Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 10:30 PM EDT

PDB ID	:	4IRO / pdb_00004iro
Title	:	Crystal structure of T-state carbonmonoxy hemoglobin from Trematomus bernacchii at pH 8.4
Authors	:	Merlino, A.; Balsamo, A.; Mazzarella, L.; Vergara, A.
Deposited on	:	2013-01-15
Resolution	:	2.20 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:

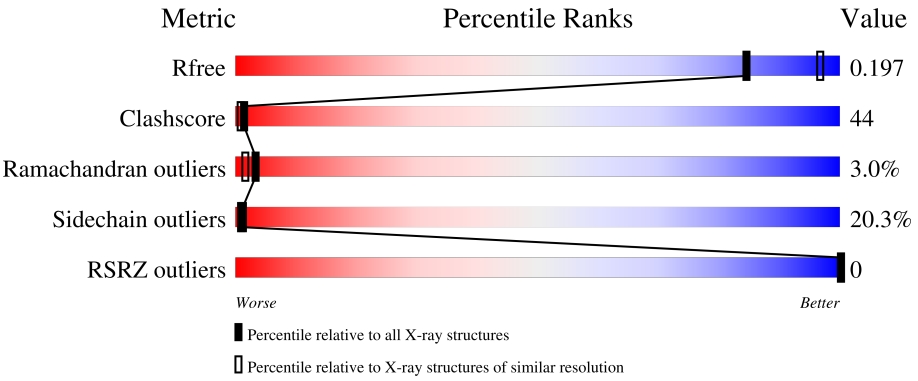
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	143	30% 52% 18%
1	C	143	32% 55% 13%
2	B	146	32% 56% 12%
2	D	146	27% 55% 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4695 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1104	710	190	199	5			
1	C	143	Total	C	N	O	S	0	0	0
			1104	710	190	199	5			

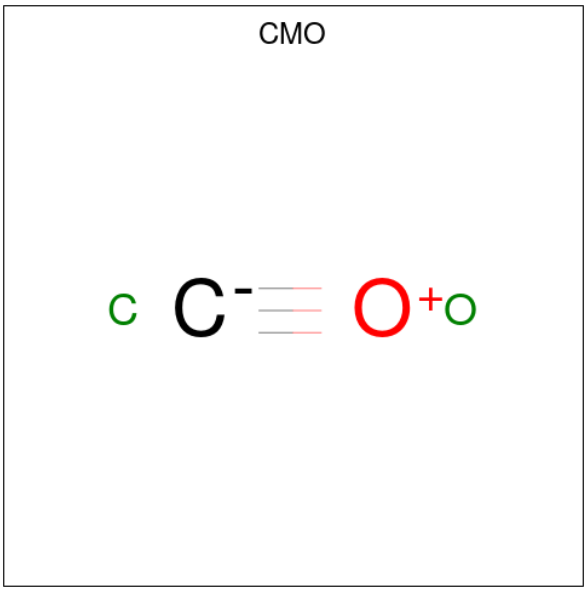
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P80043
C	0	ACE	-	acetylation	UNP P80043

- Molecule 2 is a protein called Hemoglobin subunit beta.

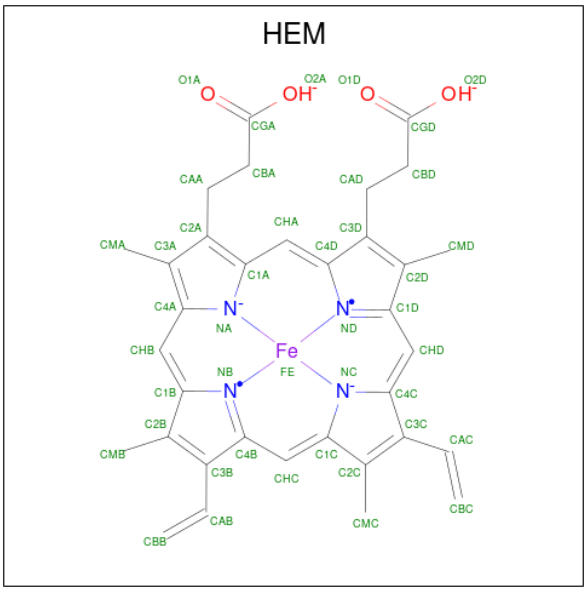
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	726	196	211	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	726	196	211	5			

- Molecule 3 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	6	Total	O	0	0
			6	6		
5	C	16	Total	O	0	0
			16	16		
5	D	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

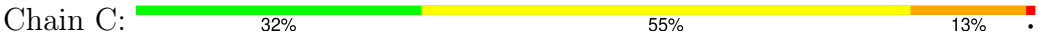
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

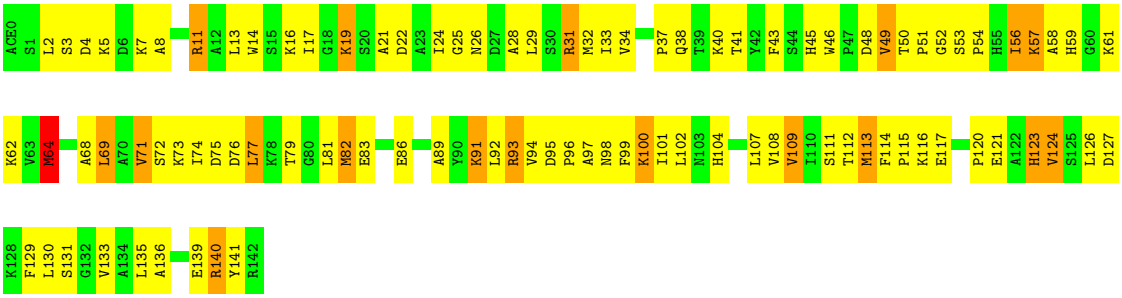
• Molecule 1: Hemoglobin subunit alpha

Chain A:

• Molecule 1: Hemoglobin subunit alpha

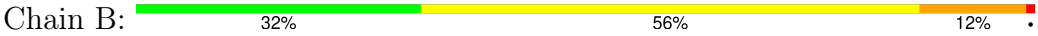
Chain C:

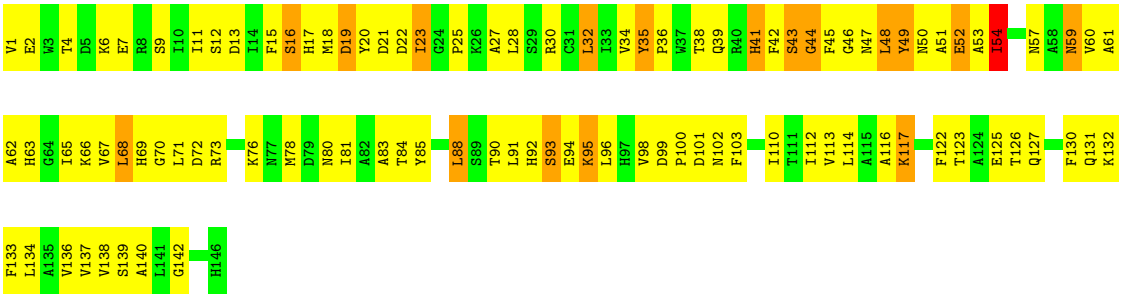




• Molecule 2: Hemoglobin subunit beta

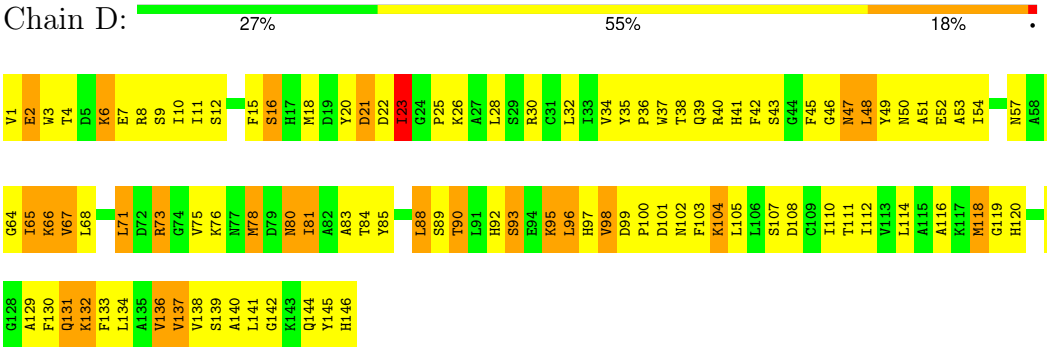
Chain B:





• Molecule 2: Hemoglobin subunit beta

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	61.54Å 104.80Å 61.62Å 90.00° 90.36° 90.00°	Depositor
Resolution (Å)	72.17 – 2.20 61.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (72.17-2.20) 77.5 (61.62-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.06Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.219 , (Not available) 0.197 , 0.197	Depositor DCC
R_{free} test set	1519 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 25.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.043 for l,k,-h 0.064 for h,-k,-l 0.288 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4695	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.06% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ACE, CMO

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	0.39	0/1127	1.41	14/1523 (0.9%)
1	C	0.37	0/1127	1.24	4/1523 (0.3%)
2	B	1.65	1/1164 (0.1%)	1.33	4/1576 (0.3%)
2	D	1.07	1/1164 (0.1%)	1.19	1/1576 (0.1%)
All	All	1.03	2/4582 (0.0%)	1.29	23/6198 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	SER	CA-CB	54.91	2.40	1.53
2	D	16	SER	CB-OG	34.67	2.11	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	16	SER	CA-CB-OG	-11.84	87.41	111.10
2	B	16	SER	N-CA-CB	-11.20	93.57	110.26
2	D	16	SER	CA-CB-OG	-7.94	95.22	111.10
1	C	64	MET	CA-C-N	6.96	127.82	120.03
1	C	64	MET	C-N-CA	6.96	127.82	120.03
1	A	10	VAL	CA-C-N	-5.97	111.41	122.09
1	A	10	VAL	C-N-CA	-5.97	111.41	122.09
1	A	22	ASP	O-C-N	5.72	127.98	122.03
1	A	107	LEU	CA-C-N	-5.64	117.19	122.66
1	A	107	LEU	C-N-CA	-5.64	117.19	122.66
2	B	19	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	112	THR	O-C-N	5.51	128.05	122.09
1	A	124	VAL	CA-C-N	5.34	129.54	120.88
1	A	124	VAL	C-N-CA	5.34	129.54	120.88
1	A	123	HIS	CA-CB-CG	5.33	119.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	35	TYR	O-C-N	5.17	125.94	121.34
1	C	109	VAL	CB-CA-C	-5.15	105.11	111.70
1	A	75	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	123	HIS	CA-CB-CG	5.11	118.91	113.80
1	A	113	MET	CA-C-N	-5.09	117.19	122.89
1	A	113	MET	C-N-CA	-5.09	117.19	122.89
1	A	22	ASP	CA-C-N	5.01	131.10	121.54
1	A	22	ASP	C-N-CA	5.01	131.10	121.54

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	1104	0	1136	101	0
1	C	1104	0	1136	90	0
2	B	1138	0	1119	119	0
2	D	1138	0	1119	120	0
3	A	2	0	0	1	0
4	A	43	0	30	4	0
4	B	43	0	30	9	0
4	C	43	0	30	7	0
4	D	43	0	30	12	0
5	A	12	0	0	0	0
5	B	6	0	0	0	0
5	C	16	0	0	0	0
5	D	3	0	0	0	0
All	All	4695	0	4630	413	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 44.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:GLY:O	2:D:48:LEU:HD23	1.56	1.04
2:B:16:SER:CB	2:B:16:SER:CA	2.40	0.99
1:A:58:ALA:HA	1:A:61:LYS:HD2	1.44	0.98
2:D:16:SER:CB	2:D:16:SER:OG	2.11	0.98
2:B:18:MET:HE2	2:B:114:LEU:HD13	1.50	0.94
2:B:92:HIS:HA	2:B:96:LEU:HB2	1.50	0.91
2:D:21:ASP:HA	2:D:65:ILE:HD11	1.53	0.91
1:C:33:ILE:HD11	1:C:51:PRO:HA	1.56	0.87
1:C:62:LYS:HD3	4:C:600:HEM:HBA1	1.55	0.87
2:B:25:PRO:HD3	2:B:65:ILE:HG13	1.58	0.86
2:D:57:ASN:HD21	2:D:59:ASN:HD22	1.23	0.85
2:D:81:ILE:HD13	2:D:136:VAL:HG11	1.61	0.83
2:B:23:ILE:HD11	2:B:117:LYS:HD2	1.64	0.79
1:A:105:CYS:O	1:A:109:VAL:HG23	1.83	0.79
1:C:54:PRO:HA	1:C:57:LYS:HD2	1.64	0.78
2:B:4:THR:OG1	2:B:7:GLU:HG3	1.84	0.78
2:D:32:LEU:HD21	2:D:42:PHE:HD2	1.48	0.77
1:A:48:ASP:HB3	1:A:53:SER:OG	1.85	0.77
1:C:7:LYS:O	1:C:11:ARG:HG3	1.83	0.77
1:C:91:LYS:HG3	1:C:92:LEU:HG	1.67	0.77
1:C:31:ARG:HG2	2:D:127:GLN:OE1	1.84	0.77
1:C:108:VAL:O	1:C:112:THR:HG23	1.85	0.76
2:D:22:ASP:O	2:D:25:PRO:HD2	1.84	0.76
2:D:89:SER:HB2	2:D:141:LEU:HA	1.66	0.76
1:A:67:ILE:O	1:A:71:VAL:HG23	1.84	0.75
2:B:47:ASN:O	2:B:53:ALA:HB1	1.87	0.75
2:D:133:PHE:O	2:D:137:VAL:HG23	1.87	0.75
1:A:54:PRO:HA	1:A:57:LYS:HG2	1.68	0.74
1:A:58:ALA:O	1:A:61:LYS:HB2	1.87	0.74
1:C:86:GLU:OE1	1:C:140:ARG:HD2	1.88	0.74
2:B:7:GLU:O	2:B:11:ILE:HG13	1.87	0.74
2:B:94:GLU:HB2	2:B:95:LYS:HZ3	1.54	0.73
1:A:26:ASN:ND2	1:A:56:ILE:HG22	2.04	0.73
2:D:92:HIS:HA	2:D:96:LEU:HD12	1.70	0.72
2:B:19:ASP:H	2:B:117:LYS:HZ1	1.36	0.72
2:B:63:HIS:HA	2:B:66:LYS:HB2	1.69	0.72
1:C:37:PRO:O	1:C:40:LYS:HG3	1.89	0.71
1:A:116:LYS:H	1:A:116:LYS:HZ2	1.39	0.71
2:B:130:PHE:O	2:B:134:LEU:HD23	1.90	0.70
2:B:11:ILE:HD12	2:B:78:MET:HE1	1.74	0.69
1:C:58:ALA:O	1:C:61:LYS:HB2	1.92	0.69
2:D:101:ASP:O	2:D:104:LYS:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LEU:O	2:B:36:PRO:HA	1.92	0.69
1:A:87:GLN:NE2	1:A:92:LEU:HD11	2.07	0.69
2:D:66:LYS:HZ1	4:D:800:HEM:HBD2	1.56	0.69
1:A:86:GLU:O	1:A:90:TYR:HB2	1.93	0.68
2:D:4:THR:OG1	2:D:7:GLU:HG3	1.92	0.68
1:A:3:SER:O	1:A:7:LYS:HG3	1.94	0.67
2:D:107:SER:HA	2:D:110:ILE:HD12	1.76	0.67
1:A:57:LYS:HE3	1:A:61:LYS:HZ2	1.60	0.66
1:A:43:PHE:O	1:A:46:TRP:HB2	1.96	0.66
1:A:124:VAL:O	1:A:128:LYS:HG3	1.96	0.66
1:A:32:MET:HG2	1:A:101:ILE:HG22	1.78	0.65
1:C:82:MET:SD	1:C:139:GLU:HG2	2.35	0.65
2:D:98:VAL:O	2:D:100:PRO:HD3	1.96	0.65
2:B:91:LEU:HA	2:B:95:LYS:HE3	1.79	0.65
2:B:99:ASP:O	2:B:102:ASN:HB2	1.96	0.65
1:A:93:ARG:HD2	2:D:40:ARG:HB2	1.78	0.65
2:B:36:PRO:O	2:B:39:GLN:HG3	1.95	0.65
2:D:36:PRO:HA	2:D:39:GLN:HE21	1.62	0.64
1:A:129:PHE:O	1:A:133:VAL:HG23	1.96	0.64
2:B:25:PRO:HG3	2:B:61:ALA:HA	1.79	0.64
2:B:81:ILE:O	2:B:84:THR:HB	1.97	0.64
2:B:21:ASP:HA	2:B:65:ILE:HG12	1.79	0.64
2:B:11:ILE:HD13	2:B:133:PHE:HB2	1.78	0.63
2:B:45:PHE:CZ	2:B:59:ASN:HB3	2.33	0.63
1:C:68:ALA:O	1:C:71:VAL:HB	1.98	0.63
2:B:94:GLU:HB2	2:B:95:LYS:NZ	2.14	0.62
2:B:63:HIS:O	2:B:67:VAL:HG23	1.99	0.62
1:A:90:TYR:CE2	1:A:140:ARG:HB3	2.34	0.62
2:B:63:HIS:HA	2:B:66:LYS:HE2	1.81	0.62
2:D:127:GLN:O	2:D:131:GLN:HB2	2.00	0.62
2:B:134:LEU:O	2:B:138:VAL:HG23	2.00	0.62
1:C:19:LYS:O	1:C:19:LYS:HD3	2.00	0.62
1:C:123:HIS:ND1	2:D:30:ARG:HD3	2.13	0.62
2:B:100:PRO:HA	2:B:103:PHE:CE2	2.34	0.62
1:C:54:PRO:O	1:C:57:LYS:HB2	2.00	0.62
2:B:35:TYR:O	2:B:38:THR:HG23	2.00	0.62
1:A:111:SER:OG	2:B:116:ALA:HB2	1.99	0.62
1:C:22:ASP:OD2	1:C:61:LYS:HG2	1.99	0.61
1:A:54:PRO:O	1:A:57:LYS:HG2	1.99	0.61
2:B:80:ASN:OD1	2:B:83:ALA:HB3	2.01	0.61
2:B:47:ASN:O	2:B:48:LEU:HD23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:OG	1:A:73:LYS:HE2	2.01	0.60
1:A:20:SER:O	1:A:24:ILE:HG13	2.01	0.60
1:A:48:ASP:HB3	1:A:53:SER:HG	1.66	0.60
1:C:14:TRP:HA	1:C:17:ILE:HG13	1.81	0.60
1:A:20:SER:O	1:A:23:ALA:HB3	2.01	0.60
2:B:92:HIS:HD2	2:B:98:VAL:HG21	1.66	0.60
2:D:137:VAL:O	2:D:140:ALA:HB3	2.00	0.60
2:D:90:THR:OG1	2:D:144:GLN:HG3	2.01	0.60
2:D:95:LYS:HE3	2:D:96:LEU:HD23	1.83	0.60
2:D:32:LEU:HD22	2:D:39:GLN:HG2	1.83	0.60
1:C:120:PRO:O	1:C:123:HIS:HB3	2.01	0.60
1:A:96:PRO:HG3	1:A:141:TYR:CE2	2.37	0.59
1:C:43:PHE:O	1:C:46:TRP:HB2	2.01	0.59
1:A:33:ILE:HG13	1:A:34:VAL:N	2.18	0.59
1:C:26:ASN:ND2	1:C:57:LYS:HA	2.17	0.59
1:C:82:MET:HE3	1:C:140:ARG:NH2	2.17	0.59
2:B:51:ALA:O	2:B:54:ILE:HB	2.01	0.59
2:B:41:HIS:CE1	2:B:98:VAL:HA	2.37	0.59
1:C:129:PHE:O	1:C:133:VAL:HG23	2.02	0.59
1:A:25:GLY:O	1:A:29:LEU:HB2	2.03	0.58
1:A:59:HIS:HE2	3:A:201:CMO:C	2.16	0.58
2:B:19:ASP:H	2:B:117:LYS:NZ	2.01	0.58
1:A:31:ARG:O	1:A:35:VAL:HG23	2.03	0.58
1:A:32:MET:O	1:A:36:TYR:HB2	2.03	0.58
2:B:71:LEU:HA	2:B:85:TYR:OH	2.04	0.58
2:B:67:VAL:HG13	4:B:400:HEM:HBB2	1.85	0.58
2:B:103:PHE:CB	2:B:138:VAL:HG13	2.34	0.58
2:D:15:PHE:CD2	2:D:75:VAL:HG21	2.38	0.58
2:B:44:GLY:O	2:B:45:PHE:HD1	1.87	0.57
2:D:39:GLN:OE1	2:D:48:LEU:HD12	2.04	0.57
2:D:100:PRO:HG3	2:D:145:TYR:CZ	2.39	0.57
2:D:35:TYR:CE1	2:D:105:LEU:HD22	2.39	0.57
1:A:95:ASP:HB3	1:A:98:ASN:ND2	2.20	0.57
2:B:28:LEU:HD23	2:B:60:VAL:O	2.05	0.57
2:B:102:ASN:HB3	4:B:400:HEM:HMC1	1.87	0.57
1:C:54:PRO:HA	1:C:57:LYS:CD	2.33	0.56
1:A:88:HIS:CE1	4:A:202:HEM:NA	2.73	0.56
1:A:26:ASN:HD21	1:A:56:ILE:HG22	1.67	0.56
1:C:24:ILE:CG2	1:C:64:MET:HE2	2.35	0.56
1:C:54:PRO:HA	1:C:57:LYS:HB2	1.86	0.56
1:A:27:ASP:HA	1:A:30:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:GLY:O	2:B:73:ARG:HG2	2.05	0.56
1:C:114:PHE:HB3	1:C:117:GLU:OE1	2.05	0.56
2:D:66:LYS:NZ	4:D:800:HEM:HBD2	2.21	0.56
1:C:76:ASP:OD2	1:C:79:THR:HB	2.06	0.56
1:C:52:GLY:O	1:C:57:LYS:HE2	2.06	0.55
1:A:82:MET:HE3	1:A:139:GLU:HG2	1.88	0.55
2:D:99:ASP:O	2:D:102:ASN:HB2	2.06	0.55
1:A:37:PRO:O	1:A:40:LYS:HB2	2.07	0.55
2:D:41:HIS:HD2	4:D:800:HEM:HBC1	1.72	0.55
2:D:32:LEU:HD21	2:D:42:PHE:CD2	2.35	0.55
1:A:65:GLY:O	1:A:68:ALA:HB3	2.07	0.55
2:B:41:HIS:CG	4:B:400:HEM:HAC	2.41	0.55
1:A:33:ILE:O	1:A:37:PRO:HA	2.07	0.55
2:B:132:LYS:O	2:B:136:VAL:HG23	2.07	0.55
4:B:400:HEM:HBD2	4:B:400:HEM:O1A	2.07	0.55
2:D:22:ASP:OD1	2:D:26:LYS:HE3	2.06	0.55
2:D:80:ASN:HD22	2:D:83:ALA:HB3	1.71	0.54
1:A:93:ARG:HD3	2:D:37:TRP:HA	1.89	0.54
1:A:114:PHE:HD1	1:A:117:GLU:OE2	1.90	0.54
1:C:24:ILE:HG21	1:C:64:MET:HE2	1.90	0.54
1:C:69:LEU:O	1:C:73:LYS:HG2	2.06	0.54
1:C:89:ALA:HA	1:C:141:TYR:HE1	1.73	0.54
2:B:95:LYS:HE2	2:B:95:LYS:N	2.22	0.54
1:A:47:PRO:HB2	1:A:55:HIS:NE2	2.23	0.53
2:D:40:ARG:O	2:D:40:ARG:HG2	2.09	0.53
2:B:45:PHE:CE1	2:B:59:ASN:HB3	2.44	0.53
2:B:48:LEU:HD22	2:B:54:ILE:HA	1.88	0.53
2:D:100:PRO:HG3	2:D:145:TYR:CE1	2.43	0.53
1:C:62:LYS:CD	4:C:600:HEM:HBA1	2.35	0.53
1:A:123:HIS:CE1	2:B:112:ILE:HD13	2.44	0.53
2:B:49:TYR:HD1	2:B:50:ASN:H	1.55	0.53
1:A:85:SER:OG	1:A:140:ARG:HG2	2.09	0.52
2:B:67:VAL:O	2:B:71:LEU:HD12	2.08	0.52
2:D:21:ASP:O	2:D:25:PRO:HG2	2.10	0.52
1:A:20:SER:OG	1:A:114:PHE:HZ	1.93	0.52
2:B:100:PRO:HA	2:B:103:PHE:CD2	2.44	0.52
1:C:22:ASP:CG	1:C:61:LYS:HG2	2.34	0.52
2:B:103:PHE:HB3	2:B:138:VAL:HG13	1.92	0.52
1:C:91:LYS:CG	1:C:92:LEU:HG	2.38	0.52
2:D:45:PHE:HB3	2:D:57:ASN:OD1	2.10	0.52
1:A:3:SER:HG	1:A:6:ASP:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LYS:O	1:C:8:ALA:HB3	2.10	0.52
1:A:13:LEU:HD23	1:A:126:LEU:HD13	1.92	0.52
1:A:31:ARG:HD3	2:B:127:GLN:OE1	2.10	0.52
2:D:2:GLU:OE1	2:D:2:GLU:HA	2.07	0.52
1:A:112:THR:O	1:A:115:PRO:HD3	2.10	0.52
1:C:14:TRP:HA	1:C:17:ILE:CG1	2.40	0.52
2:D:92:HIS:CE1	4:D:800:HEM:NA	2.78	0.52
1:C:7:LYS:NZ	1:C:75:ASP:HA	2.25	0.51
1:A:116:LYS:H	1:A:116:LYS:NZ	2.06	0.51
2:B:20:TYR:HE2	2:B:69:HIS:HA	1.75	0.51
2:B:73:ARG:HD2	2:B:85:TYR:CE1	2.45	0.51
1:C:91:LYS:HE3	1:C:92:LEU:HG	1.92	0.51
1:C:34:VAL:HG11	2:D:124:ALA:HB1	1.92	0.51
2:D:104:LYS:O	2:D:108:ASP:OD2	2.29	0.51
1:A:72:SER:O	1:A:73:LYS:HD3	2.11	0.51
1:A:93:ARG:HD3	2:D:37:TRP:O	2.11	0.51
2:B:68:LEU:HA	2:B:71:LEU:HD12	1.92	0.51
2:B:123:THR:HG1	2:B:126:THR:HG1	1.47	0.51
2:B:71:LEU:HA	2:B:85:TYR:HH	1.74	0.51
1:C:26:ASN:HD22	1:C:57:LYS:HA	1.74	0.51
2:D:64:GLY:O	2:D:67:VAL:HB	2.11	0.51
2:B:92:HIS:CA	2:B:96:LEU:HB2	2.34	0.51
1:C:98:ASN:HA	1:C:101:ILE:HD12	1.93	0.51
2:D:23:ILE:O	2:D:26:LYS:HB2	2.11	0.50
4:D:800:HEM:O2D	4:D:800:HEM:O2A	2.29	0.50
2:B:42:PHE:O	2:B:43:SER:O	2.30	0.50
1:C:54:PRO:HA	1:C:57:LYS:CG	2.42	0.50
1:C:92:LEU:HD22	4:C:600:HEM:HMD1	1.93	0.50
2:D:22:ASP:O	2:D:26:LYS:HG3	2.12	0.50
1:A:10:VAL:HG11	1:A:129:PHE:CD2	2.46	0.50
2:B:25:PRO:HG3	2:B:61:ALA:CA	2.42	0.50
2:D:30:ARG:O	2:D:34:VAL:HG23	2.12	0.50
1:A:90:TYR:HE2	1:A:140:ARG:HB3	1.75	0.50
1:A:123:HIS:ND1	2:B:30:ARG:HD3	2.26	0.50
1:C:112:THR:HB	2:D:119:GLY:O	2.12	0.50
2:D:96:LEU:HD13	4:D:800:HEM:C2D	2.47	0.50
2:B:139:SER:O	2:B:142:GLY:O	2.29	0.49
2:D:45:PHE:HB3	2:D:59:ASN:HB2	1.93	0.49
2:B:103:PHE:HB2	2:B:138:VAL:HG13	1.94	0.49
2:B:133:PHE:O	2:B:137:VAL:HG23	2.12	0.49
1:C:38:GLN:O	1:C:41:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:VAL:O	2:D:1:VAL:HG13	2.12	0.49
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.76	0.49
1:C:113:MET:HB3	1:C:114:PHE:CD2	2.47	0.49
2:D:28:LEU:HD11	2:D:42:PHE:CE2	2.48	0.49
2:B:63:HIS:CD2	2:B:66:LYS:HE2	2.47	0.49
1:C:96:PRO:HG3	1:C:141:TYR:CE2	2.48	0.49
2:D:81:ILE:HG23	2:D:85:TYR:CD2	2.48	0.49
2:B:23:ILE:HD11	2:B:117:LYS:CD	2.39	0.49
2:B:32:LEU:HB3	2:B:54:ILE:HD12	1.94	0.49
2:D:20:TYR:O	2:D:65:ILE:HG13	2.13	0.49
1:A:142:ARG:HD2	1:C:124:VAL:HG23	1.94	0.49
2:D:15:PHE:CG	2:D:75:VAL:HG21	2.48	0.49
2:B:12:SER:O	2:B:16:SER:HB3	2.13	0.48
2:D:38:THR:HG22	2:D:102:ASN:CG	2.38	0.48
2:D:81:ILE:O	2:D:85:TYR:HD2	1.95	0.48
1:C:49:VAL:O	1:C:49:VAL:HG12	2.12	0.48
2:D:63:HIS:CE1	2:D:67:VAL:HG23	2.49	0.48
1:C:135:LEU:O	1:C:135:LEU:HD12	2.12	0.48
2:D:50:ASN:CG	2:D:53:ALA:H	2.22	0.48
2:B:19:ASP:N	2:B:117:LYS:HZ1	2.09	0.48
1:C:121:GLU:OE2	2:D:51:ALA:HB1	2.14	0.48
2:D:37:TRP:HE1	2:D:105:LEU:HD11	1.79	0.48
1:A:49:VAL:HG13	1:A:49:VAL:O	2.13	0.47
1:C:2:LEU:HD21	1:C:129:PHE:HA	1.96	0.47
1:A:54:PRO:CA	1:A:57:LYS:HG2	2.40	0.47
1:C:28:ALA:HB2	1:C:109:VAL:HG21	1.96	0.47
1:C:107:LEU:O	1:C:111:SER:HB2	2.14	0.47
1:A:90:TYR:CD2	1:A:140:ARG:HB3	2.50	0.47
2:D:28:LEU:HD23	2:D:60:VAL:O	2.14	0.47
1:A:21:ALA:HB1	1:A:64:MET:HB3	1.96	0.47
2:B:63:HIS:CA	2:B:66:LYS:HB2	2.42	0.47
2:D:50:ASN:O	2:D:54:ILE:HD12	2.15	0.47
2:B:66:LYS:NZ	4:B:400:HEM:HBD2	2.28	0.47
1:C:7:LYS:HZ3	1:C:75:ASP:HA	1.79	0.47
1:A:63:VAL:HG11	1:A:102:LEU:HD21	1.95	0.47
2:D:9:SER:O	2:D:12:SER:HB3	2.15	0.47
2:D:73:ARG:HH12	2:D:88:LEU:HD22	1.79	0.47
2:D:114:LEU:HD22	2:D:130:PHE:CZ	2.50	0.47
4:B:400:HEM:O1A	4:B:400:HEM:HHA	2.15	0.46
2:B:88:LEU:HD11	4:B:400:HEM:CMA	2.45	0.46
1:A:19:LYS:HD2	1:A:19:LYS:HA	1.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HB2	1:A:40:LYS:HZ3	1.80	0.46
2:D:35:TYR:CD1	2:D:105:LEU:HD22	2.49	0.46
2:D:50:ASN:ND2	2:D:53:ALA:HB2	2.30	0.46
1:A:29:LEU:HD11	1:A:59:HIS:HD2	1.81	0.46
2:B:13:ASP:O	2:B:16:SER:OG	2.30	0.46
1:A:103:ASN:ND2	1:A:130:LEU:HB3	2.30	0.46
2:B:63:HIS:HA	2:B:66:LYS:HD3	1.98	0.46
2:B:69:HIS:O	2:B:72:ASP:HB2	2.16	0.46
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.78	0.46
2:B:70:GLY:HA2	2:B:73:ARG:CZ	2.46	0.46
2:D:35:TYR:HB3	2:D:105:LEU:HD13	1.98	0.46
1:A:59:HIS:CE1	4:A:202:HEM:HBD2	2.51	0.46
1:C:98:ASN:HD22	1:C:98:ASN:H	1.64	0.46
2:B:101:ASP:OD2	1:C:95:ASP:OD2	2.34	0.46
1:C:53:SER:O	1:C:56:ILE:HB	2.16	0.46
1:C:107:LEU:CD2	1:C:126:LEU:HD23	2.46	0.46
2:D:38:THR:HG22	2:D:102:ASN:ND2	2.31	0.45
2:B:23:ILE:HG13	2:B:117:LYS:NZ	2.31	0.45
2:D:3:TRP:HZ3	2:D:132:LYS:HD3	1.82	0.45
2:B:139:SER:OG	2:B:140:ALA:N	2.50	0.45
2:D:71:LEU:HD23	4:D:800:HEM:HMB3	1.98	0.45
2:D:93:SER:HB2	2:D:145:TYR:CE2	2.51	0.45
2:B:80:ASN:O	2:B:84:THR:OG1	2.30	0.45
1:C:45:HIS:NE2	4:C:600:HEM:O2D	2.50	0.45
2:D:53:ALA:O	2:D:57:ASN:N	2.50	0.45
2:B:57:ASN:OD1	2:B:59:ASN:N	2.50	0.45
2:B:90:THR:O	2:B:95:LYS:NZ	2.50	0.45
1:C:13:LEU:O	1:C:17:ILE:HG12	2.17	0.45
2:D:11:ILE:O	2:D:15:PHE:HD1	1.99	0.45
1:A:29:LEU:HD11	1:A:59:HIS:CD2	2.52	0.45
2:D:23:ILE:O	2:D:26:LYS:N	2.50	0.45
2:D:50:ASN:OD1	2:D:52:GLU:N	2.50	0.45
2:D:80:ASN:O	2:D:84:THR:OG1	2.29	0.45
1:A:35:VAL:HG11	2:B:131:GLN:NE2	2.32	0.45
2:B:11:ILE:CD1	2:B:133:PHE:HB2	2.44	0.45
2:B:63:HIS:HA	2:B:66:LYS:CD	2.46	0.45
1:C:77:LEU:HB3	1:C:81:LEU:CD1	2.47	0.45
2:D:32:LEU:O	2:D:39:GLN:NE2	2.50	0.45
2:D:93:SER:O	2:D:97:HIS:HA	2.17	0.45
2:B:16:SER:OG	2:B:17:HIS:N	2.50	0.45
1:A:131:SER:O	1:A:134:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:OD2	1:A:31:ARG:NE	2.49	0.44
1:A:65:GLY:O	1:A:68:ALA:N	2.50	0.44
1:A:88:HIS:HA	1:A:92:LEU:HD12	1.98	0.44
1:C:34:VAL:HG11	2:D:124:ALA:CB	2.47	0.44
2:D:3:TRP:CZ3	2:D:132:LYS:HD3	2.51	0.44
2:B:41:HIS:NE2	2:B:102:ASN:OD1	2.50	0.44
1:C:82:MET:HE3	1:C:140:ARG:HH21	1.83	0.44
2:D:118:MET:HE3	2:D:118:MET:HB3	1.75	0.44
1:A:57:LYS:HG3	1:A:58:ALA:N	2.32	0.44
1:A:101:ILE:O	1:A:104:HIS:HB3	2.17	0.44
2:B:13:ASP:OD1	2:B:17:HIS:NE2	2.50	0.44
2:B:41:HIS:O	4:B:400:HEM:HMD3	2.17	0.44
1:C:91:LYS:HG3	1:C:92:LEU:N	2.31	0.44
1:A:86:GLU:OE1	1:A:140:ARG:NE	2.50	0.44
1:A:99:PHE:HD1	4:A:202:HEM:HHC	1.82	0.44
2:B:20:TYR:HD2	2:B:69:HIS:CE1	2.35	0.44
2:B:20:TYR:CE2	2:B:69:HIS:HA	2.52	0.44
2:D:136:VAL:HG12	2:D:137:VAL:N	2.32	0.44
1:A:124:VAL:HB	2:B:34:VAL:HA	2.00	0.44
1:A:117:GLU:OE1	1:A:117:GLU:N	2.49	0.44
2:D:6:LYS:HE3	2:D:125:GLU:OE2	2.17	0.44
2:D:18:MET:HE2	2:D:114:LEU:HD13	1.99	0.44
1:A:32:MET:CG	1:A:101:ILE:HG22	2.46	0.44
2:B:41:HIS:CD2	2:B:41:HIS:H	2.34	0.44
1:C:13:LEU:O	1:C:16:LYS:HB2	2.17	0.44
1:C:62:LYS:NZ	4:C:600:HEM:O2A	2.50	0.44
1:C:115:PRO:HB3	2:D:116:ALA:HB1	1.99	0.44
1:A:10:VAL:O	1:A:10:VAL:HG12	2.18	0.43
1:A:121:GLU:OE2	2:B:52:GLU:OE2	2.36	0.43
2:B:73:ARG:HG3	2:B:84:THR:CG2	2.47	0.43
2:D:45:PHE:CD2	2:D:59:ASN:HB3	2.53	0.43
2:D:73:ARG:NH1	2:D:88:LEU:HD22	2.34	0.43
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.81	0.43
1:A:13:LEU:O	1:A:17:ILE:HG12	2.18	0.43
2:B:88:LEU:HD12	2:B:88:LEU:HA	1.78	0.43
1:C:97:ALA:O	1:C:100:LYS:HG3	2.17	0.43
2:B:46:GLY:O	2:B:47:ASN:ND2	2.50	0.43
1:C:25:GLY:O	1:C:29:LEU:HB2	2.18	0.43
1:C:121:GLU:CD	1:C:121:GLU:H	2.27	0.43
2:D:104:LYS:HE2	2:D:104:LYS:HB3	1.79	0.43
2:B:16:SER:OG	2:B:17:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:SER:HB2	2:D:140:ALA:O	2.17	0.43
2:B:127:GLN:NE2	2:B:131:GLN:OE1	2.50	0.43
1:C:46:TRP:HH2	1:C:59:HIS:CD2	2.37	0.43
1:C:98:ASN:H	1:C:98:ASN:ND2	2.15	0.43
2:B:1:VAL:HG22	2:B:2:GLU:N	2.33	0.43
2:B:47:ASN:C	2:B:48:LEU:HD23	2.44	0.43
2:B:114:LEU:HD23	2:B:122:PHE:CE1	2.54	0.43
1:A:54:PRO:C	1:A:57:LYS:HG2	2.44	0.43
2:B:99:ASP:HA	2:B:100:PRO:HD2	1.77	0.42
1:C:52:GLY:HA2	1:C:56:ILE:HG21	2.01	0.42
1:C:71:VAL:O	1:C:74:ILE:HB	2.19	0.42
1:C:99:PHE:HD1	4:C:600:HEM:HMC3	1.84	0.42
1:A:32:MET:HG2	1:A:101:ILE:CG2	2.47	0.42
2:B:15:PHE:HD1	2:B:20:TYR:OH	2.01	0.42
1:C:54:PRO:O	1:C:58:ALA:N	2.49	0.42
2:D:9:SER:O	2:D:12:SER:N	2.52	0.42
2:B:23:ILE:HG13	2:B:117:LYS:HZ3	1.84	0.42
2:B:80:ASN:CG	2:B:83:ALA:HB3	2.44	0.42
2:B:130:PHE:CE1	2:B:134:LEU:HD21	2.55	0.42
2:D:7:GLU:OE2	2:D:132:LYS:NZ	2.50	0.42
2:D:42:PHE:HB3	2:D:45:PHE:CD2	2.54	0.42
2:D:57:ASN:ND2	2:D:59:ASN:HD22	2.04	0.42
1:C:54:PRO:HA	1:C:57:LYS:CB	2.50	0.42
2:B:63:HIS:HA	2:B:66:LYS:CE	2.47	0.42
2:B:66:LYS:HZ2	4:B:400:HEM:HBD2	1.85	0.42
2:B:93:SER:OG	2:B:94:GLU:N	2.50	0.42
1:C:4:ASP:O	1:C:8:ALA:HB2	2.20	0.42
2:D:30:ARG:O	2:D:34:VAL:N	2.50	0.42
1:A:86:GLU:OE1	1:A:140:ARG:NH2	2.50	0.42
1:A:119:THR:OG1	1:A:121:GLU:HB2	2.20	0.42
1:C:71:VAL:HG12	1:C:72:SER:N	2.35	0.42
2:D:96:LEU:HD22	4:D:800:HEM:HMD3	2.02	0.42
2:D:111:THR:HG21	2:D:131:GLN:OE1	2.20	0.42
1:A:119:THR:HG1	1:A:121:GLU:HB2	1.84	0.42
1:C:62:LYS:HB3	4:C:600:HEM:HMA3	2.02	0.42
2:D:66:LYS:HB2	2:D:66:LYS:HE2	1.75	0.42
1:C:13:LEU:O	1:C:17:ILE:N	2.51	0.42
1:C:89:ALA:O	1:C:93:ARG:N	2.50	0.42
2:D:10:ILE:HG21	2:D:129:ALA:CB	2.50	0.41
2:D:66:LYS:HE3	4:D:800:HEM:HAA1	2.01	0.41
1:C:104:HIS:O	1:C:108:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD12	1:A:136:ALA:HB3	2.02	0.41
1:C:77:LEU:HB3	1:C:81:LEU:HD11	2.02	0.41
2:D:23:ILE:H	2:D:23:ILE:HG12	1.61	0.41
1:C:123:HIS:O	1:C:127:ASP:HB2	2.20	0.41
1:A:28:ALA:HB2	1:A:109:VAL:HG21	2.02	0.41
2:B:130:PHE:CZ	2:B:134:LEU:HD21	2.55	0.41
1:C:81:LEU:HD12	1:C:136:ALA:HB3	2.01	0.41
1:C:108:VAL:O	1:C:111:SER:HB3	2.20	0.41
2:D:142:GLY:HA2	2:D:145:TYR:CD1	2.55	0.41
1:A:95:ASP:HA	1:A:96:PRO:HD3	1.89	0.41
2:D:10:ILE:HD12	2:D:129:ALA:HB2	2.03	0.41
2:D:93:SER:HB2	2:D:145:TYR:CZ	2.55	0.41
2:D:63:HIS:NE2	4:D:800:HEM:ND	2.69	0.41
2:B:27:ALA:HA	2:B:113:VAL:HG21	2.03	0.41
2:B:28:LEU:HD22	2:B:63:HIS:HD1	1.85	0.41
2:D:71:LEU:HD11	2:D:134:LEU:HD23	2.03	0.41
2:D:71:LEU:HD21	4:D:800:HEM:HBB2	2.02	0.41
1:A:46:TRP:CZ3	1:A:56:ILE:HG12	2.56	0.41
1:A:69:LEU:HD11	1:A:73:LYS:HE3	2.03	0.41
2:B:48:LEU:HD13	2:B:54:ILE:HD13	2.03	0.41
2:D:78:MET:HE3	2:D:78:MET:HB3	1.91	0.41
2:D:100:PRO:HA	2:D:103:PHE:CD2	2.55	0.41
2:B:95:LYS:HE2	2:B:95:LYS:HB2	1.47	0.41
1:C:56:ILE:HG22	1:C:57:LYS:N	2.36	0.41
2:D:32:LEU:HD22	2:D:39:GLN:CG	2.51	0.41
2:D:47:ASN:OD1	2:D:49:TYR:HB2	2.21	0.41
2:D:47:ASN:OD1	2:D:49:TYR:N	2.54	0.41
2:D:95:LYS:HE3	2:D:96:LEU:CD2	2.51	0.41
1:A:7:LYS:NZ	1:A:75:ASP:HA	2.36	0.40
1:C:107:LEU:HD21	1:C:130:LEU:HD12	2.03	0.40
2:D:142:GLY:HA2	2:D:145:TYR:CE1	2.56	0.40
1:A:32:MET:HE3	1:A:32:MET:HB3	1.89	0.40
1:A:47:PRO:HD2	1:A:55:HIS:CD2	2.57	0.40
1:A:53:SER:HA	1:A:54:PRO:HD2	1.69	0.40
1:A:95:ASP:OD2	2:D:101:ASP:OD2	2.39	0.40
1:A:99:PHE:CD1	4:A:202:HEM:HHC	2.56	0.40
2:B:1:VAL:HG22	2:B:2:GLU:H	1.85	0.40
2:D:66:LYS:CE	4:D:800:HEM:HAA1	2.51	0.40
2:D:71:LEU:HD13	2:D:133:PHE:CE2	2.57	0.40
2:B:32:LEU:HB3	2:B:54:ILE:CD1	2.52	0.40
1:A:47:PRO:HB2	1:A:55:HIS:HE2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ILE:O	2:B:23:ILE:HG22	2.21	0.40
2:D:99:ASP:O	2:D:102:ASN:N	2.50	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	141/143 (99%)	124 (88%)	12 (8%)	5 (4%)	3	1
1	C	141/143 (99%)	120 (85%)	17 (12%)	4 (3%)	4	2
2	B	144/146 (99%)	111 (77%)	27 (19%)	6 (4%)	2	1
2	D	144/146 (99%)	116 (81%)	26 (18%)	2 (1%)	9	7
All	All	570/578 (99%)	471 (83%)	82 (14%)	17 (3%)	3	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
2	B	43	SER
2	D	23	ILE
1	A	93	ARG
2	B	44	GLY
2	B	49	TYR
2	B	93	SER
1	C	21	ALA
2	D	47	ASN
1	C	49	VAL
1	C	57	LYS
1	A	42	TYR
1	A	86	GLU

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Mol	Chain	Res	Type
1	C	3	SER
2	B	62	ALA
2	B	54	ILE
1	A	34	VAL

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	119/119 (100%)	96 (81%)	23 (19%)	1 1
1	C	119/119 (100%)	96 (81%)	23 (19%)	1 1
2	B	120/120 (100%)	103 (86%)	17 (14%)	3 3
2	D	120/120 (100%)	86 (72%)	34 (28%)	0 0
All	All	478/478 (100%)	381 (80%)	97 (20%)	1 1

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	11	ARG
1	A	19	LYS
1	A	29	LEU
1	A	32	MET
1	A	40	LYS
1	A	44	SER
1	A	49	VAL
1	A	50	THR
1	A	56	ILE
1	A	57	LYS
1	A	82	MET
1	A	84	LEU
1	A	87	GLN
1	A	100	LYS
1	A	107	LEU
1	A	116	LYS

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Mol	Chain	Res	Type
1	A	119	THR
1	A	126	LEU
1	A	128	LYS
1	A	131	SER
1	A	137	LEU
1	A	142	ARG
2	B	6	LYS
2	B	9	SER
2	B	22	ASP
2	B	23	ILE
2	B	32	LEU
2	B	41	HIS
2	B	48	LEU
2	B	52	GLU
2	B	54	ILE
2	B	59	ASN
2	B	68	LEU
2	B	76	LYS
2	B	88	LEU
2	B	95	LYS
2	B	110	ILE
2	B	117	LYS
2	B	125	GLU
1	C	11	ARG
1	C	19	LYS
1	C	31	ARG
1	C	32	MET
1	C	48	ASP
1	C	50	THR
1	C	56	ILE
1	C	64	MET
1	C	69	LEU
1	C	71	VAL
1	C	77	LEU
1	C	82	MET
1	C	83	GLU
1	C	91	LYS
1	C	93	ARG
1	C	94	VAL
1	C	100	LYS
1	C	102	LEU
1	C	113	MET

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Mol	Chain	Res	Type
1	C	116	LYS
1	C	124	VAL
1	C	131	SER
1	C	140	ARG
2	D	2	GLU
2	D	6	LYS
2	D	8	ARG
2	D	21	ASP
2	D	23	ILE
2	D	43	SER
2	D	48	LEU
2	D	65	ILE
2	D	66	LYS
2	D	67	VAL
2	D	68	LEU
2	D	71	LEU
2	D	73	ARG
2	D	76	LYS
2	D	78	MET
2	D	80	ASN
2	D	81	ILE
2	D	88	LEU
2	D	90	THR
2	D	93	SER
2	D	95	LYS
2	D	96	LEU
2	D	98	VAL
2	D	104	LYS
2	D	112	ILE
2	D	118	MET
2	D	120	HIS
2	D	131	GLN
2	D	132	LYS
2	D	136	VAL
2	D	137	VAL
2	D	138	VAL
2	D	139	SER
2	D	146	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
2	B	47	ASN
2	B	77	ASN
2	B	144	GLN
2	B	146	HIS
1	C	26	ASN
2	D	17	HIS
2	D	59	ASN
2	D	80	ASN
2	D	97	HIS
2	D	102	ASN
2	D	144	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)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CMO	A	201	-	0,1,1	-	-	-		
4	HEM	A	202	1	50,50,50	1.22	5 (10%)	67,82,82	0.86	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HEM	B	400	2	50,50,50	1.22	7 (14%)	67,82,82	0.89	3 (4%)
4	HEM	C	600	1	50,50,50	1.21	7 (14%)	67,82,82	0.88	1 (1%)
4	HEM	D	800	2	50,50,50	1.33	10 (20%)	67,82,82	0.86	3 (4%)

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	HEM	A	202	1	-	9/14/54/54	-
4	HEM	B	400	2	-	5/14/54/54	-
4	HEM	C	600	1	-	6/14/54/54	-
4	HEM	D	800	2	-	9/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	800	HEM	FE-NB	3.20	2.04	1.94
4	D	800	HEM	CAC-C3C	2.92	1.55	1.47
4	B	400	HEM	CAB-C3B	2.75	1.54	1.47
4	A	202	HEM	CAC-C3C	2.74	1.54	1.47
4	C	600	HEM	CAB-C3B	2.74	1.54	1.47
4	C	600	HEM	CAC-C3C	2.71	1.54	1.47
4	D	800	HEM	CAB-C3B	2.70	1.54	1.47
4	A	202	HEM	CAB-C3B	2.69	1.54	1.47
4	B	400	HEM	CAC-C3C	2.69	1.54	1.47
4	D	800	HEM	FE-NC	2.67	2.04	1.95
4	D	800	HEM	FE-ND	2.57	2.02	1.94
4	D	800	HEM	FE-NA	2.56	2.03	1.95
4	C	600	HEM	FE-NC	2.37	2.03	1.95
4	B	400	HEM	FE-NC	2.28	2.02	1.95
4	A	202	HEM	FE-ND	2.27	2.01	1.94
4	B	400	HEM	FE-NB	2.25	2.01	1.94
4	C	600	HEM	FE-ND	2.24	2.01	1.94
4	B	400	HEM	FE-NA	2.21	2.02	1.95
4	B	400	HEM	FE-ND	2.13	2.01	1.94
4	A	202	HEM	CMD-C2D	2.10	1.55	1.50
4	A	202	HEM	FE-NC	2.10	2.02	1.95
4	B	400	HEM	CMB-C2B	2.08	1.55	1.50
4	D	800	HEM	CMB-C2B	2.06	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	800	HEM	CMC-C2C	2.04	1.55	1.50
4	C	600	HEM	CMB-C2B	2.04	1.54	1.50
4	D	800	HEM	CMA-C3A	2.03	1.54	1.50
4	C	600	HEM	CMD-C2D	2.02	1.54	1.50
4	D	800	HEM	CMD-C2D	2.01	1.54	1.50
4	C	600	HEM	CMC-C2C	2.00	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	400	HEM	CBA-CAA-C2A	2.82	120.32	112.53
4	A	202	HEM	CBA-CAA-C2A	2.43	119.25	112.53
4	B	400	HEM	CBD-CAD-C3D	2.41	119.20	112.53
4	D	800	HEM	CBA-CAA-C2A	2.37	119.09	112.53
4	C	600	HEM	CBA-CAA-C2A	2.31	118.92	112.53
4	D	800	HEM	CBD-CAD-C3D	2.28	118.83	112.53
4	B	400	HEM	O1A-CGA-CBA	-2.12	116.36	123.09
4	A	202	HEM	O1A-CGA-CBA	-2.10	116.42	123.09
4	D	800	HEM	O1D-CGD-CBD	-2.01	116.71	123.09

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	202	HEM	C2A-CAA-CBA-CGA
4	B	400	HEM	C1A-C2A-CAA-CBA
4	C	600	HEM	C1A-C2A-CAA-CBA
4	C	600	HEM	C3A-C2A-CAA-CBA
4	D	800	HEM	C2C-C3C-CAC-CBC
4	D	800	HEM	C4C-C3C-CAC-CBC
4	A	202	HEM	C1A-C2A-CAA-CBA
4	B	400	HEM	C3A-C2A-CAA-CBA
4	B	400	HEM	C2A-CAA-CBA-CGA
4	D	800	HEM	C2D-C3D-CAD-CBD
4	A	202	HEM	C3A-C2A-CAA-CBA
4	D	800	HEM	C4D-C3D-CAD-CBD
4	A	202	HEM	C2B-C3B-CAB-CBB
4	A	202	HEM	C4B-C3B-CAB-CBB
4	A	202	HEM	CAD-CBD-CGD-O2D
4	A	202	HEM	CAA-CBA-CGA-O2A
4	A	202	HEM	CAA-CBA-CGA-O1A
4	A	202	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
4	D	800	HEM	C2A-CAA-CBA-CGA
4	C	600	HEM	CAD-CBD-CGD-O2D
4	C	600	HEM	CAA-CBA-CGA-O1A
4	C	600	HEM	CAD-CBD-CGD-O1D
4	D	800	HEM	CAD-CBD-CGD-O2D
4	D	800	HEM	CAA-CBA-CGA-O2A
4	C	600	HEM	CAA-CBA-CGA-O2A
4	B	400	HEM	C2D-C3D-CAD-CBD
4	D	800	HEM	CAD-CBD-CGD-O1D
4	D	800	HEM	CAA-CBA-CGA-O1A
4	B	400	HEM	CAD-CBD-CGD-O2D

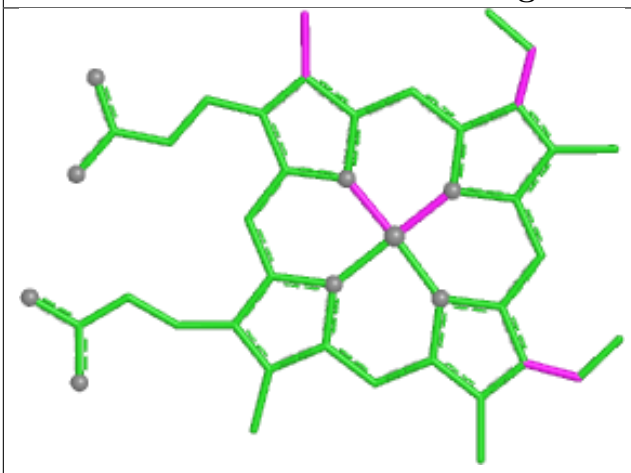
There are no ring outliers.

5 monomers are involved in 33 short contacts:

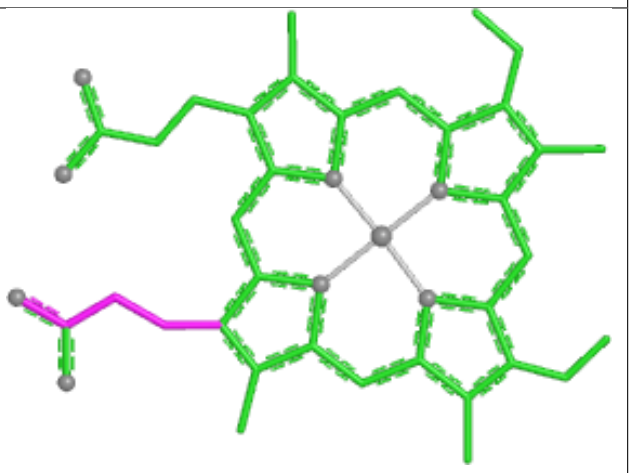
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	CMO	1	0
4	A	202	HEM	4	0
4	B	400	HEM	9	0
4	C	600	HEM	7	0
4	D	800	HEM	12	0

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.

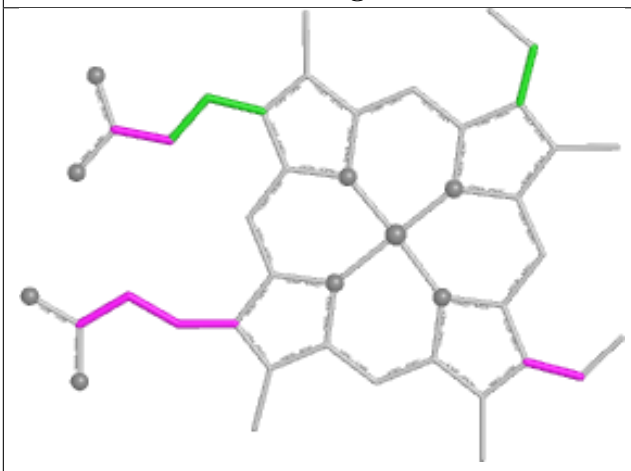
Ligand HEM A 202



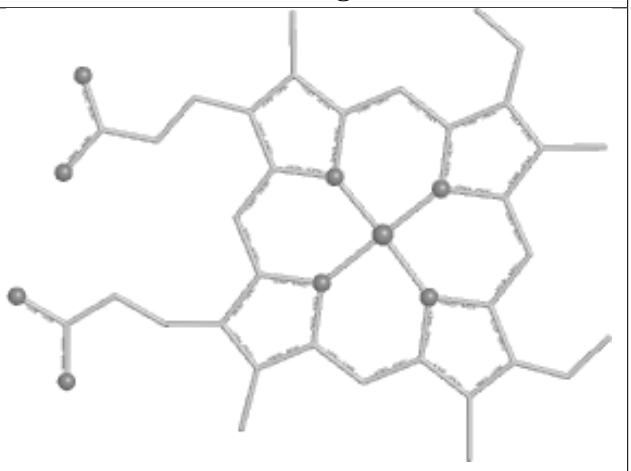
Bond lengths



Bond angles

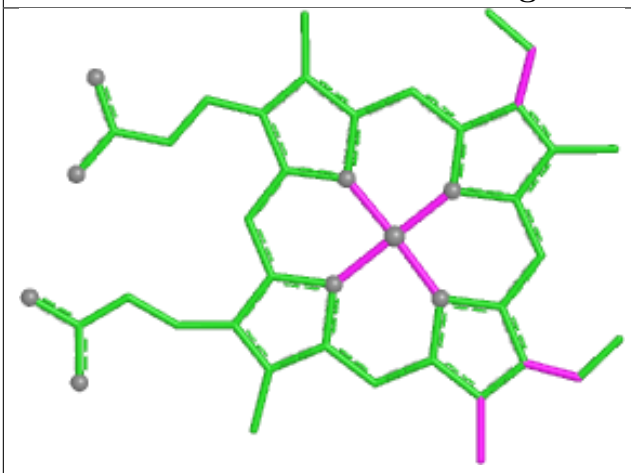


Torsions

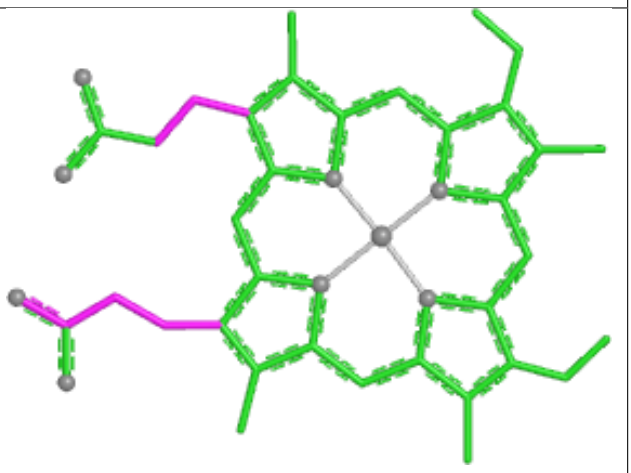


Rings

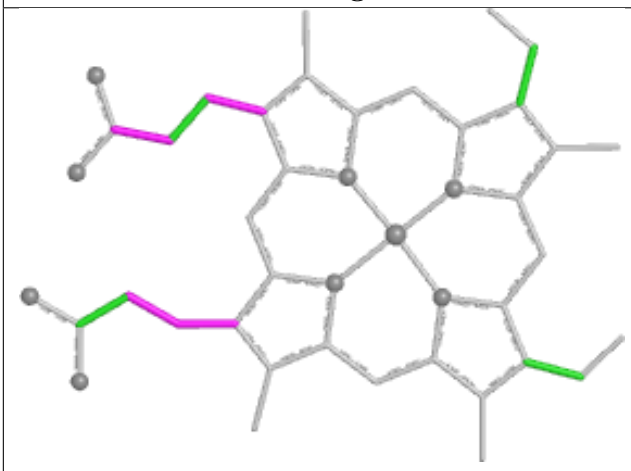
Ligand HEM B 400



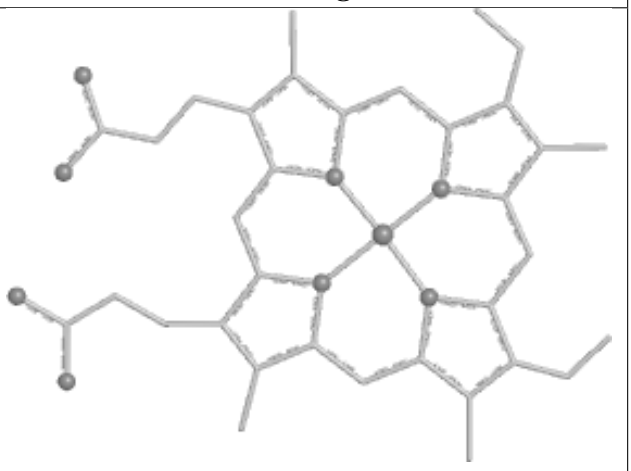
Bond lengths



Bond angles

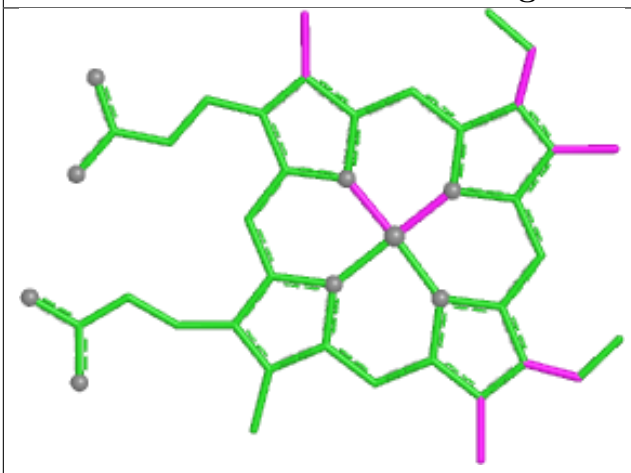


Torsions

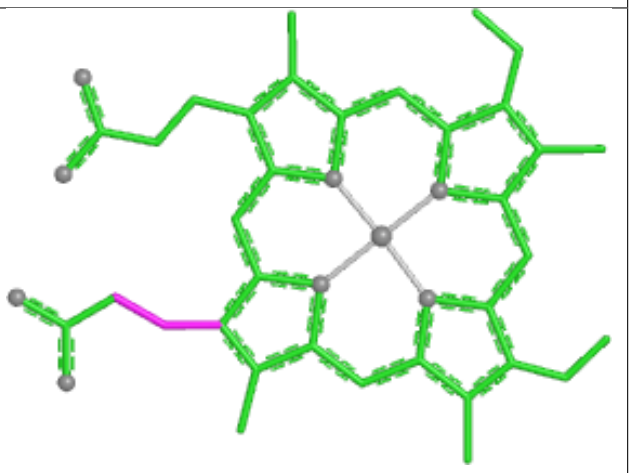


Rings

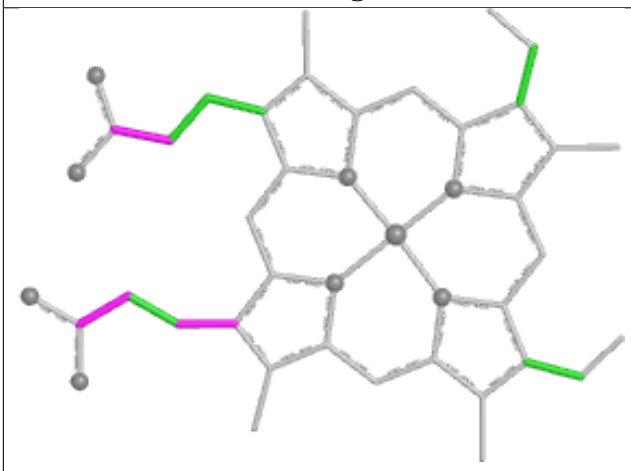
Ligand HEM C 600



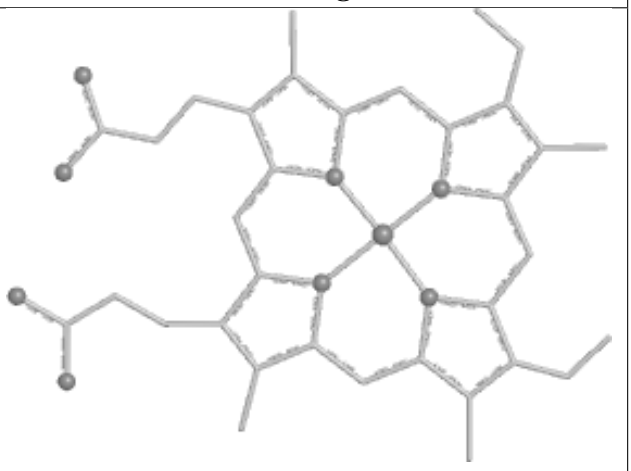
Bond lengths



Bond angles

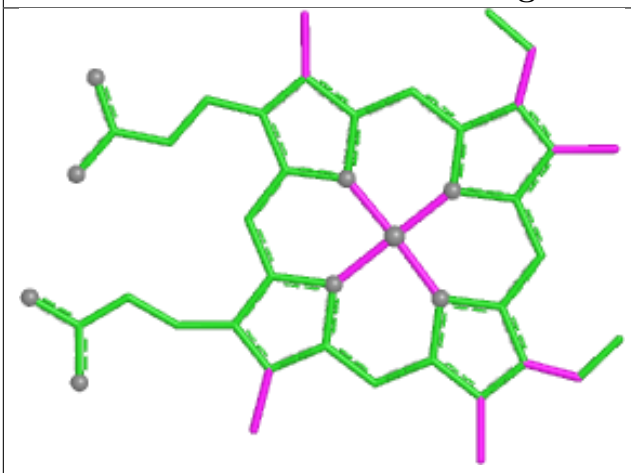


Torsions

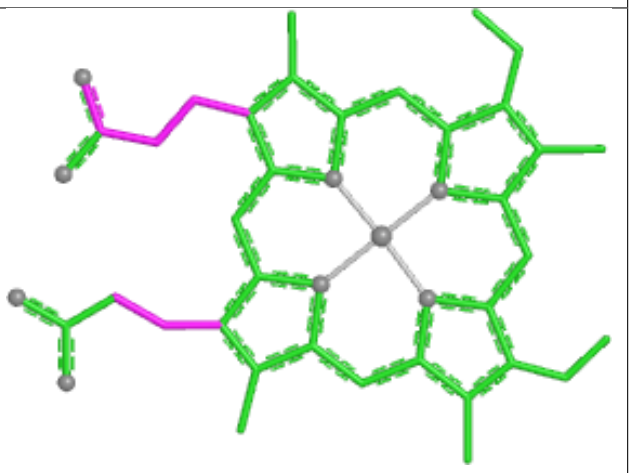


Rings

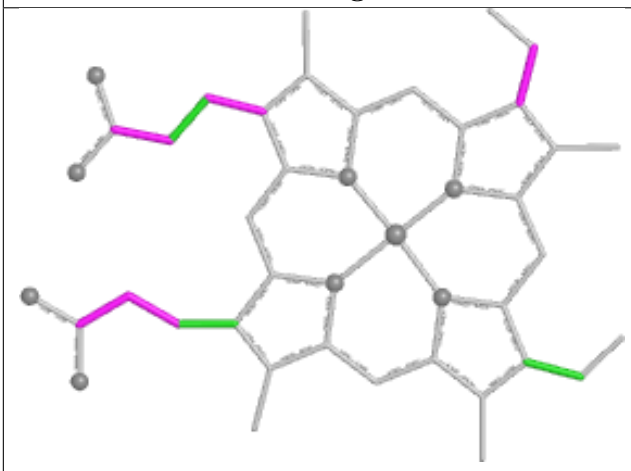
Ligand HEM D 800



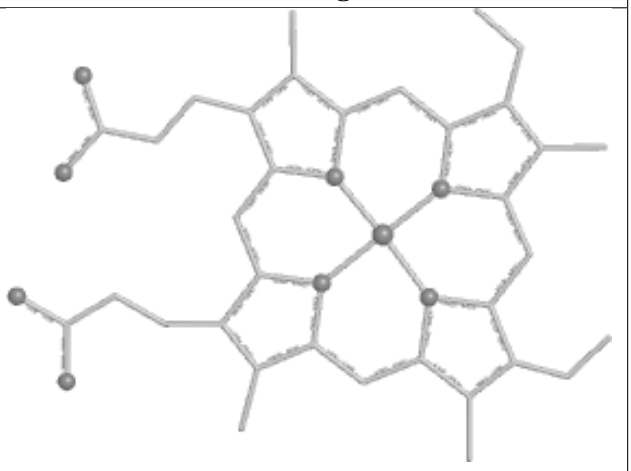
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	142/143 (99%)	-1.15	0	100	100	20, 36, 58, 66	0
1	C	142/143 (99%)	-1.14	0	100	100	27, 40, 71, 80	0
2	B	146/146 (100%)	-1.03	0	100	100	25, 45, 68, 77	0
2	D	146/146 (100%)	-0.98	0	100	100	23, 47, 76, 88	0
All	All	576/578 (99%)	-1.07	0	100	100	20, 41, 69, 88	0

There are no RSRZ outliers to report.

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

There are no oligosaccharides in this entry.

6.4 Ligands

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
3	CMO	A	201	2/2	0.98	0.07	48,48,48,48	0
4	HEM	A	202	43/43	0.99	0.04	28,37,42,59	0
4	HEM	B	400	43/43	0.99	0.05	48,52,56,59	0
4	HEM	C	600	43/43	0.99	0.04	40,47,52,55	0

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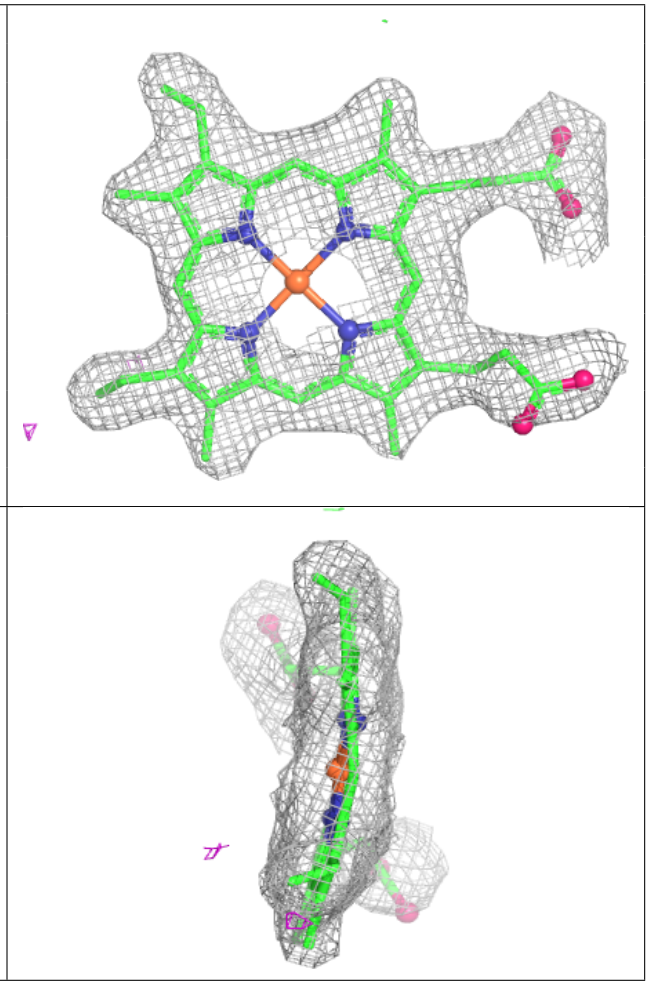
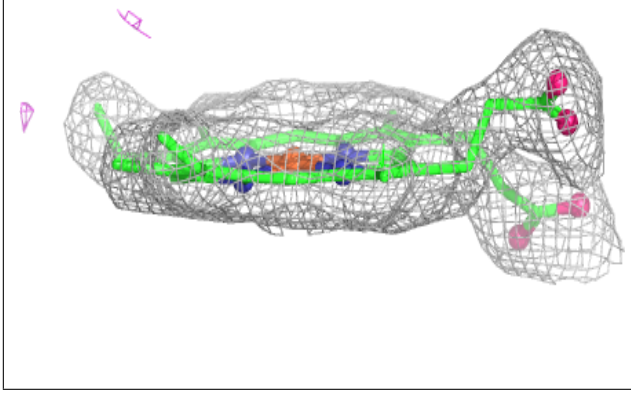
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HEM	D	800	43/43	0.99	0.04	60,66,68,69	0

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 HEM A 202:

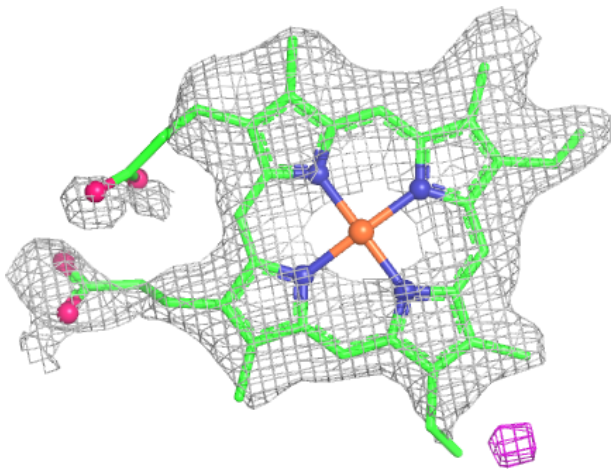
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

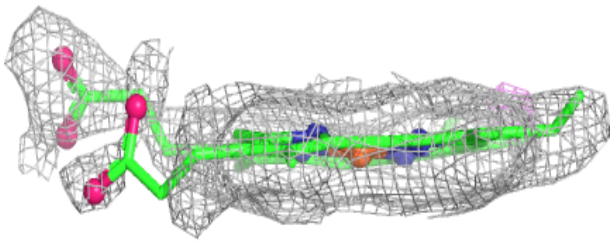


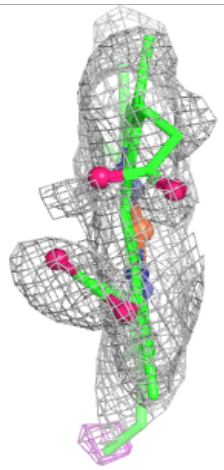


Electron density around HEM B 400:

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

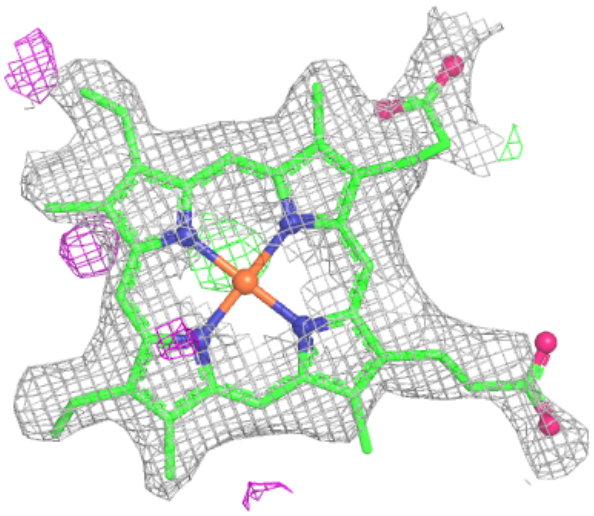


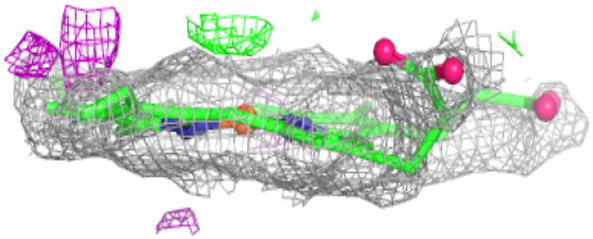


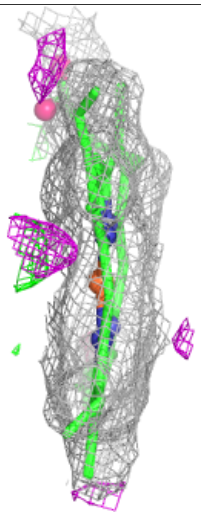


Electron density around HEM C 600:

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

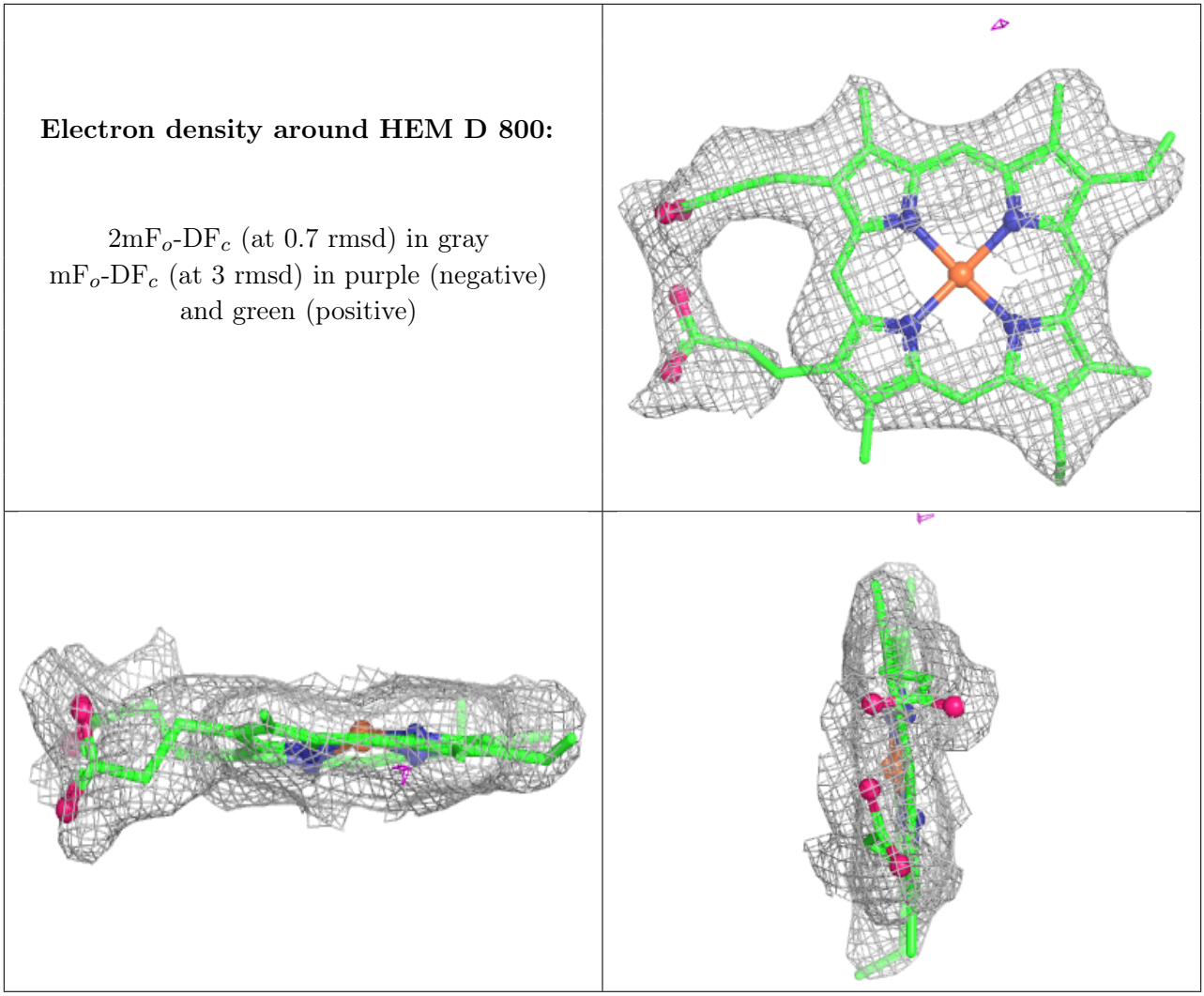






Electron density around HEM D 800:

$2mF_o$-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

There are no such residues in this entry.