Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 11:33 PM EDT

PDB ID	:	4JWS / pdb_00004jws
Title	:	Crystal structure of Cytochrome P450cam-putidaredoxin complex
Authors	:	Tripathi, S.M.; Li, H.; Poulos, T.L.
Deposited on	:	2013-03-27
Resolution	:	2.15 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 (i) 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 (i)) were used in the production of this report:

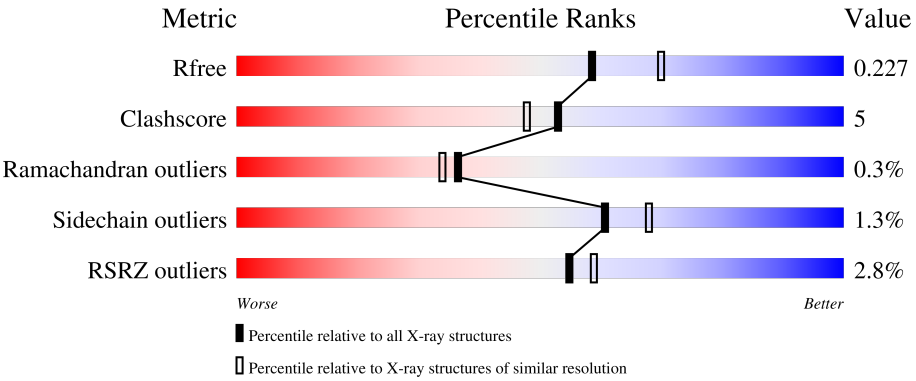
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	415	3% 81% 12% • 6%
1	B	415	3% 82% 13% • 5%
2	C	112	2% 81% 13% 5%
2	D	112	% 79% 13% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	FES	D	201	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8154 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 Camphor 5-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3097	1963	543	577	14			
1	B	395	Total	C	N	O	S	0	0	0
			3102	1966	542	580	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	SER	CYS	engineered mutation	UNP P00183
A	85	SER	CYS	engineered mutation	UNP P00183
A	136	SER	CYS	engineered mutation	UNP P00183
A	285	SER	CYS	engineered mutation	UNP P00183
A	334	ALA	CYS	engineered mutation	UNP P00183
A	344	CYS	LYS	engineered mutation	UNP P00183
B	58	SER	CYS	engineered mutation	UNP P00183
B	85	SER	CYS	engineered mutation	UNP P00183
B	136	SER	CYS	engineered mutation	UNP P00183
B	285	SER	CYS	engineered mutation	UNP P00183
B	334	ALA	CYS	engineered mutation	UNP P00183
B	344	CYS	LYS	engineered mutation	UNP P00183

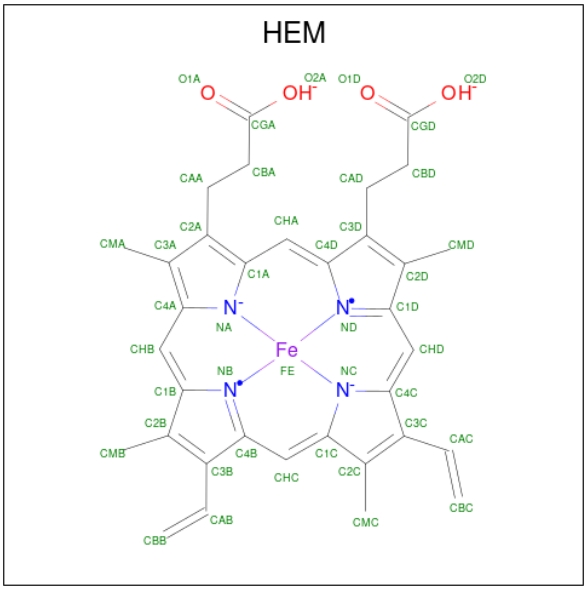
- Molecule 2 is a protein called Putidaredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	106	Total	C	N	O	S	0	0	0
			794	488	136	161	9			
2	D	106	Total	C	N	O	S	0	0	0
			794	488	136	161	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P00259
C	-4	HIS	-	expression tag	UNP P00259
C	-3	HIS	-	expression tag	UNP P00259
C	-2	HIS	-	expression tag	UNP P00259
C	-1	HIS	-	expression tag	UNP P00259
C	0	HIS	-	expression tag	UNP P00259
D	-5	HIS	-	expression tag	UNP P00259
D	-4	HIS	-	expression tag	UNP P00259
D	-3	HIS	-	expression tag	UNP P00259
D	-2	HIS	-	expression tag	UNP P00259
D	-1	HIS	-	expression tag	UNP P00259
D	0	HIS	-	expression tag	UNP P00259

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

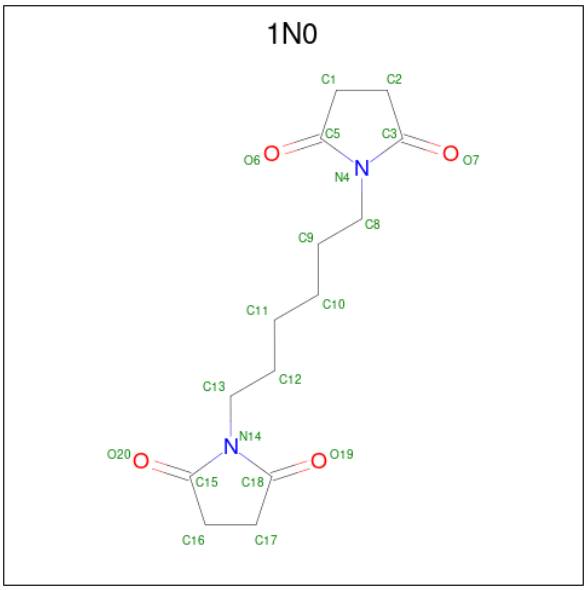
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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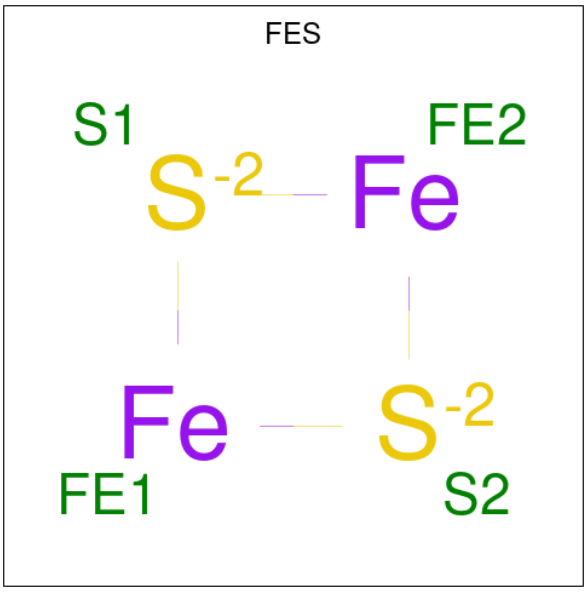
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is 1,1'-hexane-1,6-diyldipyrrolidine-2,5-dione (CCD ID: 1N0) (formula: $C_{14}H_{20}N_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 20 14 2 4	0	0
5	B	1	Total C N O 20 14 2 4	0	0

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Fe S 4 2 2	0	0
6	D	1	Total Fe S 4 2 2	0	0

- Molecule 7 is water.

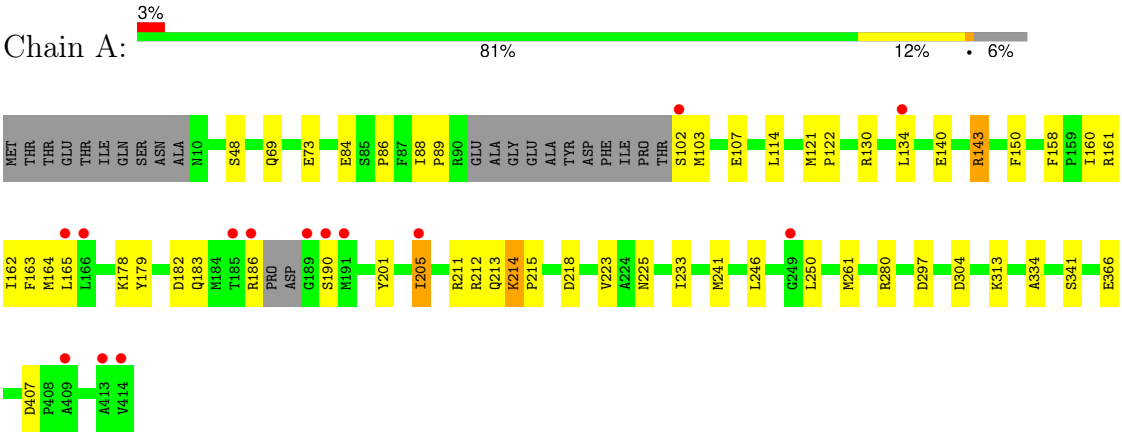
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	101	Total O 101 101	0	0
7	B	85	Total O 85 85	0	0
7	C	25	Total O 25 25	0	0
7	D	20	Total O 20 20	0	0

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.

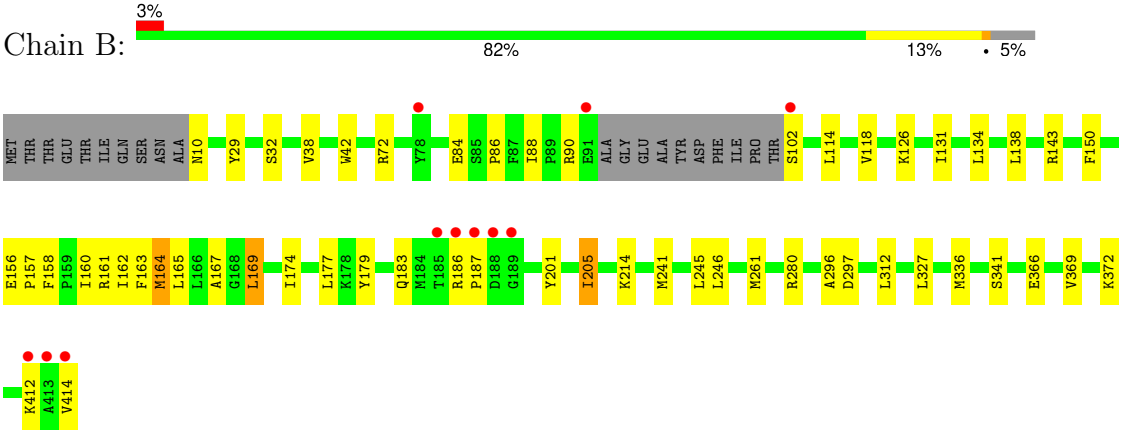
• Molecule 1: Camphor 5-monooxygenase

Chain A:



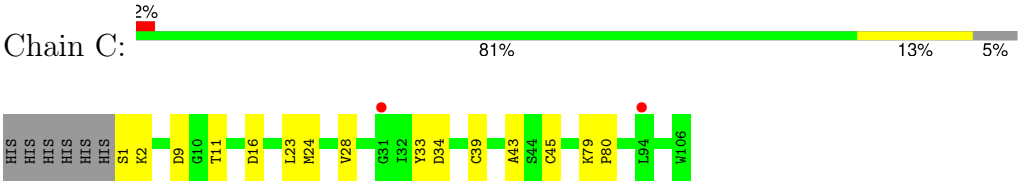
• Molecule 1: Camphor 5-monooxygenase

Chain B:



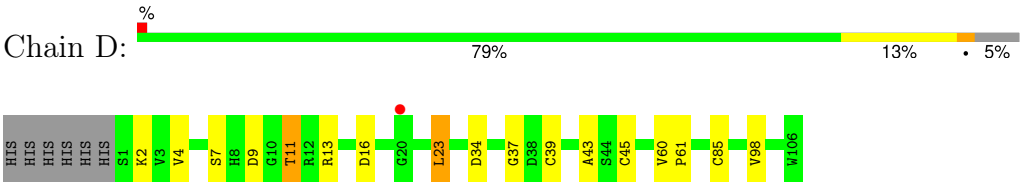
• Molecule 2: Putidaredoxin

Chain C:



• Molecule 2: Putidaredoxin

Chain D:


%
79%
13%
5%
HIS
HIS
HIS
HIS
HIS
HIS
S1
K2
V3
V4
S7
H8
D9
G10
T11
R12
R13
D16
G20
L23
D34
G37
D38
C39
A43
S44
C45
V60
P61
C85
V98
W106

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.59Å 106.72Å 88.70Å 90.00° 107.91° 90.00°	Depositor
Resolution (Å)	54.80 – 2.15 54.80 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (54.80-2.15) 99.9 (54.80-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.175 , 0.225 0.179 , 0.227	Depositor DCC
R_{free} test set	2781 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8154	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: 1N0, FES, CA, HEM

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	0.62	1/3170 (0.0%)	0.91	8/4303 (0.2%)
1	B	0.53	0/3176	0.87	11/4316 (0.3%)
2	C	0.54	0/805	0.89	0/1093
2	D	0.54	0/805	0.87	0/1093
All	All	0.57	1/7956 (0.0%)	0.89	19/10805 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	ALA	CA-CB	5.78	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	LYS	CA-C-N	9.30	130.79	120.66
1	A	214	LYS	C-N-CA	9.30	130.79	120.66
1	B	143	ARG	CA-C-N	-6.59	114.11	120.83
1	B	143	ARG	C-N-CA	-6.59	114.11	120.83
1	B	214	LYS	CA-C-N	-6.38	114.06	120.31
1	B	214	LYS	C-N-CA	-6.38	114.06	120.31
1	A	205	ILE	CB-CA-C	-6.24	107.74	114.35
1	B	187	PRO	N-CA-CB	6.14	109.69	103.25
1	A	48	SER	N-CA-C	5.54	117.32	111.28
1	B	296	ALA	CA-C-N	-5.52	114.87	122.16
1	B	296	ALA	C-N-CA	-5.52	114.87	122.16
1	A	143	ARG	CA-C-N	-5.45	115.27	120.83
1	A	143	ARG	C-N-CA	-5.45	115.27	120.83
1	A	407	ASP	CA-C-N	5.43	125.10	119.56
1	A	407	ASP	C-N-CA	5.43	125.10	119.56
1	B	205	ILE	CB-CA-C	-5.20	108.84	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	32	SER	N-CA-C	5.19	117.34	111.11
1	B	156	GLU	CA-C-N	-5.09	114.42	119.56
1	B	156	GLU	C-N-CA	-5.09	114.42	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3097	0	3049	28	0
1	B	3102	0	3033	29	0
2	C	794	0	769	8	0
2	D	794	0	769	9	0
3	A	43	0	30	2	0
3	B	43	0	30	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	17	0	0
5	B	20	0	17	0	0
6	C	4	0	0	1	0
6	D	4	0	0	2	0
7	A	101	0	0	1	0
7	B	85	0	0	4	0
7	C	25	0	0	0	0
7	D	20	0	0	0	0
All	All	8154	0	7714	78	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 (78) 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:114:LEU:HD23	1:B:241:MET:HE3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD11	1:B:161:ARG:HD3	1.64	0.80
3:B:501:HEM:HHC	3:B:501:HEM:HBB2	1.68	0.75
1:A:114:LEU:HD23	1:A:241:MET:HE3	1.69	0.73
3:A:501:HEM:HMB1	3:A:501:HEM:HBB2	1.74	0.70
1:B:126:LYS:NZ	7:B:663:HOH:O	2.24	0.70
1:A:103:MET:HE2	1:A:107:GLU:HB3	1.76	0.68
1:B:10:ASN:N	7:B:674:HOH:O	2.28	0.66
2:D:2:LYS:NZ	2:D:16:ASP:OD1	2.30	0.65
1:A:280:ARG:NH2	1:A:341:SER:OG	2.30	0.64
1:B:280:ARG:NH2	1:B:341:SER:OG	2.30	0.64
1:A:134:LEU:HD11	1:A:161:ARG:HD3	1.82	0.61
3:B:501:HEM:HBC2	3:B:501:HEM:HHD	1.83	0.60
1:A:84:GLU:OE1	1:A:102:SER:N	2.34	0.60
1:B:201:TYR:O	1:B:205:ILE:HG13	2.02	0.60
1:A:69:GLN:NE2	1:A:73:GLU:OE2	2.28	0.59
1:A:182:ASP:O	1:A:186:ARG:N	2.37	0.57
1:B:163:PHE:CD2	1:B:246:LEU:HD13	2.39	0.57
2:D:39:CYS:HB3	2:D:45:CYS:HB3	1.87	0.56
1:B:84:GLU:OE2	1:B:102:SER:N	2.38	0.56
1:B:167:ALA:HB3	1:B:169:LEU:HD22	1.89	0.55
1:A:179:TYR:O	1:A:183:GLN:HG2	2.07	0.54
1:A:160:ILE:O	1:A:164:MET:HG2	2.08	0.54
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.42	0.54
1:A:213:GLN:C	1:A:215:PRO:HD3	2.32	0.54
1:B:118:VAL:HG11	1:B:245:LEU:HD13	1.88	0.54
1:B:179:TYR:O	1:B:183:GLN:HG2	2.09	0.53
2:D:4:VAL:HB	2:D:98:VAL:HG22	1.89	0.53
1:B:280:ARG:NH1	7:B:655:HOH:O	2.40	0.53
1:B:29:TYR:OH	1:B:88:ILE:O	2.18	0.52
1:A:86:PRO:O	1:A:297:ASP:HB2	2.10	0.51
2:C:39:CYS:HB3	2:C:45:CYS:HB3	1.92	0.51
1:A:201:TYR:O	1:A:205:ILE:HG13	2.11	0.50
1:A:211:ARG:NH1	1:A:218:ASP:OD2	2.44	0.50
2:C:34:ASP:OD1	2:C:34:ASP:N	2.39	0.50
1:A:212:ARG:C	1:A:214:LYS:H	2.20	0.49
2:D:43:ALA:HA	6:D:201:FES:S1	2.53	0.49
2:D:7:SER:OG	2:D:13:ARG:NH2	2.46	0.48
1:B:158:PHE:CZ	1:B:162:ILE:HD11	2.48	0.48
1:A:158:PHE:CZ	1:A:162:ILE:HD11	2.49	0.48
1:B:327:LEU:HD22	1:B:336:MET:HE1	1.97	0.47
1:B:164:MET:HE2	1:B:169:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HD13	1:B:366:GLU:HG2	1.96	0.47
1:A:130:ARG:HD2	1:A:165:LEU:HD11	1.98	0.46
2:D:9:ASP:OD1	2:D:11:THR:OG1	2.28	0.46
2:D:23:LEU:HB2	2:D:85:CYS:HB2	1.97	0.46
1:A:215:PRO:HB3	1:A:225:ASN:ND2	2.31	0.45
1:B:161:ARG:HA	1:B:164:MET:HG3	1.97	0.45
2:C:2:LYS:NZ	2:C:16:ASP:OD1	2.34	0.45
2:C:9:ASP:OD1	2:C:11:THR:OG1	2.29	0.45
1:B:157:PRO:HA	1:B:160:ILE:HG22	1.99	0.44
1:A:162:ILE:HD13	1:A:366:GLU:HG2	1.98	0.44
1:A:223:VAL:O	1:A:233:ILE:HG21	2.18	0.44
1:B:72:ARG:NH1	7:B:624:HOH:O	2.51	0.44
1:A:178:LYS:NZ	7:A:684:HOH:O	2.43	0.43
1:B:412:LYS:HG2	1:B:414:VAL:HG13	2.01	0.43
1:B:138:LEU:HD12	1:B:138:LEU:HA	1.92	0.42
1:B:164:MET:HE3	1:B:177:LEU:HD22	2.01	0.42
3:A:501:HEM:HBB2	3:A:501:HEM:CMB	2.48	0.42
3:B:501:HEM:HBC2	3:B:501:HEM:CHD	2.48	0.42
2:C:79:LYS:HB3	2:C:80:PRO:HD2	2.01	0.42
1:A:163:PHE:CD2	1:A:246:LEU:HD13	2.55	0.42
1:A:122:PRO:HG3	2:C:33:TYR:CG	2.55	0.42
1:B:86:PRO:O	1:B:297:ASP:HB2	2.20	0.42
2:D:37:GLY:HA2	6:D:201:FES:S2	2.60	0.42
1:A:88:ILE:HA	1:A:89:PRO:HA	1.83	0.42
1:A:213:GLN:O	1:A:215:PRO:HD3	2.20	0.41
1:B:131:ILE:HG22	1:B:369:VAL:HG11	2.01	0.41
2:C:24:MET:O	2:C:28:VAL:HG23	2.20	0.41
1:A:304:ASP:OD1	1:A:313:LYS:HD2	2.20	0.41
2:C:43:ALA:HA	6:C:201:FES:S1	2.61	0.41
2:D:60:VAL:HA	2:D:61:PRO:HD2	1.83	0.41
1:B:38:VAL:O	1:B:42:TRP:HD1	2.04	0.41
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.55	0.41
1:A:140:GLU:OE2	1:A:143:ARG:NE	2.50	0.41
1:B:164:MET:SD	1:B:174:ILE:HG12	2.61	0.40
1:B:261:MET:HE3	1:B:261:MET:HB3	1.98	0.40
1:A:121:MET:HB3	1:A:122:PRO:HD3	2.03	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	386/415 (93%)	375 (97%)	10 (3%)	1 (0%)	36	34
1	B	391/415 (94%)	376 (96%)	13 (3%)	2 (0%)	24	20
2	C	104/112 (93%)	102 (98%)	2 (2%)	0	100	100
2	D	104/112 (93%)	103 (99%)	1 (1%)	0	100	100
All	All	985/1054 (94%)	956 (97%)	26 (3%)	3 (0%)	36	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	ARG
1	B	90	ARG
1	A	190	SER

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	337/358 (94%)	336 (100%)	1 (0%)	86	91
1	B	335/358 (94%)	330 (98%)	5 (2%)	57	64
2	C	89/95 (94%)	87 (98%)	2 (2%)	45	51
2	D	89/95 (94%)	86 (97%)	3 (3%)	32	33
All	All	850/906 (94%)	839 (99%)	11 (1%)	61	68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	LEU
1	B	164	MET
1	B	165	LEU
1	B	169	LEU
1	B	312	LEU
1	B	372	LYS
2	C	1	SER
2	C	23	LEU
2	D	11	THR
2	D	23	LEU
2	D	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	145	GLN
1	A	272	GLN
1	B	225	ASN
1	B	272	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
6	FES	C	201	2	0,4,4	-	-	-		
3	HEM	A	501	1,7	50,50,50	2.02	12 (24%)	67,82,82	1.35	9 (13%)
5	1N0	A	503	1,2	21,21,21	3.98	12 (57%)	28,28,28	2.07	5 (17%)
6	FES	D	201	2	0,4,4	-	-	-		
5	1N0	B	503	1,2	21,21,21	4.00	13 (61%)	28,28,28	1.69	4 (14%)
3	HEM	B	501	1	50,50,50	1.96	10 (20%)	67,82,82	1.41	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FES	C	201	2	-	-	0/1/1/1
3	HEM	A	501	1,7	-	2/14/54/54	-
5	1N0	A	503	1,2	-	4/9/35/35	0/2/2/2
6	FES	D	201	2	-	-	0/1/1/1
5	1N0	B	503	1,2	-	4/9/35/35	0/2/2/2
3	HEM	B	501	1	-	2/14/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	1N0	O20-C15	8.23	1.40	1.23
5	B	503	1N0	O20-C15	8.15	1.40	1.23
3	A	501	HEM	C3D-C2D	7.78	1.53	1.36
5	B	503	1N0	O6-C5	7.70	1.39	1.23
3	B	501	HEM	C3D-C2D	7.67	1.53	1.36
5	A	503	1N0	O6-C5	7.63	1.39	1.23
5	A	503	1N0	O19-C18	7.02	1.38	1.23
5	B	503	1N0	O19-C18	6.89	1.37	1.23
5	B	503	1N0	O7-C3	6.00	1.36	1.23
5	A	503	1N0	O7-C3	5.69	1.35	1.23
3	A	501	HEM	FE-NC	4.94	2.11	1.95
3	B	501	HEM	FE-ND	4.91	2.10	1.94
5	A	503	1N0	C1-C2	-4.86	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	1N0	C1-C2	-4.85	1.40	1.52
5	A	503	1N0	C17-C16	-4.71	1.41	1.52
3	A	501	HEM	FE-NA	4.61	2.10	1.95
5	B	503	1N0	C17-C16	-4.56	1.41	1.52
3	B	501	HEM	FE-NB	4.28	2.08	1.94
5	A	503	1N0	C16-C15	-3.94	1.39	1.51
5	A	503	1N0	C17-C18	-3.87	1.40	1.51
5	B	503	1N0	C17-C18	-3.84	1.40	1.51
5	B	503	1N0	C16-C15	-3.78	1.40	1.51
3	A	501	HEM	FE-ND	3.78	2.06	1.94
3	B	501	HEM	FE-NA	3.77	2.07	1.95
5	B	503	1N0	C1-C5	-3.75	1.40	1.51
5	A	503	1N0	C1-C5	-3.66	1.40	1.51
5	B	503	1N0	C3-N4	-3.55	1.33	1.38
5	A	503	1N0	C2-C3	-3.26	1.41	1.51
5	A	503	1N0	C3-N4	-3.22	1.33	1.38
5	B	503	1N0	C2-C3	-3.07	1.42	1.51
3	A	501	HEM	CAB-C3B	3.06	1.55	1.47
3	B	501	HEM	CAC-C3C	3.03	1.55	1.47
3	A	501	HEM	CAC-C3C	2.92	1.55	1.47
3	B	501	HEM	CMC-C2C	2.89	1.56	1.50
3	B	501	HEM	CAB-C3B	2.82	1.54	1.47
3	A	501	HEM	FE-NB	2.62	2.03	1.94
5	B	503	1N0	C18-N14	-2.54	1.34	1.38
3	A	501	HEM	CMB-C2B	2.52	1.55	1.50
3	B	501	HEM	C3B-C2B	-2.44	1.32	1.37
5	B	503	1N0	C15-N14	-2.41	1.35	1.38
3	B	501	HEM	CMA-C3A	2.38	1.55	1.50
5	A	503	1N0	C18-N14	-2.34	1.35	1.38
3	B	501	HEM	C3C-C2C	-2.32	1.32	1.37
3	A	501	HEM	CMC-C2C	2.23	1.55	1.50
3	A	501	HEM	O1D-CGD	2.19	1.29	1.22
3	A	501	HEM	CMD-C2D	2.18	1.55	1.50
3	A	501	HEM	CMA-C3A	2.12	1.55	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	503	1N0	C18-N14-C15	-7.04	109.86	112.94
5	B	503	1N0	C18-N14-C15	-6.24	110.21	112.94
3	B	501	HEM	C4D-ND-C1D	5.36	111.56	105.21
3	A	501	HEM	C4D-ND-C1D	5.22	111.39	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	503	1N0	C5-N4-C3	-5.18	110.67	112.94
5	B	503	1N0	C5-N4-C3	-3.59	111.37	112.94
5	A	503	1N0	O20-C15-N14	2.88	127.03	123.94
3	B	501	HEM	CMC-C2C-C1C	2.79	129.63	124.73
3	A	501	HEM	CAC-C3C-C4C	2.77	131.44	124.82
3	A	501	HEM	CHC-C4B-NB	2.69	127.32	124.42
3	A	501	HEM	CBD-CAD-C3D	-2.63	105.26	112.53
3	A	501	HEM	CHD-C4C-C3C	2.59	129.57	125.21
5	A	503	1N0	C9-C8-N4	2.47	118.22	112.36
3	B	501	HEM	CMC-C2C-C3C	-2.36	122.71	128.43
5	B	503	1N0	C2-C1-C5	2.36	107.66	105.24
3	B	501	HEM	C3B-C2B-C1B	2.36	108.18	106.41
3	B	501	HEM	CAC-C3C-C4C	2.36	130.44	124.82
3	B	501	HEM	CAB-C3B-C2B	-2.33	120.84	128.43
3	A	501	HEM	CAC-C3C-C2C	-2.28	121.02	128.43
3	A	501	HEM	C2A-C1A-NA	-2.26	107.64	110.15
3	A	501	HEM	CHD-C1D-ND	2.21	126.81	124.42
3	A	501	HEM	CAD-C3D-C4D	2.20	128.54	124.70
3	B	501	HEM	CAC-C3C-C2C	-2.20	121.29	128.43
5	B	503	1N0	O6-C5-N4	2.14	126.24	123.94
5	A	503	1N0	C2-C1-C5	2.02	107.31	105.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	1N0	C11-C12-C13-N14
5	B	503	1N0	C11-C12-C13-N14
5	A	503	1N0	N4-C8-C9-C10
5	B	503	1N0	C11-C10-C9-C8
3	B	501	HEM	C4B-C3B-CAB-CBB
5	B	503	1N0	C9-C10-C11-C12
3	A	501	HEM	C4C-C3C-CAC-CBC
3	B	501	HEM	C4C-C3C-CAC-CBC
5	A	503	1N0	C12-C13-N14-C15
5	B	503	1N0	N4-C8-C9-C10
5	A	503	1N0	C12-C13-N14-C18
3	A	501	HEM	CAD-CBD-CGD-O2D

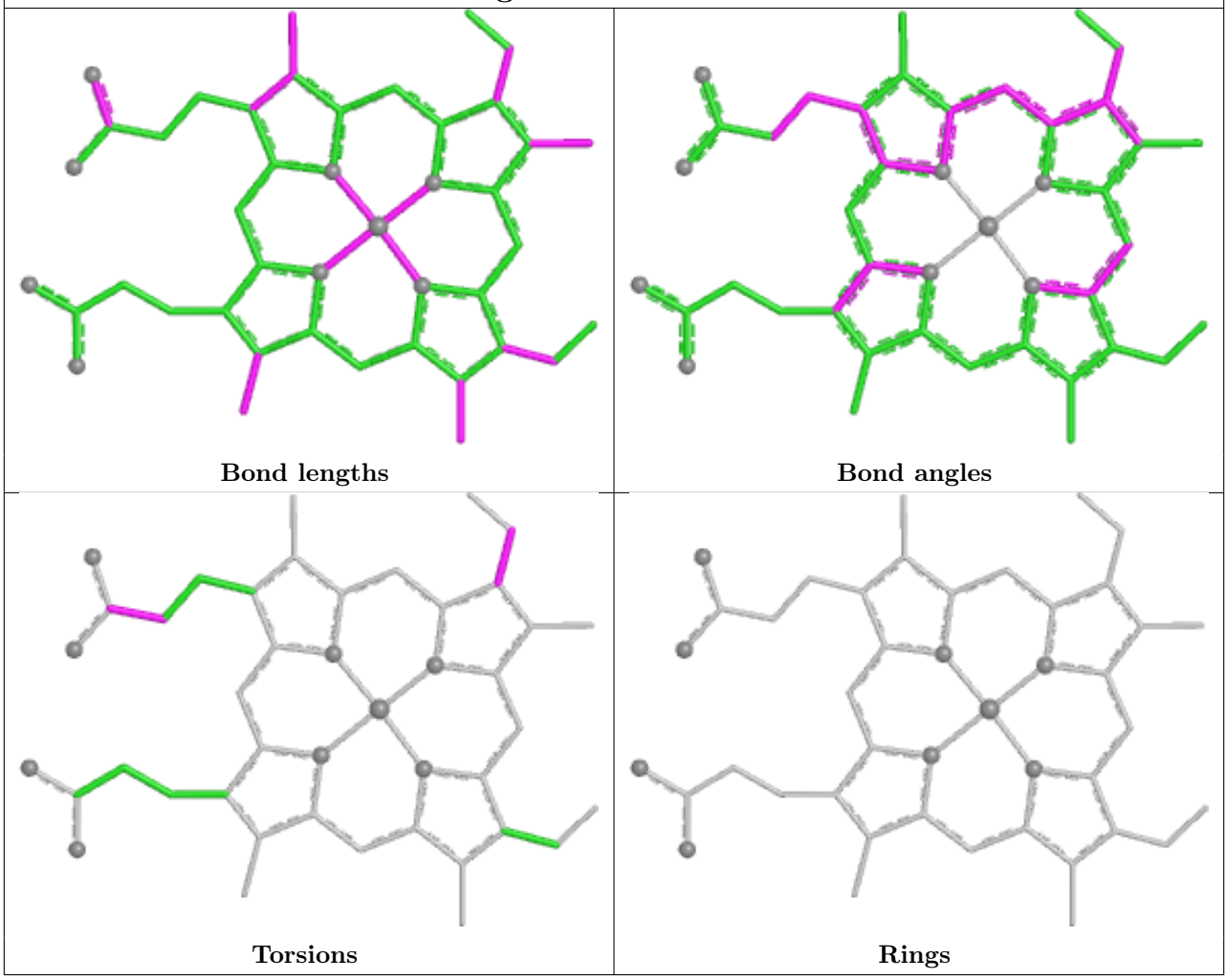
There are no ring outliers.

4 monomers are involved in 8 short contacts:

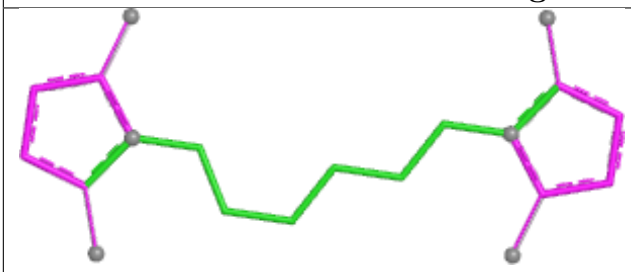
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	FES	1	0
3	A	501	HEM	2	0
6	D	201	FES	2	0
3	B	501	HEM	3	0

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

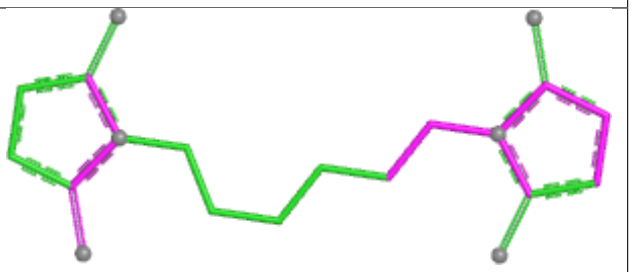
Ligand HEM A 501



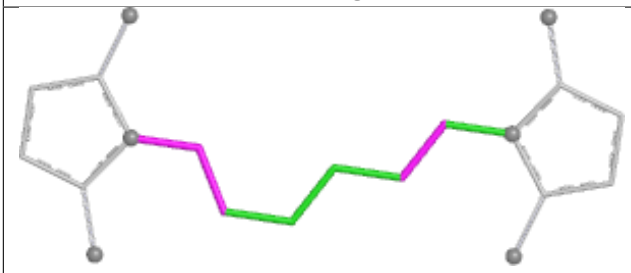
Ligand 1N0 A 503



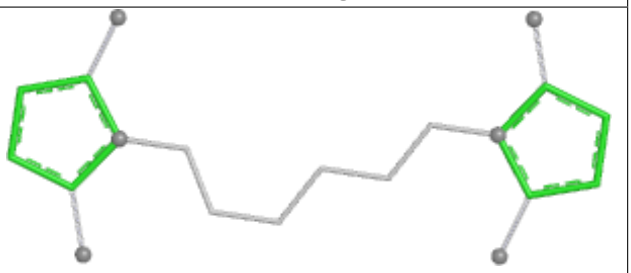
Bond lengths



Bond angles

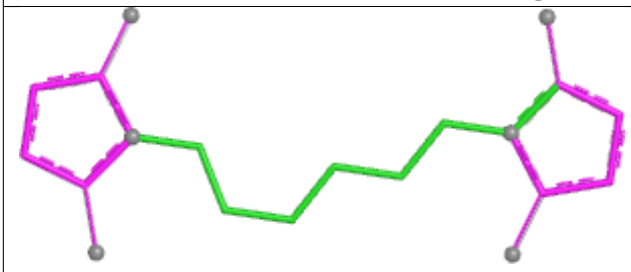


Torsions

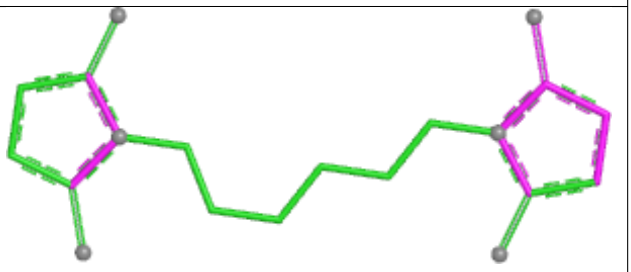


Rings

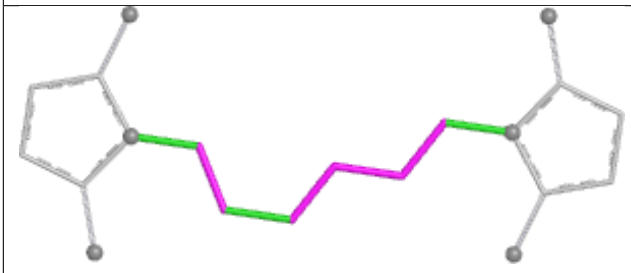
Ligand 1N0 B 503



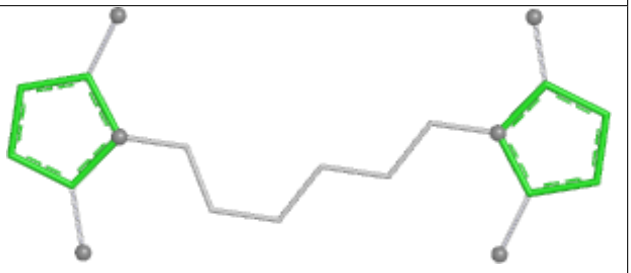
Bond lengths



Bond angles

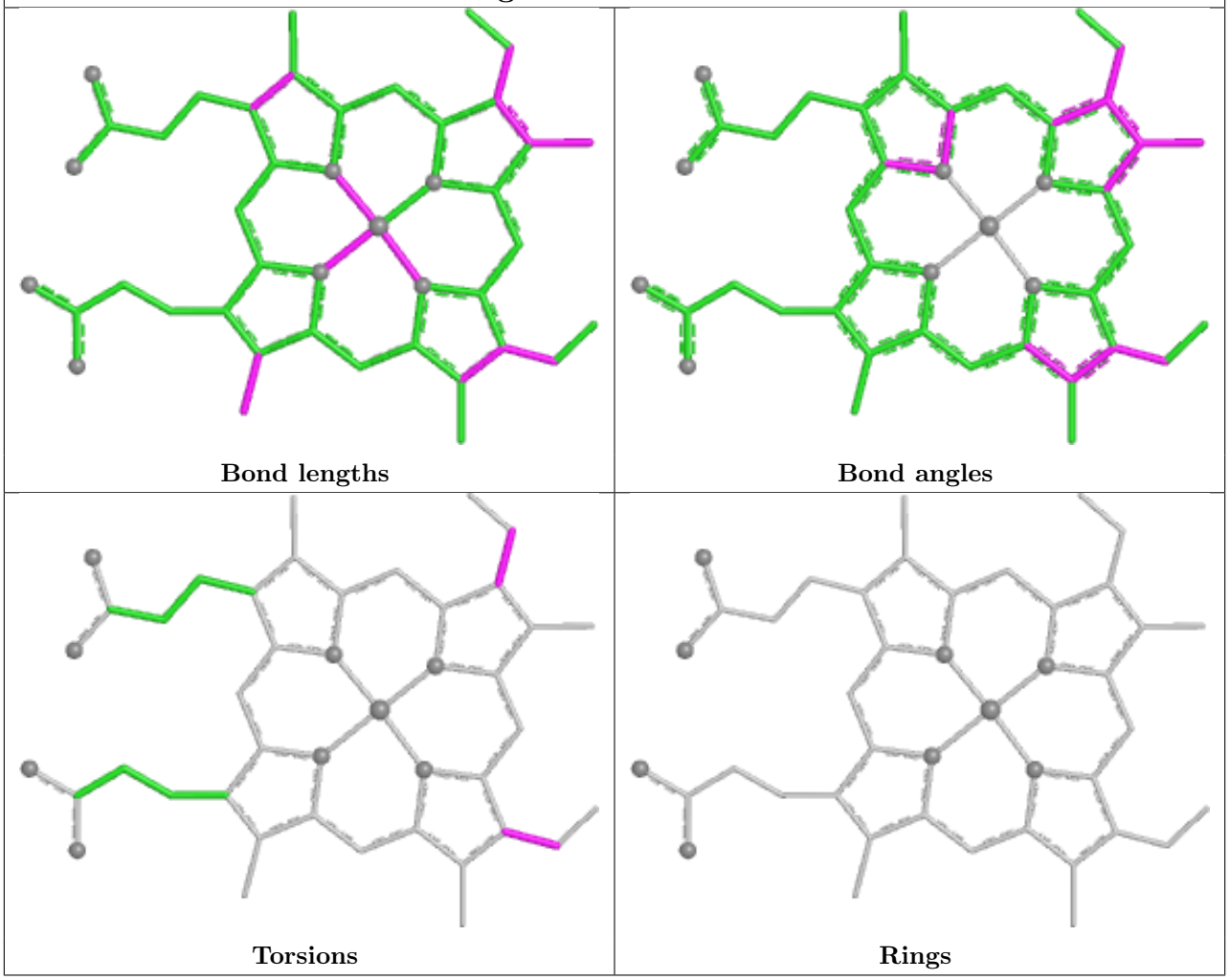


Torsions



Rings

Ligand HEM B 501



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	392/415 (94%)	0.18	14 (3%)	46	50	25, 51, 91, 117	0
1	B	395/415 (95%)	0.34	11 (2%)	55	59	37, 56, 88, 115	0
2	C	106/112 (94%)	0.23	2 (1%)	66	70	31, 57, 94, 107	0
2	D	106/112 (94%)	0.35	1 (0%)	81	83	41, 62, 88, 111	0
All	All	999/1054 (94%)	0.27	28 (2%)	55	59	25, 55, 91, 117	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	SER	5.1
1	B	187	PRO	4.5
1	B	414	VAL	3.6
1	A	165	LEU	3.5
1	A	186	ARG	3.5
1	B	91	GLU	3.5
1	A	414	VAL	3.2
1	A	102	SER	3.1
1	A	189	GLY	3.1
1	B	412	LYS	2.9
1	B	188	ASP	2.8
1	A	205	ILE	2.7
1	A	409	ALA	2.7
1	B	413	ALA	2.6
1	B	186	ARG	2.4
1	A	134	LEU	2.3
1	B	189	GLY	2.3
1	B	78	TYR	2.3
1	A	190	SER	2.2
1	A	413	ALA	2.2
1	B	185	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	94	LEU	2.1
1	A	249	GLY	2.1
2	C	31	GLY	2.1
1	A	166	LEU	2.1
1	A	191	MET	2.1
2	D	20	GLY	2.1
1	A	185	THR	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 oligosaccharides in this entry.

6.4 Ligands (i)

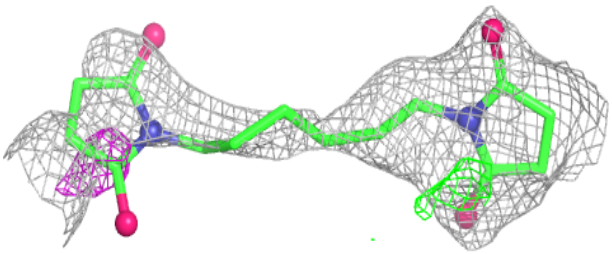
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

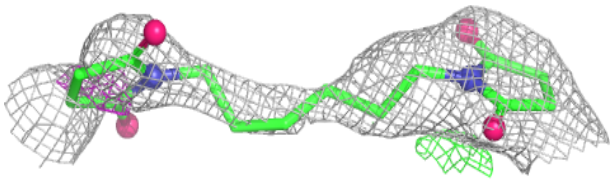
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1N0	B	503	20/20	0.84	0.15	58,89,118,118	0
5	1N0	A	503	20/20	0.89	0.13	42,77,110,112	0
4	CA	A	502	1/1	0.97	0.04	54,54,54,54	0
4	CA	B	502	1/1	0.98	0.07	54,54,54,54	0
3	HEM	B	501	43/43	0.98	0.08	22,34,51,63	0
3	HEM	A	501	43/43	0.98	0.07	21,30,46,71	0
6	FES	D	201	4/4	0.98	0.06	41,42,43,44	0
6	FES	C	201	4/4	0.99	0.02	32,32,33,34	0

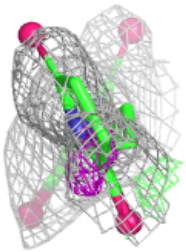
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1N0 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)

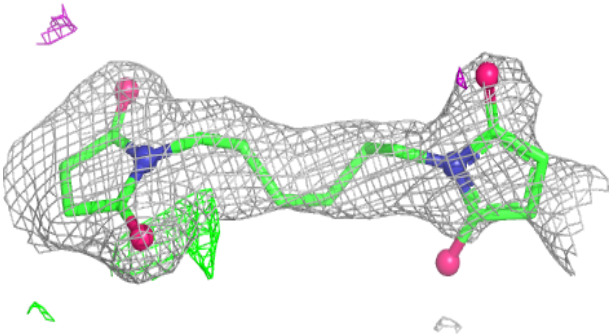


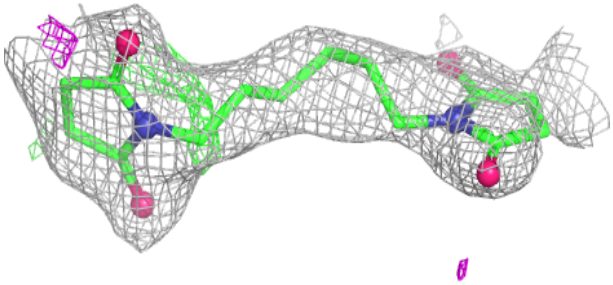


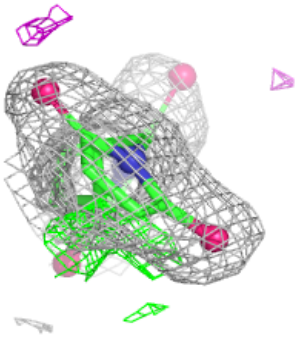


Electron density around 1N0 A 503:

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

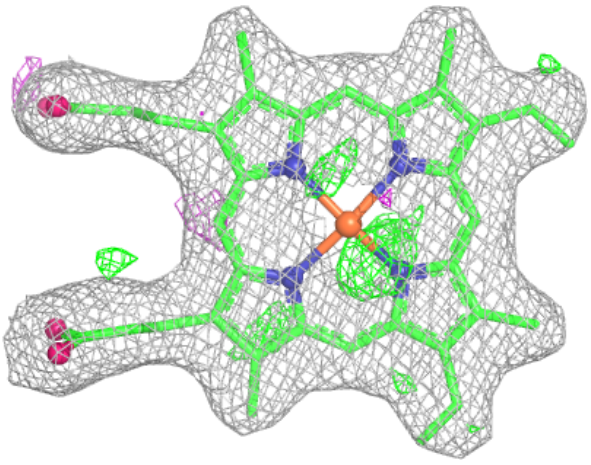


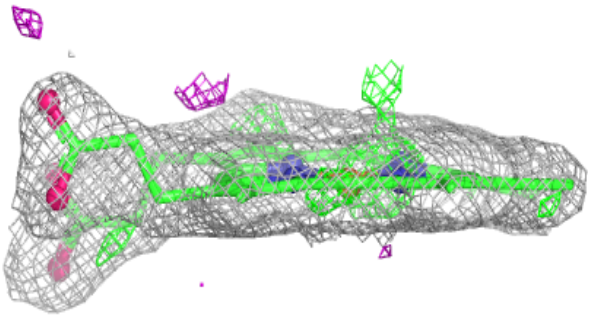




Electron density around HEM B 501:

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

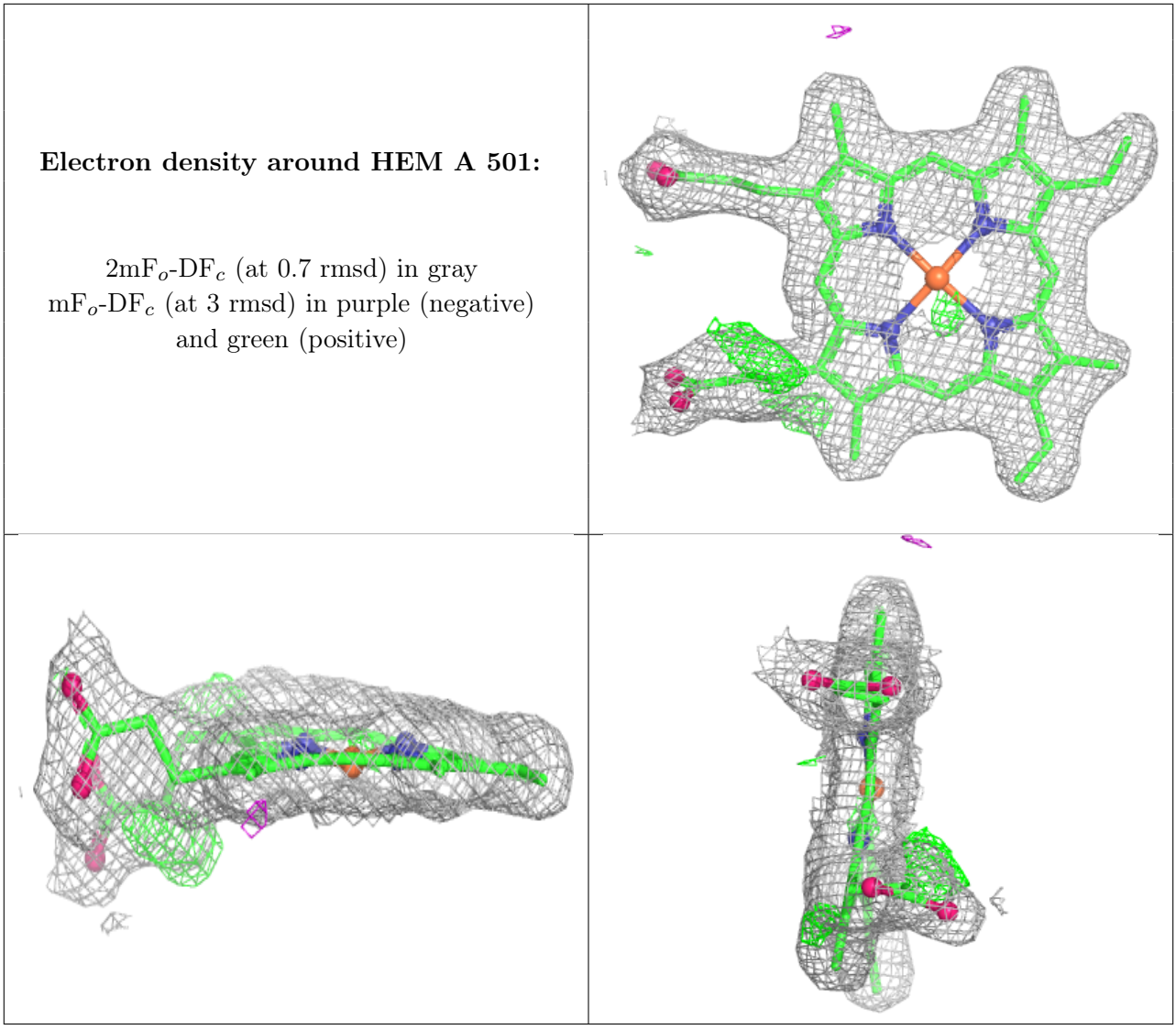






Electron density around HEM A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.