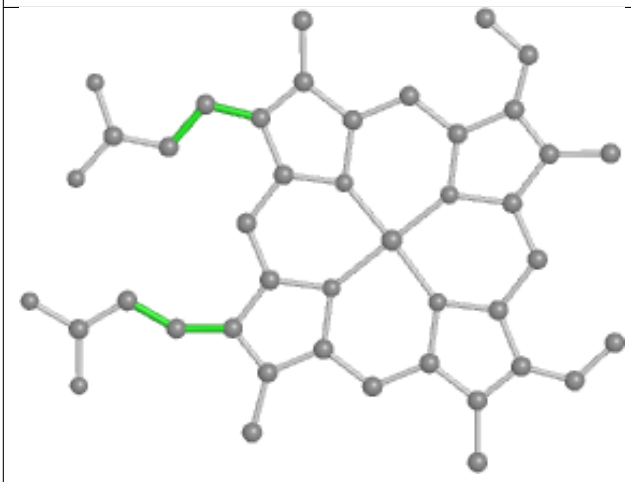
Ligand HEM C 1517



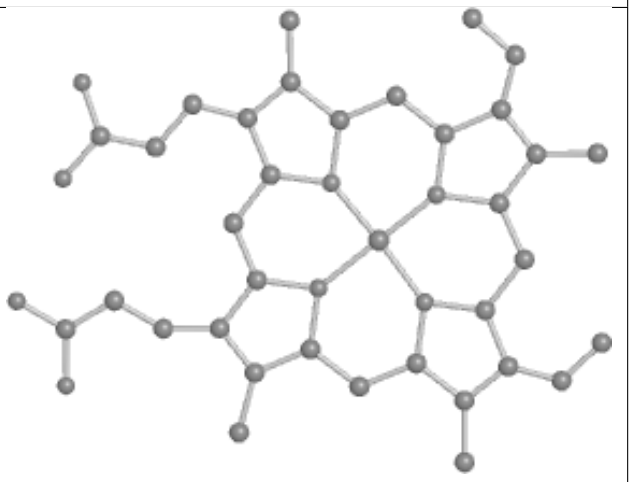
Bond lengths



Bond angles

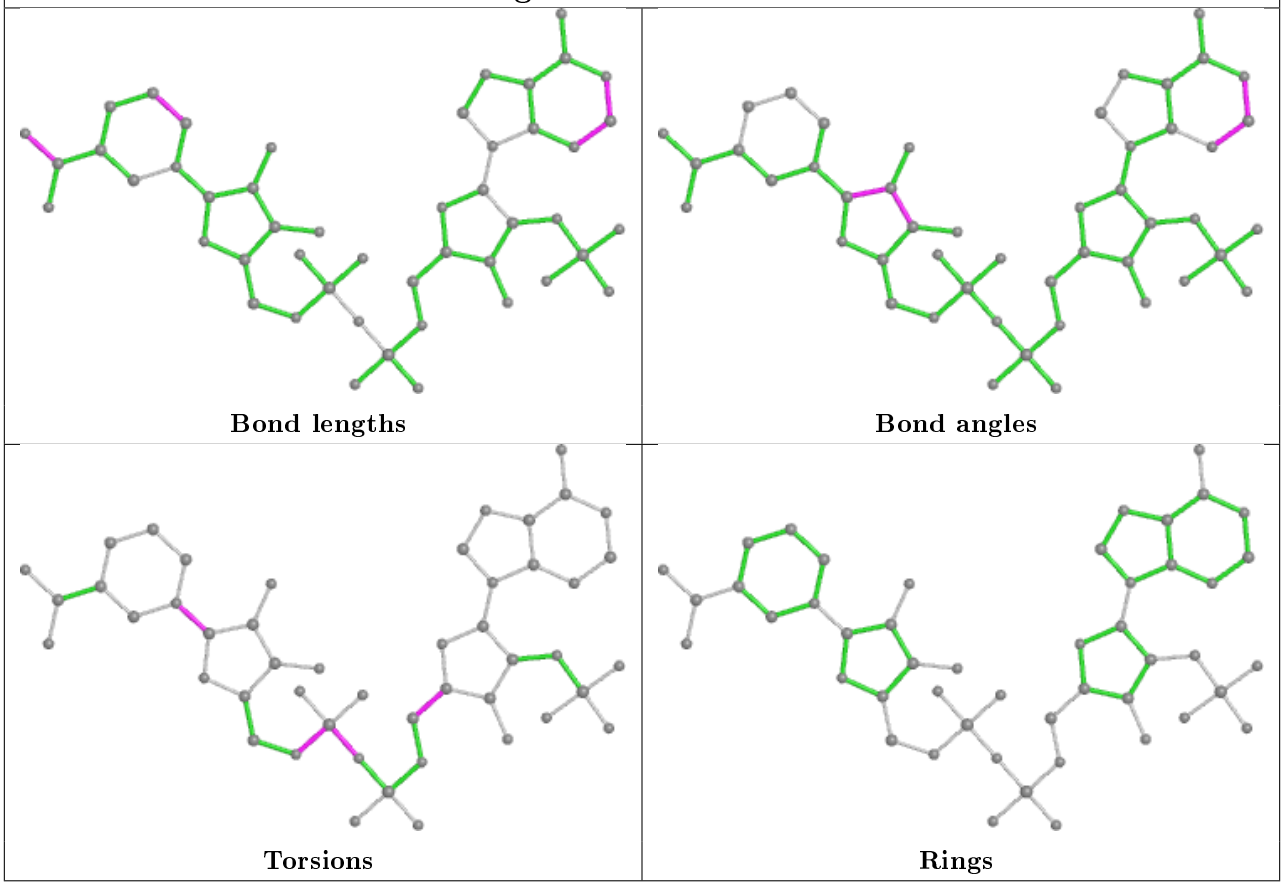


Torsions



Rings

Ligand NDP B 1518



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	419:ASN	C	420:HIS	N	1.12
1	A	419:ASN	C	420:HIS	N	1.09

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	419:ASN	C	420:HIS	N	1.08
1	B	419:ASN	C	420:HIS	N	1.06

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	515/515 (100%)	-0.01	4 (0%)	86	84	7, 11, 20, 83	0
1	B	514/515 (99%)	-0.02	2 (0%)	92	91	7, 12, 22, 76	0
1	C	514/515 (99%)	0.01	5 (0%)	82	80	7, 12, 22, 73	0
1	D	514/515 (99%)	0.01	4 (0%)	86	84	7, 12, 22, 84	0
All	All	2057/2060 (99%)	-0.00	15 (0%)	87	86	7, 12, 22, 84	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	ALA	11.8
1	A	2	SER	11.2
1	A	516	ALA	10.9
1	B	516	ALA	9.1
1	D	516	ALA	7.7
1	D	3	GLU	4.4
1	A	3	GLU	3.6
1	D	4	LYS	3.2
1	C	261	TYR	2.6
1	C	3	GLU	2.6
1	C	388[A]	TYR	2.5
1	C	9	GLN	2.4
1	A	388[A]	TYR	2.2
1	B	388[A]	TYR	2.2
1	D	388[A]	TYR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

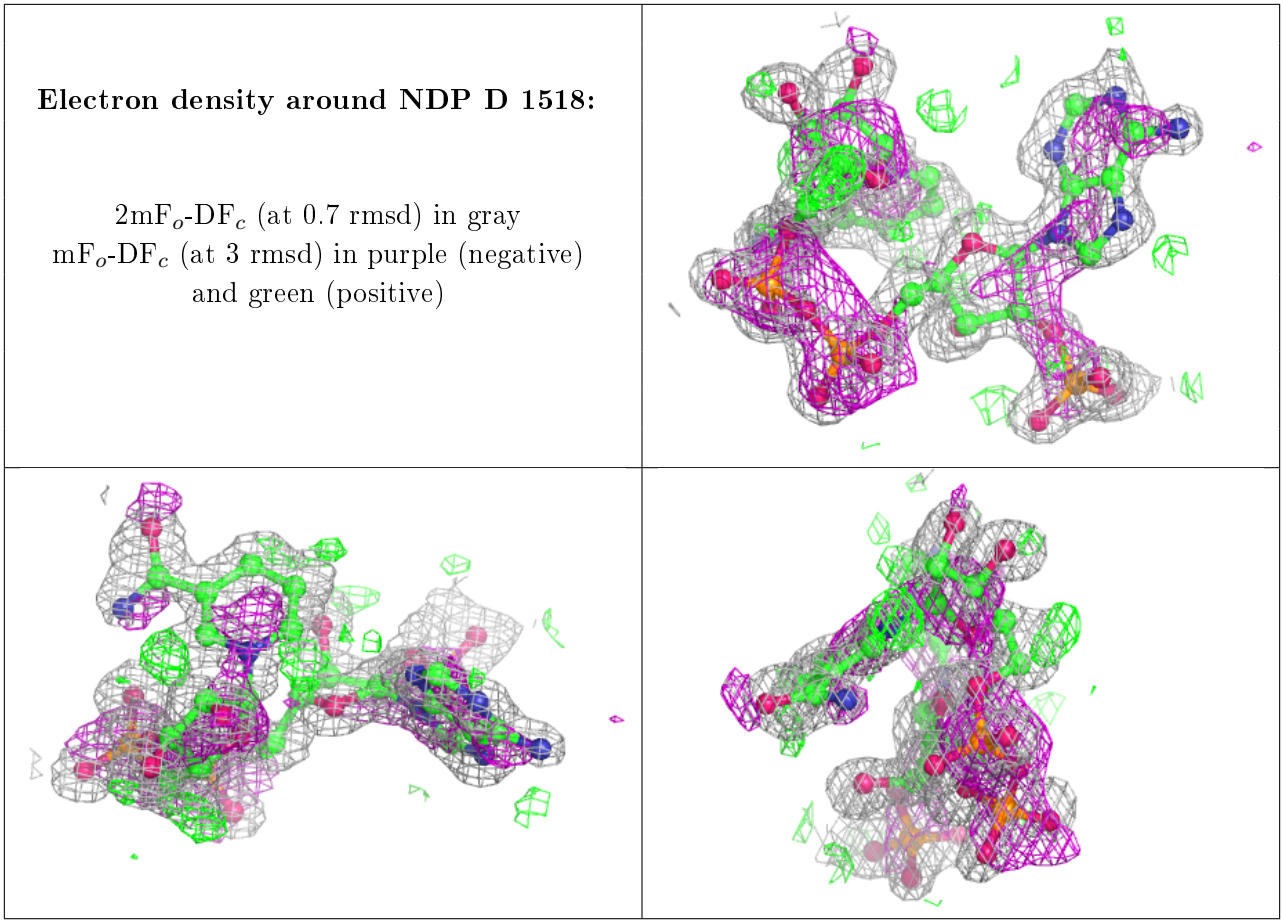
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NDP	D	1518	48/48	0.80	0.27	22,26,31,33	0
5	NDP	C	1519	48/48	0.81	0.26	19,25,33,34	0
6	BTB	D	1519	14/14	0.84	0.20	23,29,39,48	0
6	BTB	B	1520	14/14	0.88	0.16	22,24,39,43	0
6	BTB	C	1518	14/14	0.88	0.20	22,29,40,41	0
6	BTB	B	1521	14/14	0.91	0.14	20,24,31,35	0
5	NDP	B	1518	48/48	0.91	0.19	19,21,24,26	0
5	NDP	A	1520	48/48	0.92	0.15	15,17,21,21	0
3	NO	D	1520	2/2	0.96	0.13	20,20,20,20	0
3	NO	C	1520	2/2	0.97	0.11	20,20,20,20	0
3	NO	A	1518	2/2	0.98	0.12	20,20,20,20	0
3	NO	B	1522	2/2	0.98	0.12	20,20,20,20	0
2	HEM	B	1517	43/43	0.98	0.08	7,9,11,12	0
2	HEM	D	1517	43/43	0.98	0.08	7,8,11,13	0
2	HEM	C	1517	43/43	0.99	0.08	7,8,10,12	0
2	HEM	A	1517	43/43	0.99	0.08	7,8,10,13	0
4	CL	A	1519	1/1	1.00	0.06	14,14,14,14	0
4	CL	B	1519	1/1	1.00	0.05	14,14,14,14	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.

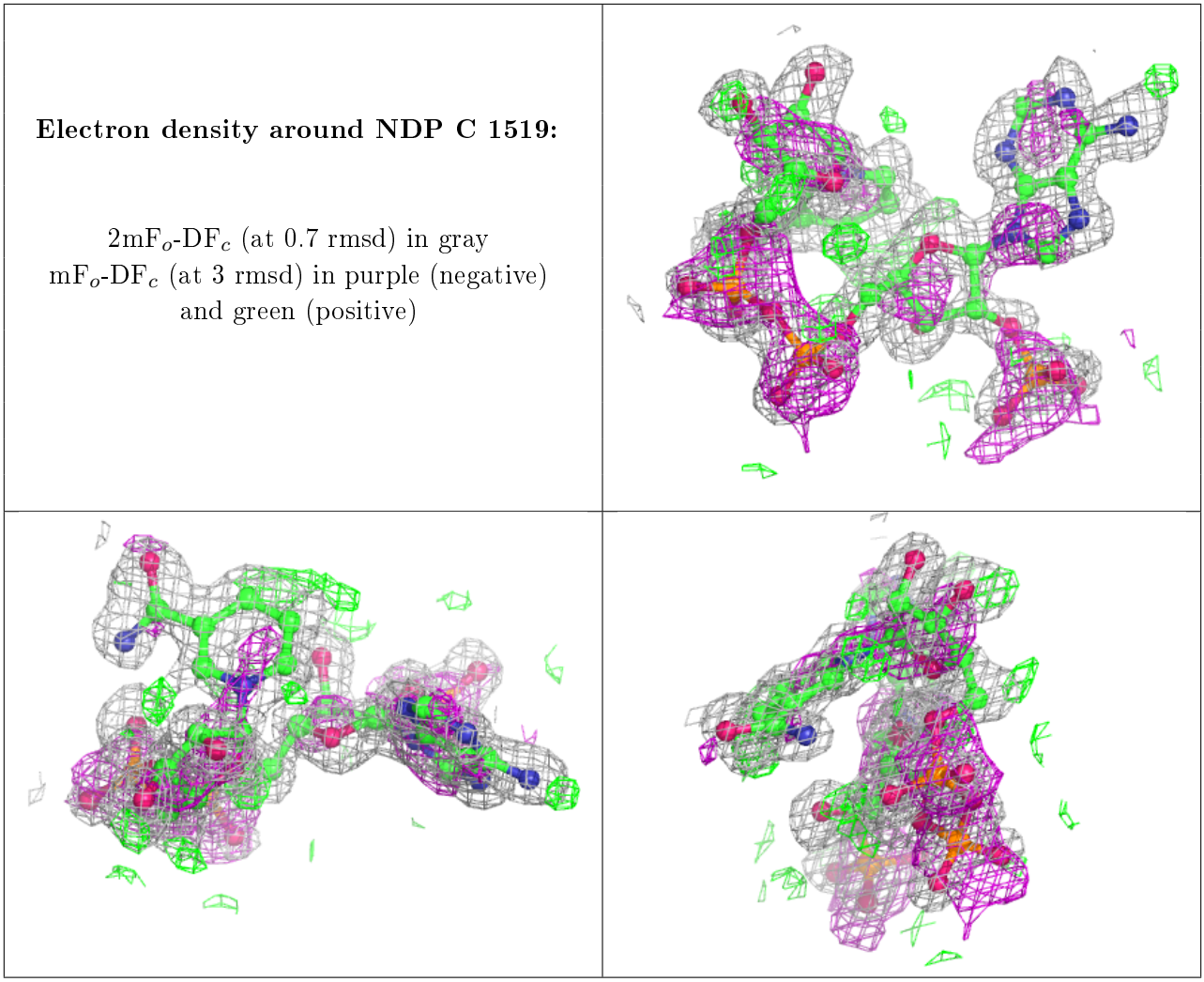
Electron density around NDP D 1518:

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



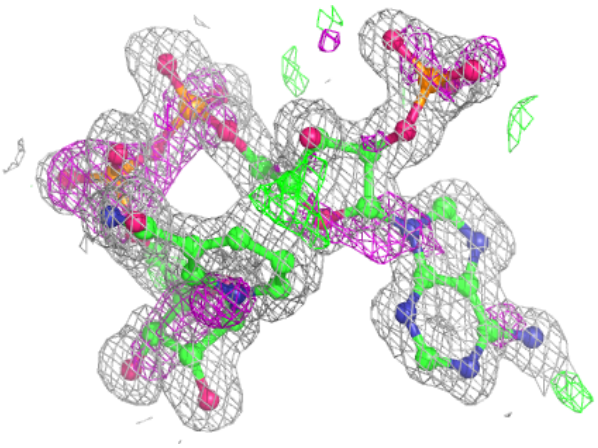
Electron density around NDP C 1519:

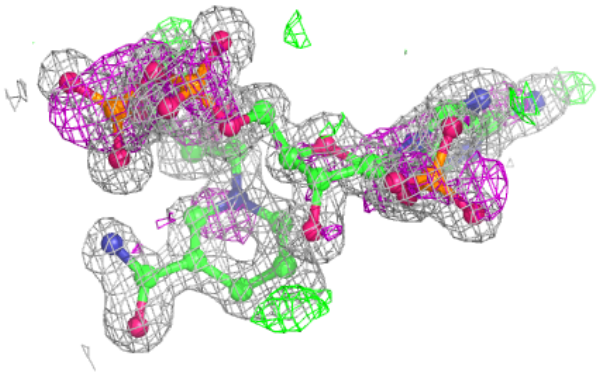
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

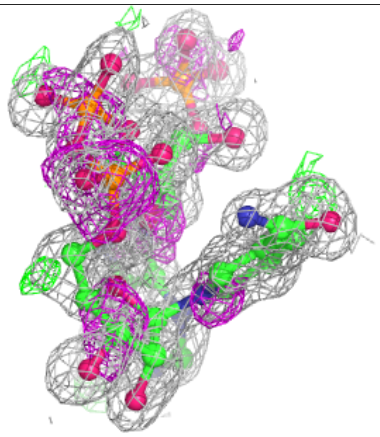


Electron density around NDP B 1518:

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

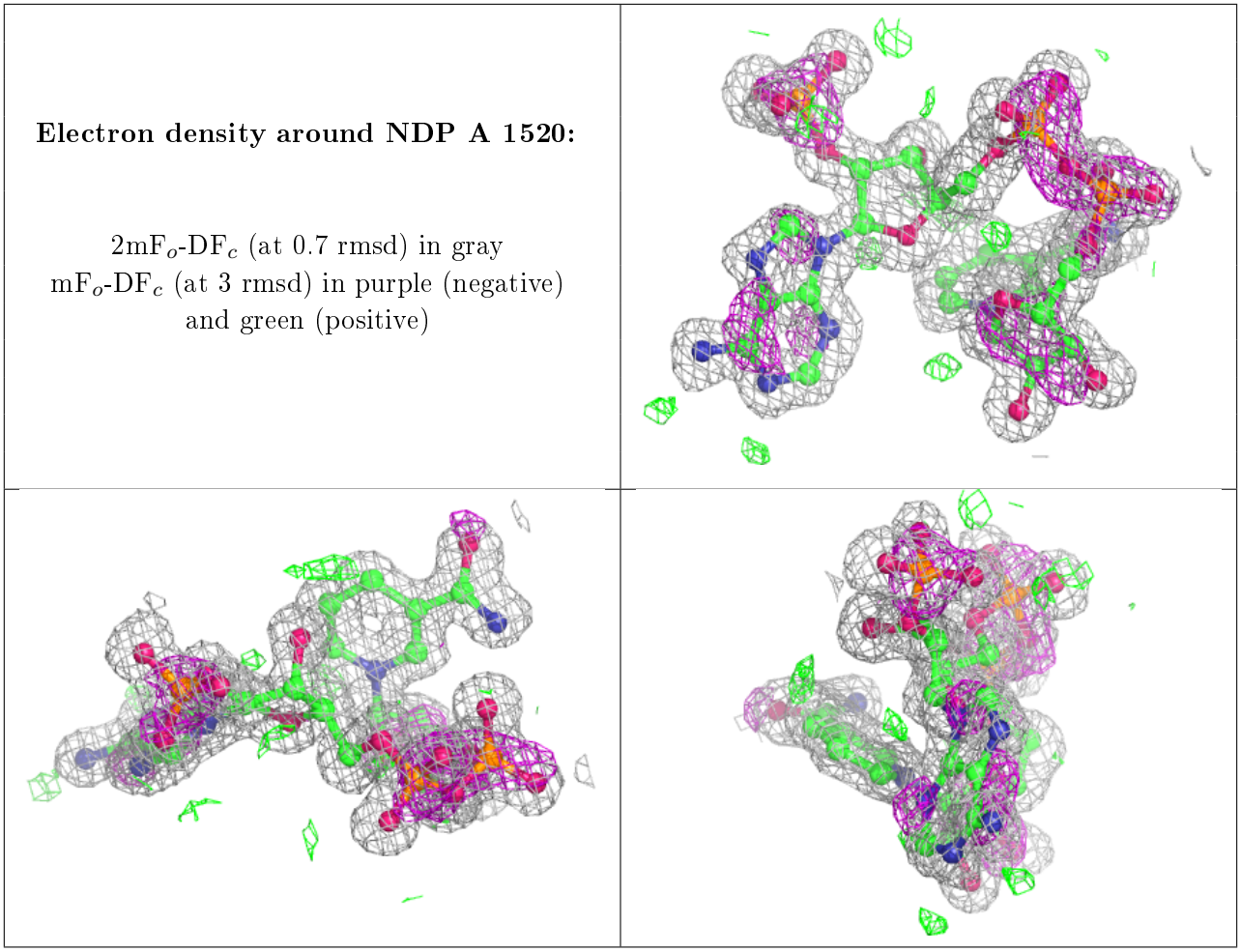






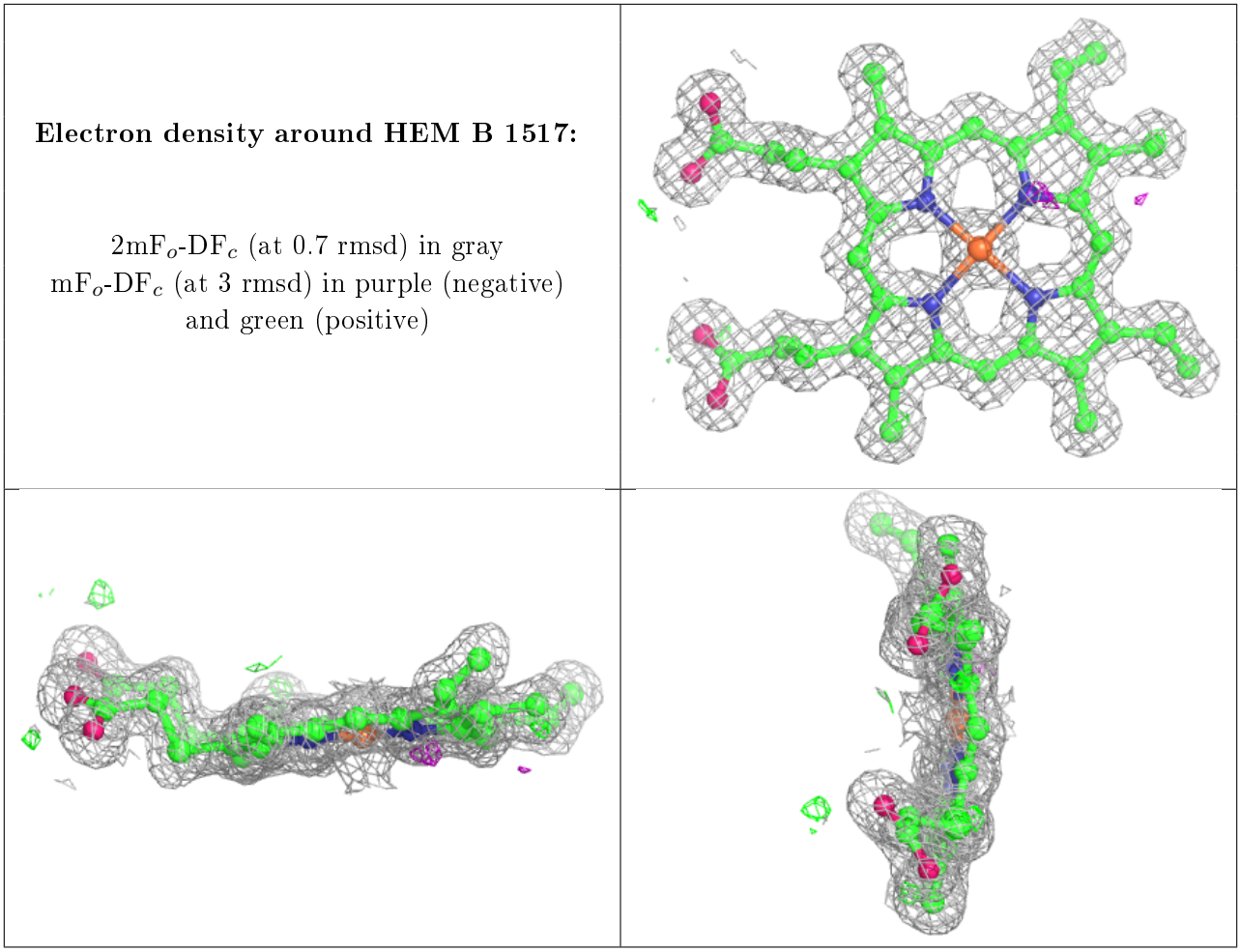
Electron density around NDP A 1520:

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



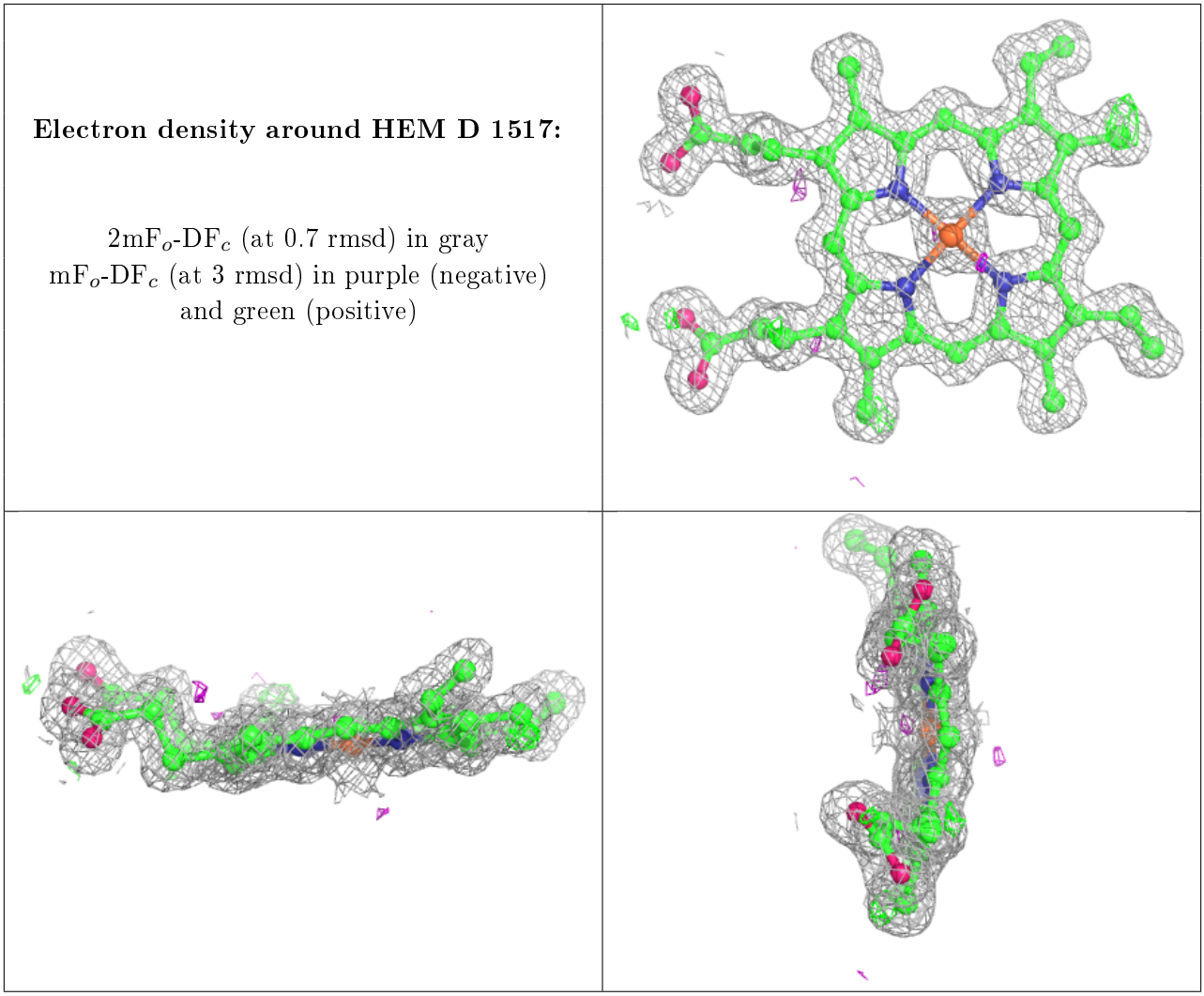
Electron density around HEM B 1517:

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



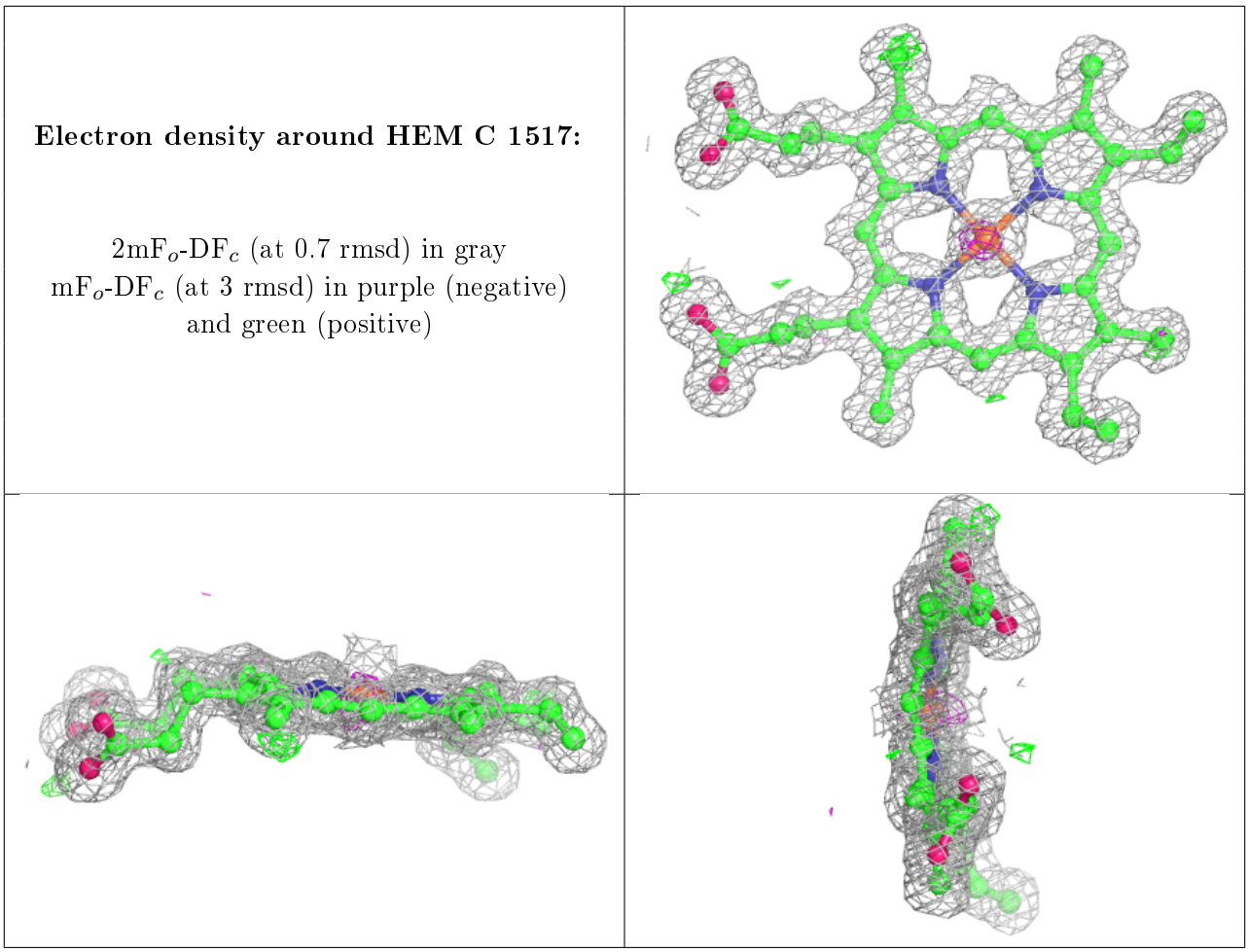
Electron density around HEM D 1517:

$2mF_o$-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 1517:

$2mF_o$-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 1517:

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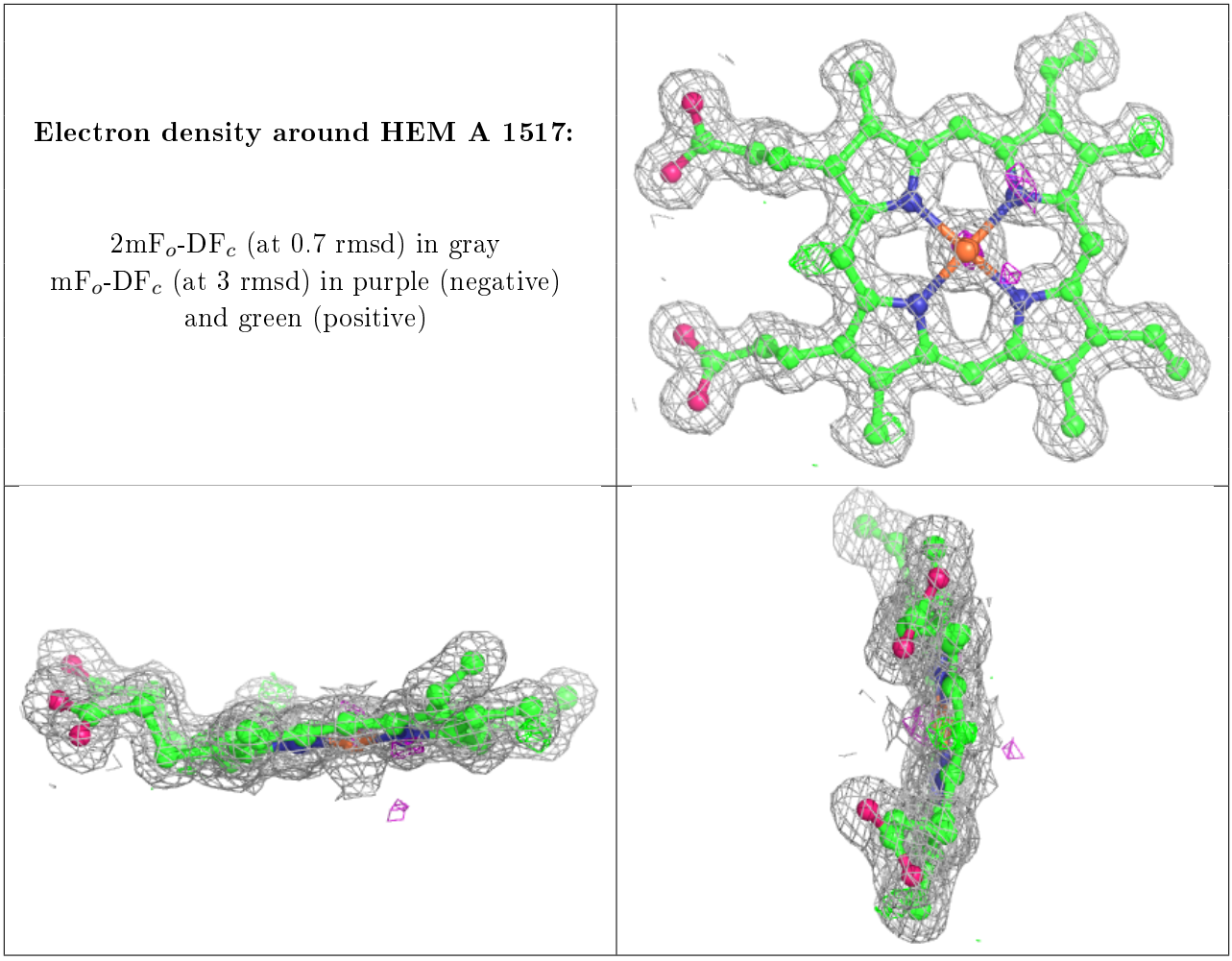
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.