Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 03:45 PM EST

PDB ID	:	3Q09
Title	:	Crystal Structure of Chlorite Dismutase from D. Aromatica at pH 9.0
Authors	:	Goblirsch, B.R.; Wilmot, C.M.
Deposited on	:	2010-12-15
Resolution	:	3.00 Å(reported)

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

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

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

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

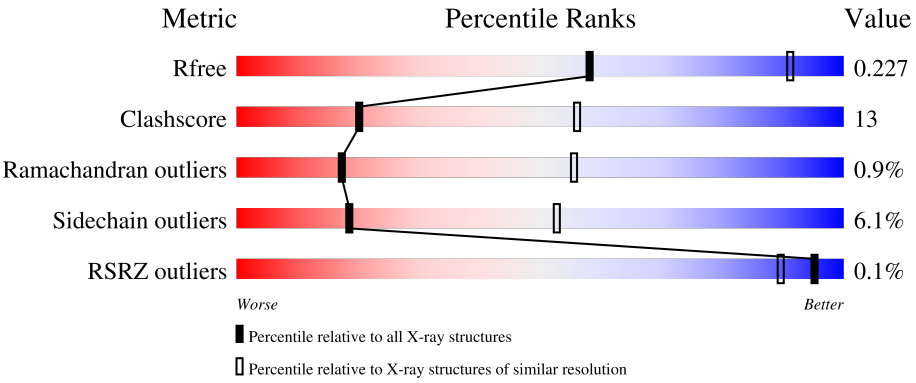
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	248	70% 25%
1	B	248	72% 22%
1	C	248	73% 20%
1	D	248	73% 22%
1	E	248	71% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	248	71% 25%
1	G	248	70% 24%
1	H	248	76% 19%
1	I	248	75% 19%
1	J	248	73% 20%
1	K	248	75% 21%
1	L	248	74% 20%
1	M	248	74% 21%
1	N	248	70% 24%
1	O	248	76% 19%
1	P	248	70% 24%
1	Q	248	67% 25% 5%
1	R	248	70% 24%
1	S	248	% 67% 28%
1	T	248	62% 31% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39520 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 Chlorite dismutase.

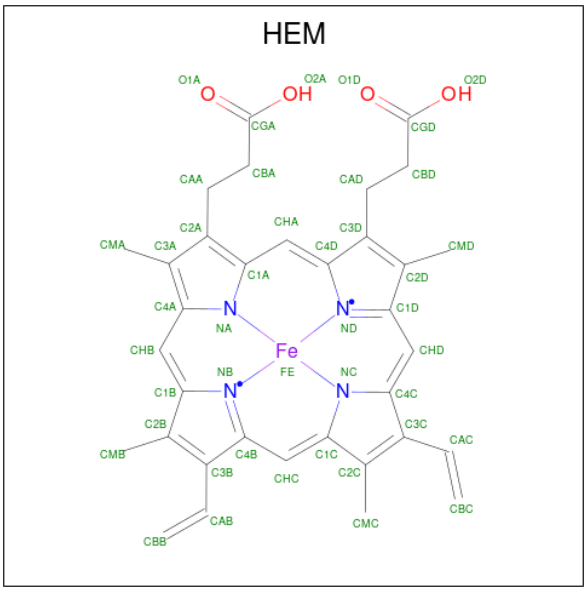
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	B	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	C	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	D	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	E	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	F	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	G	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	H	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	I	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	J	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	K	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	L	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	M	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	N	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	O	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	P	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	R	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	S	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	T	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			

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



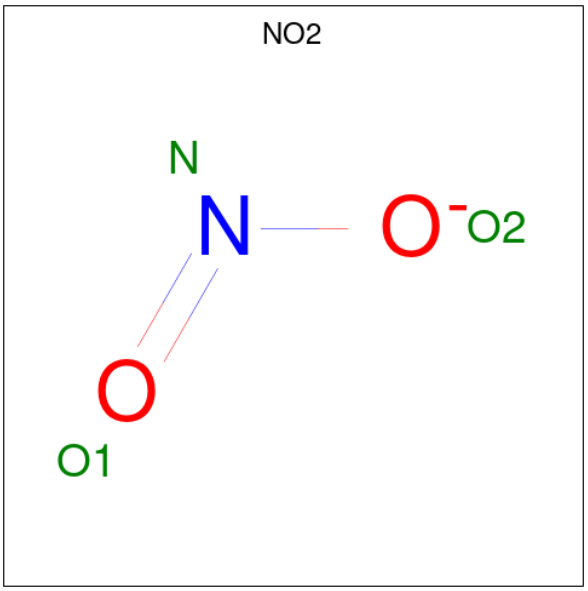
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 3 1 2	0	0
3	B	1	Total N O 3 1 2	0	0
3	C	1	Total N O 3 1 2	0	0
3	D	1	Total N O 3 1 2	0	0
3	E	1	Total N O 3 1 2	0	0
3	F	1	Total N O 3 1 2	0	0
3	G	1	Total N O 3 1 2	0	0
3	H	1	Total N O 3 1 2	0	0
3	I	1	Total N O 3 1 2	0	0
3	J	1	Total N O 3 1 2	0	0
3	K	1	Total N O 3 1 2	0	0
3	L	1	Total N O 3 1 2	0	0
3	M	1	Total N O 3 1 2	0	0
3	N	1	Total N O 3 1 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total N O 3 1 2	0	0
3	P	1	Total N O 3 1 2	0	0
3	Q	1	Total N O 3 1 2	0	0
3	R	1	Total N O 3 1 2	0	0
3	S	1	Total N O 3 1 2	0	0
3	T	1	Total N O 3 1 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0
4	G	1	Total Ca 1 1	0	0
4	H	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	J	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0
4	M	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total Ca 1 1	0	0
4	O	1	Total Ca 1 1	0	0
4	P	1	Total Ca 1 1	0	0
4	Q	1	Total Ca 1 1	0	0
4	R	1	Total Ca 1 1	0	0
4	S	1	Total Ca 1 1	0	0
4	T	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	E	1	Total O 1 1	0	0
5	F	1	Total O 1 1	0	0
5	G	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0
5	I	1	Total O 1 1	0	0
5	J	1	Total O 1 1	0	0
5	K	1	Total O 1 1	0	0
5	L	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

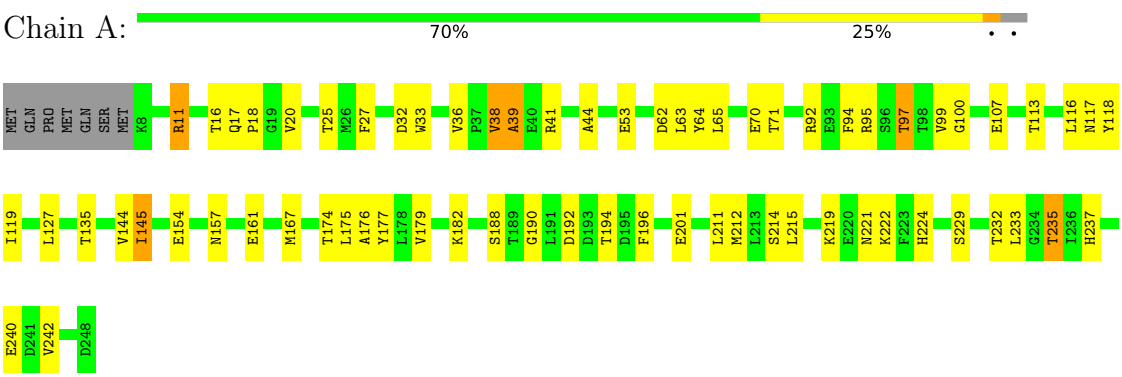
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total O 1 1	0	0
5	N	1	Total O 1 1	0	0
5	O	1	Total O 1 1	0	0
5	P	1	Total O 1 1	0	0
5	Q	1	Total O 1 1	0	0
5	R	1	Total O 1 1	0	0
5	S	1	Total O 1 1	0	0
5	T	1	Total O 1 1	0	0

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.

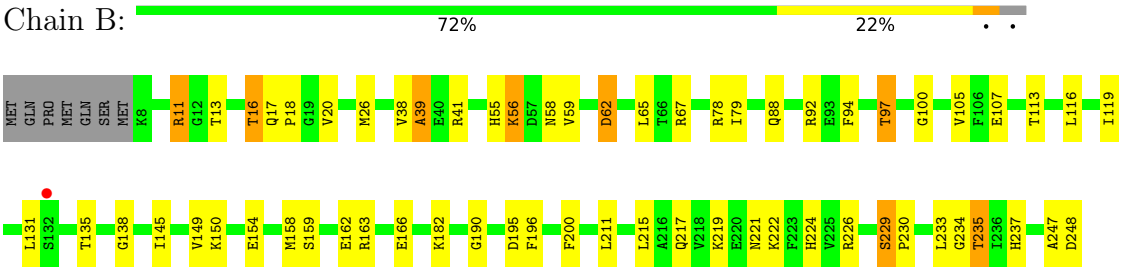
• Molecule 1: Chlorite dismutase

Chain A:



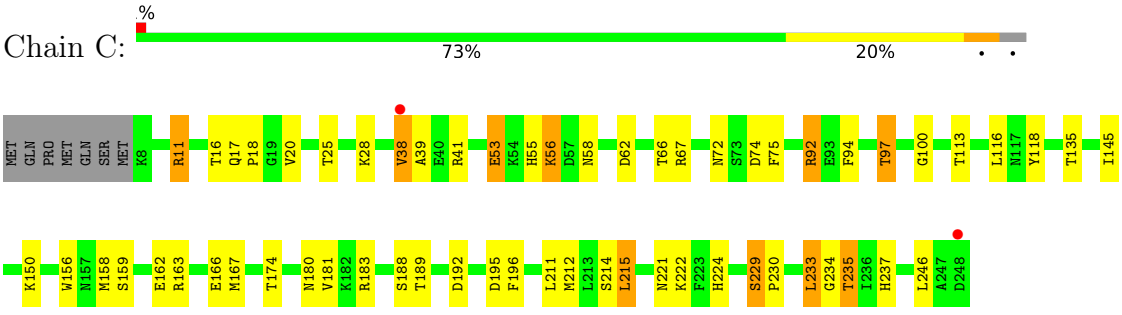
• Molecule 1: Chlorite dismutase

Chain B:



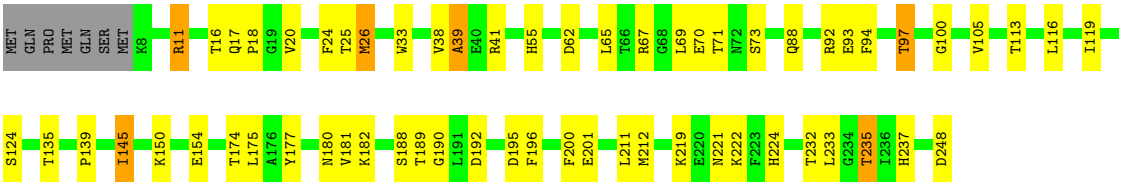
• Molecule 1: Chlorite dismutase

Chain C:



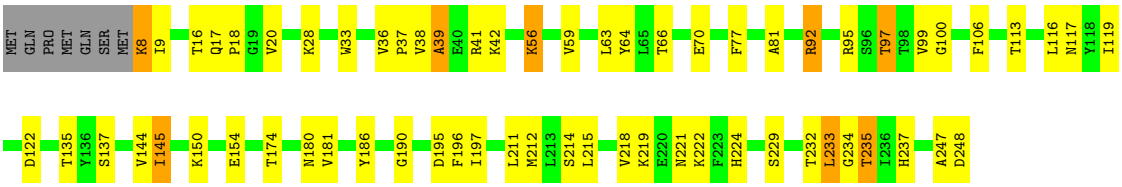
• Molecule 1: Chlorite dismutase

Chain D:



• Molecule 1: Chlorite dismutase

Chain E:



• Molecule 1: Chlorite dismutase

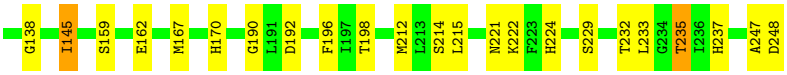
Chain F:

• Molecule 1: Chlorite dismutase

Chain G:

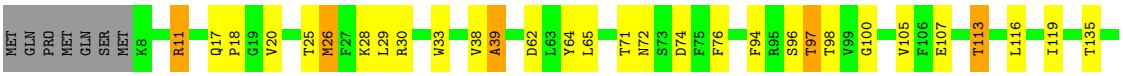
• Molecule 1: Chlorite dismutase

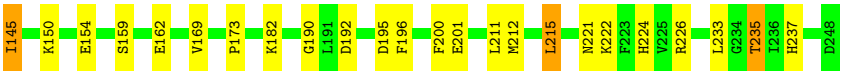
Chain H:



• Molecule 1: Chlorite dismutase

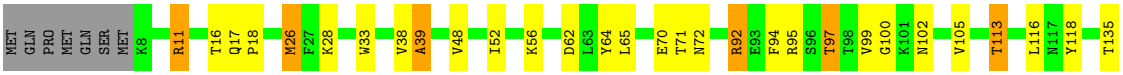
Chain I:

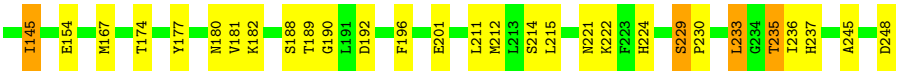




• Molecule 1: Chlorite dismutase

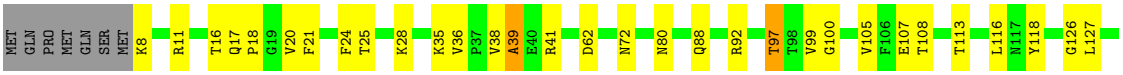
Chain J:





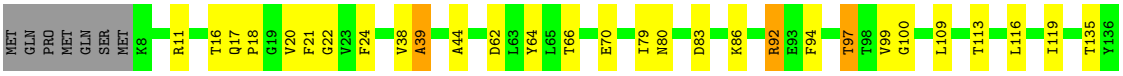
• Molecule 1: Chlorite dismutase

Chain K:



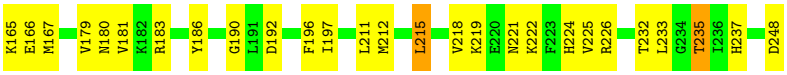
• Molecule 1: Chlorite dismutase

Chain L:



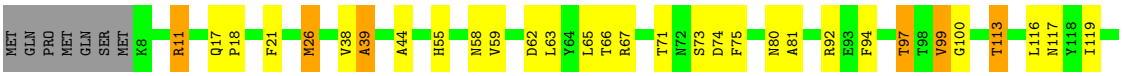
• Molecule 1: Chlorite dismutase

Chain M:



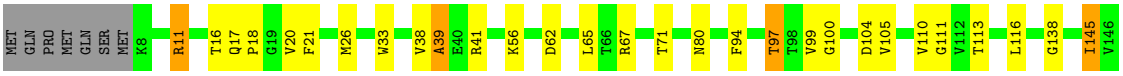
• Molecule 1: Chlorite dismutase

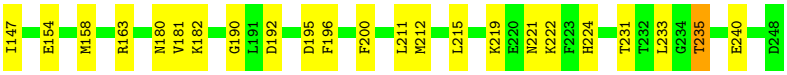
Chain N:



• Molecule 1: Chlorite dismutase

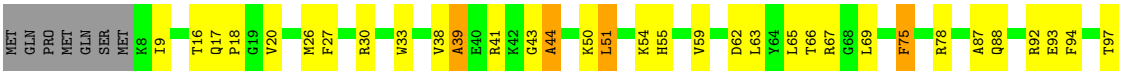
Chain O:

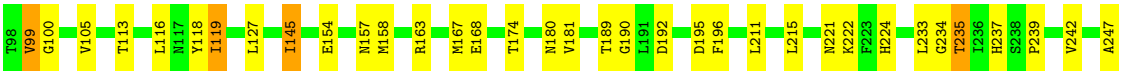




• Molecule 1: Chlorite dismutase

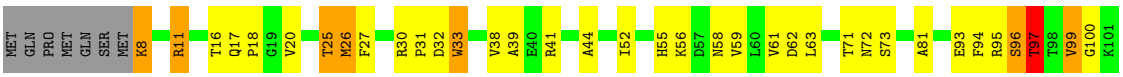
Chain P:

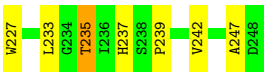




• Molecule 1: Chlorite dismutase

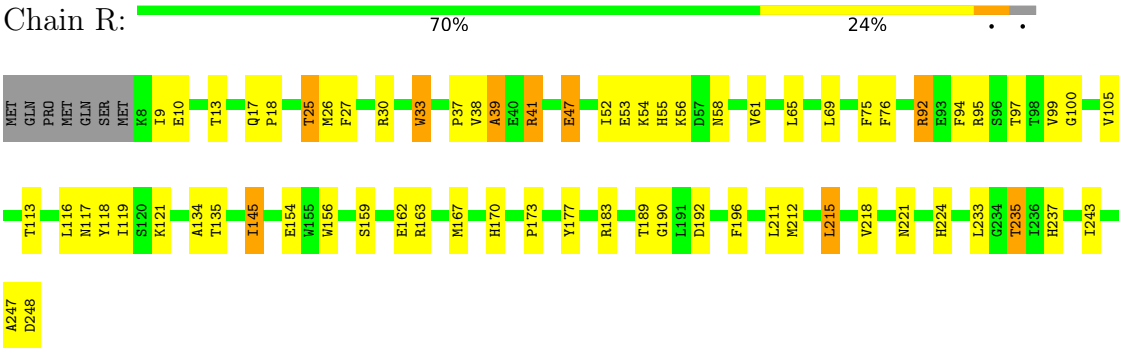
Chain Q:





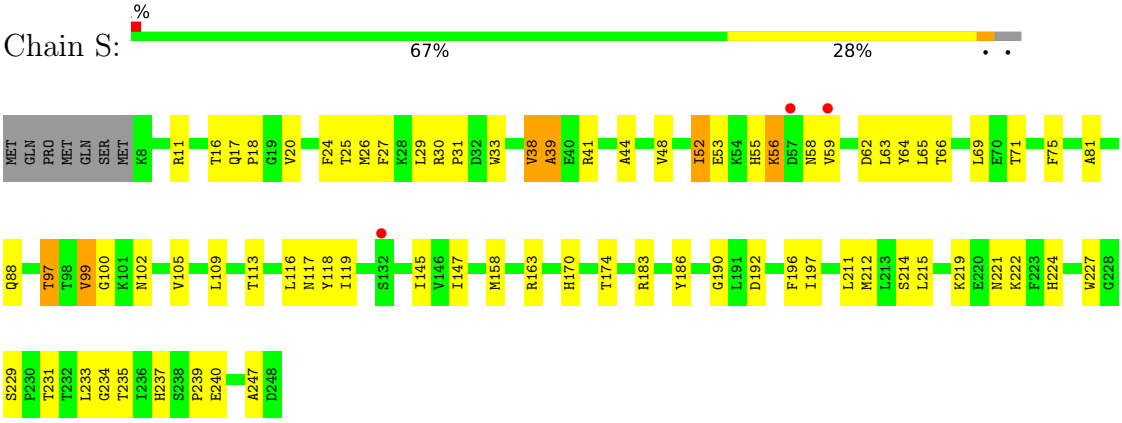
• Molecule 1: Chlorite dismutase

Chain R:



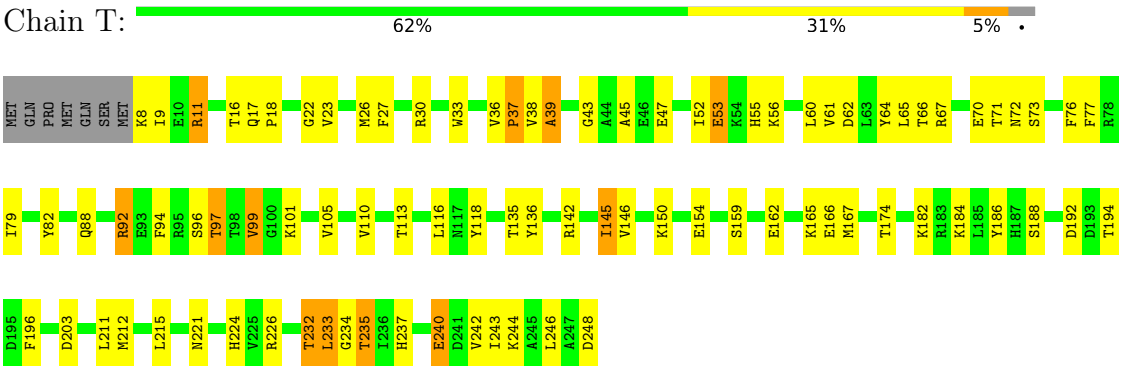
• Molecule 1: Chlorite dismutase

Chain S:



• Molecule 1: Chlorite dismutase

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.70Å 202.85Å 247.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 3.00 48.31 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.31-3.00) 99.7 (48.31-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.59 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.234 0.183 , 0.227	Depositor DCC
R_{free} test set	6174 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 17.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	39520	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, NO2, CA

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	0.83	2/1973 (0.1%)	0.86	2/2676 (0.1%)
1	B	0.87	0/1973	0.89	2/2676 (0.1%)
1	C	0.85	1/1973 (0.1%)	0.85	1/2676 (0.0%)
1	D	0.80	0/1973	0.83	0/2676
1	E	0.84	0/1973	0.86	2/2676 (0.1%)
1	F	0.75	1/1973 (0.1%)	0.81	0/2676
1	G	0.77	0/1973	0.81	0/2676
1	H	0.76	0/1973	0.83	0/2676
1	I	0.80	0/1973	0.84	0/2676
1	J	0.75	0/1973	0.81	0/2676
1	K	0.76	0/1973	0.83	0/2676
1	L	0.76	0/1973	0.79	0/2676
1	M	0.80	1/1973 (0.1%)	0.85	1/2676 (0.0%)
1	N	0.75	1/1973 (0.1%)	0.79	0/2676
1	O	0.71	0/1973	0.77	1/2676 (0.0%)
1	P	0.82	6/1973 (0.3%)	0.83	5/2676 (0.2%)
1	Q	0.99	6/1973 (0.3%)	0.88	6/2676 (0.2%)
1	R	0.78	4/1973 (0.2%)	0.77	1/2676 (0.0%)
1	S	0.76	1/1973 (0.1%)	0.73	0/2676
1	T	0.88	7/1973 (0.4%)	0.83	1/2676 (0.0%)
All	All	0.80	30/39460 (0.1%)	0.82	22/53520 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	L	0	1
1	M	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
All	All	0	5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	93	GLU	CD-OE1	16.32	1.43	1.25
1	Q	33	TRP	CG-CD1	11.41	1.52	1.36
1	Q	33	TRP	CB-CG	10.37	1.69	1.50
1	R	33	TRP	CB-CG	8.30	1.65	1.50
1	Q	96	SER	CB-OG	7.63	1.52	1.42
1	T	53	GLU	CD-OE2	7.52	1.33	1.25
1	A	53	GLU	CG-CD	7.42	1.63	1.51
1	R	41	ARG	CZ-NH2	7.24	1.42	1.33
1	M	162	GLU	CG-CD	6.37	1.61	1.51
1	C	53	GLU	CG-CD	6.37	1.61	1.51
1	N	142	ARG	CZ-NH2	6.27	1.41	1.33
1	P	43	GLY	C-O	6.22	1.33	1.23
1	Q	33	TRP	CD1-NE1	-5.95	1.27	1.38
1	S	52	ILE	CB-CG1	5.87	1.70	1.54
1	Q	97	THR	C-O	-5.86	1.12	1.23
1	R	47	GLU	CB-CG	5.84	1.63	1.52
1	P	44	ALA	C-N	5.73	1.47	1.34
1	F	54	LYS	CD-CE	5.61	1.65	1.51
1	T	47	GLU	CD-OE2	5.52	1.31	1.25
1	P	75	PHE	CD2-CE2	5.46	1.50	1.39
1	T	82	TYR	CE1-CZ	-5.45	1.31	1.38
1	A	161	GLU	CG-CD	5.43	1.60	1.51
1	P	51	LEU	C-O	5.33	1.33	1.23
1	T	82	TYR	CG-CD2	-5.33	1.32	1.39
1	T	43	GLY	C-O	5.31	1.32	1.23
1	R	54	LYS	CA-CB	5.31	1.65	1.53
1	P	54	LYS	N-CA	5.26	1.56	1.46
1	P	55	HIS	CD2-NE2	5.10	1.52	1.42
1	T	53	GLU	CB-CG	5.04	1.61	1.52
1	T	43	GLY	C-N	5.03	1.45	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	33	TRP	CD1-CG-CD2	-8.99	99.11	106.30
1	P	75	PHE	CB-CG-CD1	8.80	126.96	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	33	TRP	CG-CD2-CE3	-8.24	126.48	133.90
1	Q	33	TRP	CB-CG-CD2	8.17	137.22	126.60
1	Q	131	LEU	CA-CB-CG	7.86	133.39	115.30
1	R	41	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	P	65	LEU	CB-CG-CD1	6.57	122.17	111.00
1	Q	33	TRP	CE2-CD2-CE3	6.31	126.27	118.70
1	C	215	LEU	CB-CG-CD1	6.06	121.31	111.00
1	E	92	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	P	55	HIS	CA-CB-CG	-5.98	103.44	113.60
1	A	92	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	P	55	HIS	CG-ND1-CE1	5.82	116.34	108.20
1	P	54	LYS	CA-CB-CG	5.59	125.70	113.40
1	M	215	LEU	CA-CB-CG	5.58	128.14	115.30
1	E	122	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	78	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	T	55	HIS	CA-C-N	-5.33	105.48	117.20
1	Q	33	TRP	CG-CD1-NE1	5.25	115.34	110.10
1	O	104	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	92	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	62	ASP	CB-CG-OD1	-5.09	113.72	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	138	GLY	Peptide
1	L	138	GLY	Peptide
1	M	133	SER	Peptide
1	M	179	VAL	Peptide
1	O	138	GLY	Peptide

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	1928	0	1938	57	0
1	B	1928	0	1938	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1928	0	1938	50	0
1	D	1928	0	1938	57	0
1	E	1928	0	1938	54	0
1	F	1928	0	1938	54	0
1	G	1928	0	1938	65	0
1	H	1928	0	1938	43	0
1	I	1928	0	1938	49	0
1	J	1928	0	1938	56	0
1	K	1928	0	1938	41	0
1	L	1928	0	1938	47	0
1	M	1928	0	1938	41	0
1	N	1928	0	1938	59	0
1	O	1928	0	1938	41	0
1	P	1928	0	1938	58	0
1	Q	1928	0	1938	60	0
1	R	1928	0	1938	60	0
1	S	1928	0	1938	62	0
1	T	1928	0	1938	61	0
2	A	43	0	30	8	0
2	B	43	0	30	6	0
2	C	43	0	30	7	0
2	D	43	0	30	9	0
2	E	43	0	30	8	0
2	F	43	0	30	11	0
2	G	43	0	30	15	0
2	H	43	0	30	9	0
2	I	43	0	30	7	0
2	J	43	0	30	10	0
2	K	43	0	30	5	0
2	L	43	0	30	7	0
2	M	43	0	30	6	0
2	N	43	0	30	10	0
2	O	43	0	30	5	0
2	P	43	0	30	3	0
2	Q	43	0	30	10	0
2	R	43	0	30	14	0
2	S	43	0	30	9	0
2	T	43	0	30	6	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	1	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	1	0
3	M	3	0	0	0	0
3	N	3	0	0	0	0
3	O	3	0	0	0	0
3	P	3	0	0	0	0
3	Q	3	0	0	0	0
3	R	3	0	0	0	0
3	S	3	0	0	0	0
3	T	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	2	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	H	1	0	0	2	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	2	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
All	All	39520	0	39360	988	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 13.

All (988) 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:O:97:THR:HG22	1:O:100:GLY:H	1.10	1.15
1:C:18:PRO:HA	1:C:113:THR:HG22	1.23	1.15
1:J:18:PRO:HA	1:J:113:THR:HG22	1.26	1.12
1:K:18:PRO:HA	1:K:113:THR:HG22	1.33	1.10
1:N:18:PRO:HA	1:N:113:THR:HG22	1.28	1.10
1:L:18:PRO:HA	1:L:113:THR:HG22	1.33	1.10
1:M:97:THR:HG22	1:M:100:GLY:H	1.16	1.10
1:L:17:GLN:O	1:L:113:THR:HG21	1.51	1.09
1:G:18:PRO:HA	1:G:113:THR:HG22	1.35	1.08
1:B:138:GLY:HA2	1:F:115:PRO:HG2	1.35	1.08
1:E:18:PRO:HA	1:E:113:THR:HG22	1.28	1.07
1:L:196:PHE:CZ	2:L:1000:HEM:O2D	2.07	1.06
1:D:18:PRO:HA	1:D:113:THR:HG22	1.38	1.06
1:A:18:PRO:HA	1:A:113:THR:HG22	1.32	1.05
1:C:18:PRO:HA	1:C:113:THR:CG2	1.86	1.05
1:C:97:THR:HG22	1:C:100:GLY:H	1.14	1.05
1:M:18:PRO:HA	1:M:113:THR:HG22	1.35	1.05
1:G:221:ASN:HD22	1:G:224:HIS:CD2	1.75	1.05
1:H:97:THR:HG22	1:H:100:GLY:H	1.17	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:PHE:CZ	2:D:1000:HEM:O2D	2.12	1.03
1:I:18:PRO:HA	1:I:113:THR:HG22	1.39	1.03
1:K:17:GLN:O	1:K:113:THR:HG21	1.59	1.02
1:K:196:PHE:CZ	2:K:1000:HEM:O2D	2.13	1.01
1:G:97:THR:HG22	1:G:100:GLY:H	1.24	1.01
1:N:221:ASN:HD22	1:N:224:HIS:CD2	1.77	1.01
1:C:221:ASN:HD22	1:C:224:HIS:CD2	1.76	1.01
1:E:221:ASN:HD22	1:E:224:HIS:CD2	1.79	1.01
1:I:97:THR:HG22	1:I:100:GLY:H	1.25	1.00
1:A:174:THR:HB	2:A:1000:HEM:HBB2	1.44	0.99
1:O:17:GLN:O	1:O:113:THR:HG21	1.62	0.99
1:G:221:ASN:ND2	1:G:224:HIS:HD2	1.60	0.98
1:M:17:GLN:O	1:M:113:THR:HG21	1.64	0.98
1:D:97:THR:HG22	1:D:100:GLY:H	1.28	0.97
1:A:221:ASN:HD22	1:A:224:HIS:HD2	0.99	0.97
1:E:221:ASN:ND2	1:E:224:HIS:HD2	1.63	0.97
1:R:18:PRO:HA	1:R:113:THR:HG22	1.45	0.97
1:Q:97:THR:HG22	1:Q:100:GLY:H	1.29	0.97
1:B:97:THR:HG22	1:B:100:GLY:H	1.28	0.96
1:H:221:ASN:HD22	1:H:224:HIS:HD2	1.13	0.96
1:N:221:ASN:ND2	1:N:224:HIS:HD2	1.64	0.96
1:P:18:PRO:HA	1:P:113:THR:HG22	1.43	0.96
1:S:221:ASN:HD22	1:S:224:HIS:CD2	1.83	0.96
1:C:221:ASN:ND2	1:C:224:HIS:HD2	1.62	0.95
1:J:18:PRO:HA	1:J:113:THR:CG2	1.95	0.95
2:L:1000:HEM:HHC	2:L:1000:HEM:HBB2	1.48	0.95
1:F:18:PRO:HA	1:F:113:THR:HG22	1.49	0.95
1:H:18:PRO:HA	1:H:113:THR:HG22	1.45	0.95
1:B:221:ASN:HD22	1:B:224:HIS:HD2	0.98	0.95
1:P:221:ASN:HD22	1:P:224:HIS:HD2	1.12	0.95
1:T:18:PRO:HA	1:T:113:THR:HG22	1.50	0.94
1:F:221:ASN:HD22	1:F:224:HIS:HD2	1.04	0.94
1:L:221:ASN:HD22	1:L:224:HIS:HD2	1.00	0.94
1:N:18:PRO:HA	1:N:113:THR:CG2	1.97	0.94
1:B:221:ASN:HD22	1:B:224:HIS:CD2	1.86	0.94
1:O:221:ASN:HD22	1:O:224:HIS:HD2	0.97	0.94
1:C:196:PHE:CZ	2:C:1000:HEM:O2D	2.21	0.94
1:Q:17:GLN:O	1:Q:113:THR:HG21	1.68	0.93
1:D:221:ASN:HD22	1:D:224:HIS:HD2	1.03	0.93
2:H:1000:HEM:HHC	2:H:1000:HEM:HBB2	1.48	0.93
1:A:221:ASN:HD22	1:A:224:HIS:CD2	1.87	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:221:ASN:HD22	1:J:224:HIS:HD2	1.03	0.93
1:J:221:ASN:HD22	1:J:224:HIS:CD2	1.86	0.93
1:I:221:ASN:HD22	1:I:224:HIS:CD2	1.87	0.93
1:F:196:PHE:CZ	2:F:1000:HEM:O2D	2.22	0.93
1:R:221:ASN:HD22	1:R:224:HIS:HD2	1.05	0.93
1:A:196:PHE:CZ	2:A:1000:HEM:O2D	2.21	0.93
1:N:17:GLN:O	1:N:113:THR:HG21	1.69	0.93
1:G:211:LEU:HD11	2:G:1000:HEM:HBB2	1.49	0.93
1:O:221:ASN:HD22	1:O:224:HIS:CD2	1.87	0.92
1:E:97:THR:HG22	1:E:100:GLY:H	1.34	0.92
1:Q:145:ILE:HD13	1:Q:233:LEU:HD13	1.52	0.92
1:A:97:THR:HG22	1:A:100:GLY:H	1.33	0.92
1:N:221:ASN:HD22	1:N:224:HIS:HD2	0.94	0.92
1:C:17:GLN:O	1:C:113:THR:HG21	1.70	0.92
1:N:159:SER:OG	1:N:162:GLU:HG3	1.70	0.92
1:C:221:ASN:HD22	1:C:224:HIS:HD2	0.95	0.92
1:A:235:THR:HG23	1:A:237:HIS:NE2	1.85	0.91
1:K:221:ASN:HD22	1:K:224:HIS:CD2	1.88	0.91
1:T:221:ASN:HD22	1:T:224:HIS:HD2	1.16	0.91
1:I:17:GLN:O	1:I:113:THR:HG21	1.71	0.91
1:T:196:PHE:CZ	2:T:1000:HEM:O2D	2.22	0.91
1:A:18:PRO:HA	1:A:113:THR:CG2	2.00	0.91
1:D:221:ASN:HD22	1:D:224:HIS:CD2	1.88	0.90
1:H:196:PHE:CZ	2:H:1000:HEM:O2D	2.24	0.90
1:L:221:ASN:HD22	1:L:224:HIS:CD2	1.89	0.90
1:S:18:PRO:HA	1:S:113:THR:HG22	1.50	0.90
1:K:221:ASN:HD22	1:K:224:HIS:HD2	0.96	0.90
1:G:18:PRO:HA	1:G:113:THR:CG2	2.00	0.90
1:K:18:PRO:HA	1:K:113:THR:CG2	2.01	0.90
1:I:18:PRO:HA	1:I:113:THR:CG2	2.01	0.89
1:S:33:TRP:CH2	1:S:99:VAL:HG13	2.08	0.89
1:H:221:ASN:HD22	1:H:224:HIS:CD2	1.89	0.89
1:S:48:VAL:O	1:S:52:ILE:HG13	1.72	0.89
1:B:18:PRO:HA	1:B:113:THR:HG22	1.54	0.88
1:I:221:ASN:HD22	1:I:224:HIS:HD2	0.95	0.88
1:L:18:PRO:HA	1:L:113:THR:CG2	2.02	0.88
1:J:17:GLN:O	1:J:113:THR:HG21	1.73	0.88
1:S:97:THR:HG22	1:S:100:GLY:H	1.39	0.87
1:S:221:ASN:HD22	1:S:224:HIS:HD2	0.91	0.87
1:A:17:GLN:O	1:A:113:THR:HG21	1.75	0.87
1:T:211:LEU:HD11	2:T:1000:HEM:HBB2	1.54	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:PHE:O	1:D:97:THR:HB	1.73	0.87
1:E:221:ASN:HD22	1:E:224:HIS:HD2	0.91	0.86
1:G:221:ASN:HD22	1:G:224:HIS:HD2	0.89	0.86
1:E:196:PHE:CZ	2:E:1000:HEM:O2D	2.28	0.86
1:B:221:ASN:ND2	1:B:224:HIS:HD2	1.73	0.86
1:B:94:PHE:O	1:B:97:THR:HB	1.76	0.86
1:B:196:PHE:CZ	2:B:1000:HEM:O2D	2.29	0.85
1:R:196:PHE:CZ	2:R:1000:HEM:O2D	2.30	0.85
1:P:69:LEU:HG	1:T:88:GLN:HG3	1.56	0.85
1:L:97:THR:HG22	1:L:100:GLY:H	1.41	0.85
1:B:17:GLN:O	1:B:113:THR:HG21	1.75	0.85
1:R:17:GLN:O	1:R:113:THR:HG21	1.76	0.85
1:D:18:PRO:HA	1:D:113:THR:CG2	2.06	0.84
1:J:196:PHE:CZ	2:J:1000:HEM:O2D	2.29	0.84
1:O:97:THR:HG22	1:O:100:GLY:N	1.91	0.84
1:P:94:PHE:O	1:P:97:THR:HG22	1.77	0.84
1:A:221:ASN:ND2	1:A:224:HIS:HD2	1.75	0.84
1:B:235:THR:HG23	1:B:237:HIS:NE2	1.93	0.84
1:O:18:PRO:HA	1:O:113:THR:HG22	1.58	0.84
1:O:221:ASN:ND2	1:O:224:HIS:HD2	1.74	0.84
1:O:97:THR:CG2	1:O:100:GLY:H	1.89	0.83
1:E:97:THR:CG2	1:E:100:GLY:H	1.91	0.83
1:Q:196:PHE:CZ	2:Q:1000:HEM:O2D	2.32	0.82
1:N:97:THR:HG22	1:N:100:GLY:H	1.44	0.82
1:E:17:GLN:O	1:E:113:THR:HG21	1.78	0.82
1:I:212:MET:HG3	1:J:190:GLY:CA	2.10	0.82
1:E:18:PRO:HA	1:E:113:THR:CG2	2.09	0.82
1:H:221:ASN:ND2	1:H:224:HIS:HD2	1.77	0.82
1:J:221:ASN:ND2	1:J:224:HIS:HD2	1.76	0.82
1:O:196:PHE:CZ	2:O:1000:HEM:O2D	2.34	0.81
1:C:94:PHE:O	1:C:97:THR:HB	1.80	0.81
1:L:221:ASN:ND2	1:L:224:HIS:HD2	1.77	0.81
1:S:221:ASN:ND2	1:S:224:HIS:HD2	1.75	0.81
1:D:221:ASN:ND2	1:D:224:HIS:HD2	1.77	0.81
1:A:97:THR:CG2	1:A:100:GLY:H	1.94	0.81
1:L:196:PHE:HZ	2:L:1000:HEM:O2D	1.64	0.80
1:P:27:PHE:HB2	1:P:75:PHE:CZ	2.17	0.80
1:M:97:THR:CG2	1:M:100:GLY:H	1.93	0.79
1:A:174:THR:CB	2:A:1000:HEM:HBB2	2.12	0.79
1:K:97:THR:HG22	1:K:100:GLY:H	1.46	0.79
1:C:97:THR:HG22	1:C:100:GLY:N	1.95	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:221:ASN:HD22	1:R:224:HIS:CD2	1.97	0.78
1:P:221:ASN:HD22	1:P:224:HIS:CD2	1.99	0.78
1:M:97:THR:HG22	1:M:100:GLY:N	1.97	0.78
1:J:97:THR:HG22	1:J:100:GLY:H	1.49	0.77
1:Q:212:MET:HG3	1:R:190:GLY:HA3	1.65	0.77
1:F:17:GLN:O	1:F:113:THR:HG21	1.84	0.77
1:O:94:PHE:O	1:O:97:THR:HB	1.85	0.77
1:I:196:PHE:CZ	2:I:1000:HEM:O2D	2.39	0.76
1:R:211:LEU:HD11	2:R:1000:HEM:HBB2	1.67	0.76
1:K:221:ASN:ND2	1:K:224:HIS:HD2	1.80	0.76
1:S:221:ASN:HA	1:S:224:HIS:CD2	2.20	0.75
1:E:235:THR:HG23	1:E:237:HIS:NE2	2.01	0.75
1:J:97:THR:CG2	1:J:100:GLY:H	1.99	0.75
1:S:66:THR:HG22	1:S:234:GLY:HA3	1.69	0.75
1:M:18:PRO:HA	1:M:113:THR:CG2	2.13	0.74
1:G:196:PHE:CZ	2:G:1000:HEM:O2D	2.40	0.74
1:H:212:MET:HG3	1:I:190:GLY:CA	2.17	0.74
1:M:221:ASN:HD22	1:M:224:HIS:CD2	2.05	0.74
1:N:212:MET:HG3	1:O:190:GLY:CA	2.16	0.74
1:G:65:LEU:HB3	1:G:235:THR:HG22	1.69	0.74
1:T:53:GLU:O	1:T:56:LYS:HG3	1.87	0.74
1:K:212:MET:HG3	1:L:190:GLY:CA	2.18	0.74
1:F:145:ILE:HD13	1:F:233:LEU:HD13	1.70	0.74
1:I:94:PHE:O	1:I:97:THR:HB	1.86	0.74
1:T:221:ASN:HD22	1:T:224:HIS:CD2	2.04	0.74
1:D:17:GLN:O	1:D:113:THR:HG21	1.87	0.73
1:H:97:THR:HG22	1:H:100:GLY:N	2.00	0.73
1:L:235:THR:HG23	1:L:237:HIS:NE2	2.02	0.73
1:G:212:MET:HG3	1:H:190:GLY:HA3	1.68	0.73
1:N:59:VAL:HG12	1:N:81:ALA:HB2	1.70	0.73
1:H:145:ILE:HD13	1:H:233:LEU:HD13	1.70	0.73
1:J:235:THR:HG23	1:J:237:HIS:NE2	2.02	0.73
1:B:190:GLY:CA	1:D:212:MET:HG3	2.19	0.73
1:J:65:LEU:HB3	1:J:235:THR:HG22	1.70	0.72
1:L:97:THR:CG2	1:L:100:GLY:H	2.02	0.72
1:P:196:PHE:CZ	2:P:1000:HEM:O2D	2.43	0.72
1:F:221:ASN:HD22	1:F:224:HIS:CD2	1.97	0.72
1:I:211:LEU:HD11	2:I:1000:HEM:HBB2	1.71	0.72
1:P:105:VAL:HG12	1:S:71:THR:HG23	1.71	0.72
1:G:94:PHE:O	1:G:97:THR:HB	1.89	0.72
1:F:212:MET:HG3	1:G:190:GLY:CA	2.18	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:MET:HG3	1:G:190:GLY:HA3	1.69	0.72
1:I:221:ASN:ND2	1:I:224:HIS:HD2	1.79	0.72
1:H:18:PRO:HA	1:H:113:THR:CG2	2.20	0.72
1:Q:221:ASN:HD22	1:Q:224:HIS:CD2	2.08	0.72
1:B:105:VAL:HG12	1:D:71:THR:HG23	1.72	0.71
1:A:154:GLU:OE1	1:E:222:LYS:HE2	1.90	0.71
1:O:65:LEU:HB3	1:O:235:THR:HG22	1.70	0.71
1:A:71:THR:HG23	1:D:105:VAL:HG12	1.71	0.71
1:B:18:PRO:HA	1:B:113:THR:CG2	2.19	0.71
1:M:221:ASN:HD22	1:M:224:HIS:HD2	1.38	0.71
1:H:212:MET:HG3	1:I:190:GLY:HA3	1.72	0.71
1:G:17:GLN:O	1:G:113:THR:HG21	1.89	0.71
1:K:180:ASN:HB3	1:K:181:VAL:HG23	1.71	0.71
1:S:97:THR:CG2	1:S:100:GLY:H	2.03	0.70
1:I:212:MET:HG3	1:J:190:GLY:HA2	1.74	0.70
1:F:190:GLY:HA3	1:J:212:MET:HG3	1.73	0.70
1:E:211:LEU:HD11	2:E:1000:HEM:HBB2	1.74	0.70
1:S:235:THR:HG23	1:S:237:HIS:NE2	2.06	0.70
1:K:235:THR:HG23	1:K:237:HIS:NE2	2.07	0.70
1:F:38:VAL:HB	1:F:41:ARG:NH1	2.07	0.69
1:N:196:PHE:CZ	2:N:1000:HEM:O2D	2.45	0.69
1:C:211:LEU:HD11	2:C:1000:HEM:HBB2	1.75	0.69
1:A:190:GLY:HA3	1:E:212:MET:HG3	1.73	0.69
1:R:118:TYR:HE2	2:R:1000:HEM:O1D	1.76	0.69
1:R:212:MET:HG3	1:S:190:GLY:HA3	1.73	0.69
1:N:18:PRO:CA	1:N:113:THR:HG22	2.15	0.69
1:P:190:GLY:HA3	1:S:212:MET:HG3	1.72	0.69
1:A:97:THR:HG22	1:A:100:GLY:N	2.06	0.69
1:K:221:ASN:HA	1:K:224:HIS:CD2	2.28	0.69
1:P:17:GLN:O	1:P:113:THR:HG21	1.92	0.69
1:S:196:PHE:CZ	2:S:1000:HEM:O2D	2.45	0.69
1:T:26:MET:HG3	1:T:76:PHE:HB3	1.75	0.69
1:A:174:THR:HG22	1:A:211:LEU:HD11	1.75	0.69
1:G:116:LEU:HA	2:G:1000:HEM:O1A	1.93	0.69
1:K:212:MET:HG3	1:L:190:GLY:HA2	1.75	0.69
1:G:235:THR:HG23	1:G:237:HIS:NE2	2.09	0.68
1:P:66:THR:HG22	1:P:234:GLY:HA3	1.76	0.68
1:S:17:GLN:O	1:S:113:THR:HG21	1.93	0.68
1:G:145:ILE:HD13	1:G:233:LEU:HD13	1.75	0.68
1:K:145:ILE:HD13	1:K:233:LEU:HD13	1.74	0.68
1:Q:11:ARG:NH2	1:Q:62:ASP:OD1	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:LYS:HA	1:D:195:ASP:HB2	1.76	0.67
1:F:235:THR:HG23	1:F:237:HIS:NE2	2.09	0.67
1:G:212:MET:HG3	1:H:190:GLY:CA	2.24	0.67
1:K:105:VAL:HG12	1:O:71:THR:HG23	1.75	0.67
1:A:70:GLU:OE2	1:A:232:THR:HA	1.94	0.67
1:D:235:THR:HG23	1:D:237:HIS:NE2	2.09	0.67
1:P:222:LYS:HE2	1:T:154:GLU:OE1	1.95	0.67
1:Q:94:PHE:O	1:Q:97:THR:HB	1.93	0.67
1:R:235:THR:HG23	1:R:237:HIS:NE2	2.09	0.67
1:A:145:ILE:HD13	1:A:233:LEU:HD13	1.76	0.67
1:A:235:THR:CG2	1:A:237:HIS:NE2	2.56	0.67
1:Q:55:HIS:CD2	1:Q:58:ASN:HD22	2.12	0.67
1:I:71:THR:HG23	1:J:105:VAL:HG12	1.77	0.66
1:R:221:ASN:ND2	1:R:224:HIS:HD2	1.88	0.66
1:A:174:THR:HG22	1:A:211:LEU:CD1	2.26	0.66
1:M:116:LEU:HA	2:M:1000:HEM:O1A	1.95	0.66
1:P:27:PHE:HB2	1:P:75:PHE:CE2	2.31	0.66
1:A:38:VAL:O	1:A:39:ALA:CB	2.42	0.66
1:A:44:ALA:HB1	1:A:99:VAL:HG22	1.76	0.66
1:B:235:THR:CG2	1:B:237:HIS:NE2	2.58	0.66
1:L:97:THR:HG22	1:L:100:GLY:N	2.09	0.66
1:K:211:LEU:HD11	2:K:1000:HEM:HBB2	1.78	0.66
1:L:116:LEU:HA	2:L:1000:HEM:O1A	1.95	0.66
1:D:38:VAL:O	1:D:39:ALA:CB	2.44	0.66
1:F:221:ASN:ND2	1:F:224:HIS:HD2	1.87	0.66
1:N:212:MET:HG3	1:O:190:GLY:HA2	1.78	0.66
1:Q:55:HIS:HD2	1:Q:58:ASN:HD22	1.44	0.66
1:Q:116:LEU:HA	2:Q:1000:HEM:O1A	1.96	0.66
1:I:235:THR:HG23	1:I:237:HIS:NE2	2.11	0.65
1:K:116:LEU:HA	2:K:1000:HEM:O1A	1.94	0.65
1:Q:190:GLY:HA3	1:T:212:MET:HG3	1.79	0.65
1:F:118:TYR:HE2	2:F:1000:HEM:O1D	1.80	0.65
1:G:44:ALA:HB1	1:G:99:VAL:HG23	1.78	0.65
1:M:196:PHE:CZ	2:M:1000:HEM:O2D	2.50	0.65
1:O:18:PRO:HA	1:O:113:THR:CG2	2.25	0.65
1:P:44:ALA:HB1	1:P:99:VAL:HG22	1.78	0.65
1:N:235:THR:HG23	1:N:237:HIS:NE2	2.11	0.65
1:R:94:PHE:O	1:R:97:THR:HG22	1.95	0.65
1:P:221:ASN:ND2	1:P:224:HIS:HD2	1.91	0.65
1:T:221:ASN:ND2	1:T:224:HIS:HD2	1.90	0.65
1:F:180:ASN:HB3	1:F:181:VAL:HG23	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1000:HEM:HHC	2:H:1000:HEM:CBB	2.25	0.64
1:P:127:LEU:HD12	1:P:168:GLU:HG2	1.78	0.64
1:A:38:VAL:O	1:A:39:ALA:HB2	1.98	0.64
1:F:190:GLY:CA	1:J:212:MET:HG3	2.27	0.64
1:H:116:LEU:HA	2:H:1000:HEM:O1A	1.97	0.64
1:D:70:GLU:OE2	1:D:232:THR:HA	1.96	0.64
1:B:116:LEU:HA	2:B:1000:HEM:O1A	1.98	0.64
1:C:212:MET:HG3	1:E:190:GLY:HA3	1.79	0.64
1:F:222:LYS:HE2	1:G:154:GLU:OE1	1.98	0.64
1:N:212:MET:HG3	1:O:190:GLY:HA3	1.79	0.64
1:C:212:MET:HG3	1:E:190:GLY:CA	2.28	0.64
1:M:212:MET:HG3	1:N:190:GLY:HA3	1.80	0.64
1:I:212:MET:HG3	1:J:190:GLY:HA3	1.79	0.64
1:N:222:LYS:HE2	1:O:154:GLU:OE1	1.98	0.64
1:O:211:LEU:HD11	2:O:1000:HEM:HBB2	1.79	0.64
1:Q:222:LYS:HE2	1:R:154:GLU:OE1	1.98	0.63
1:B:41:ARG:NH2	1:B:247:ALA:O	2.31	0.63
1:F:18:PRO:HA	1:F:113:THR:CG2	2.26	0.63
1:R:30:ARG:O	1:R:33:TRP:HB3	1.97	0.63
1:S:59:VAL:HG12	1:S:81:ALA:HB2	1.80	0.63
1:B:190:GLY:HA2	1:D:212:MET:HG3	1.79	0.63
1:F:150:LYS:HA	1:F:195:ASP:HB2	1.79	0.63
1:F:221:ASN:HA	1:F:224:HIS:CD2	2.34	0.63
1:N:117:ASN:N	2:N:1000:HEM:O1A	2.31	0.63
1:Q:59:VAL:HG12	1:Q:81:ALA:HB2	1.81	0.63
1:P:9:ILE:O	1:P:9:ILE:HG22	1.98	0.63
1:A:190:GLY:CA	1:E:212:MET:HG3	2.29	0.62
1:H:17:GLN:O	1:H:113:THR:HG21	1.98	0.62
1:L:11:ARG:NH2	1:L:62:ASP:OD1	2.31	0.62
1:R:97:THR:CG2	1:R:100:GLY:H	2.12	0.62
1:O:33:TRP:CH2	1:O:41:ARG:HG2	2.35	0.62
1:Q:17:GLN:O	1:Q:113:THR:CG2	2.43	0.62
1:I:119:ILE:HG13	2:I:1000:HEM:HMA2	1.80	0.62
1:D:116:LEU:HD13	1:D:119:ILE:O	2.00	0.62
1:A:177:TYR:HB2	2:A:1000:HEM:HBB1	1.82	0.62
1:N:38:VAL:O	1:N:39:ALA:HB2	1.99	0.62
1:N:97:THR:CG2	1:N:100:GLY:H	2.12	0.62
1:C:235:THR:HG23	1:C:237:HIS:NE2	2.15	0.62
1:J:116:LEU:HA	2:J:1000:HEM:O1A	1.99	0.62
1:T:116:LEU:HA	2:T:1000:HEM:O1A	2.00	0.62
1:A:174:THR:HB	2:A:1000:HEM:CBB	2.26	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:LEU:HD11	2:F:1000:HEM:HBB2	1.82	0.61
1:J:201:GLU:HG2	1:J:236:ILE:HD11	1.81	0.61
1:O:116:LEU:HA	2:O:1000:HEM:O1A	2.00	0.61
1:N:150:LYS:HA	1:N:195:ASP:HB2	1.82	0.61
1:B:145:ILE:HD13	1:B:233:LEU:HD13	1.82	0.61
1:B:190:GLY:HA3	1:D:212:MET:HG3	1.81	0.61
1:K:150:LYS:HA	1:K:195:ASP:HB2	1.82	0.61
1:L:20:VAL:H	1:L:113:THR:HB	1.65	0.61
1:F:38:VAL:HB	1:F:41:ARG:HH12	1.64	0.61
1:N:67:ARG:HB2	1:N:74:ASP:HB3	1.83	0.61
1:P:20:VAL:H	1:P:113:THR:HB	1.66	0.61
1:E:97:THR:HG22	1:E:100:GLY:N	2.09	0.61
1:G:211:LEU:HD11	2:G:1000:HEM:CBB	2.28	0.61
1:J:174:THR:HB	2:J:1000:HEM:HBB2	1.83	0.61
1:P:116:LEU:HA	2:P:1000:HEM:O1A	2.00	0.61
1:L:224:HIS:HE1	5:L:3000:HOH:O	1.82	0.60
1:Q:18:PRO:HA	1:Q:113:THR:HG22	1.82	0.60
1:A:116:LEU:HA	2:A:1000:HEM:O1A	2.01	0.60
1:B:97:THR:HG22	1:B:100:GLY:N	2.09	0.60
1:T:9:ILE:HG22	1:T:9:ILE:O	2.01	0.60
1:G:97:THR:HG22	1:G:100:GLY:N	2.07	0.60
1:N:11:ARG:NH2	1:N:62:ASP:OD1	2.35	0.60
1:R:18:PRO:HA	1:R:113:THR:CG2	2.28	0.60
1:M:158:MET:O	1:M:163:ARG:NH1	2.34	0.60
1:P:97:THR:HG23	1:P:100:GLY:H	1.67	0.60
1:T:235:THR:HG23	1:T:237:HIS:NE2	2.16	0.60
1:M:221:ASN:ND2	1:M:224:HIS:HD2	2.00	0.60
1:D:174:THR:HB	2:D:1000:HEM:HBB2	1.84	0.60
1:J:48:VAL:O	1:J:52:ILE:HG13	2.01	0.60
1:L:211:LEU:O	1:L:214:SER:HB2	2.02	0.60
1:P:18:PRO:HA	1:P:113:THR:CG2	2.27	0.60
1:P:190:GLY:CA	1:S:212:MET:HG3	2.31	0.60
1:B:65:LEU:HB3	1:B:235:THR:HG22	1.82	0.59
1:F:71:THR:HG23	1:G:105:VAL:HG12	1.84	0.59
1:L:224:HIS:CE1	5:L:3000:HOH:O	2.53	0.59
1:S:97:THR:HG22	1:S:100:GLY:N	2.14	0.59
1:B:159:SER:OG	1:B:162:GLU:HG3	2.01	0.59
1:C:97:THR:CG2	1:C:100:GLY:H	2.03	0.59
1:N:71:THR:HG23	1:O:105:VAL:HG12	1.83	0.59
1:P:221:ASN:HA	1:P:224:HIS:CD2	2.38	0.59
1:B:11:ARG:NH2	1:B:62:ASP:OD1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:VAL:H	1:F:113:THR:HB	1.67	0.59
1:N:158:MET:O	1:N:163:ARG:NH1	2.36	0.59
1:M:180:ASN:HB3	1:M:181:VAL:HG23	1.84	0.59
1:A:222:LYS:HE2	1:D:154:GLU:OE1	2.03	0.59
1:K:18:PRO:CA	1:K:113:THR:HG22	2.22	0.59
1:L:70:GLU:OE2	1:L:232:THR:HA	2.03	0.59
1:N:97:THR:HG22	1:N:100:GLY:N	2.17	0.59
1:R:116:LEU:HA	2:R:1000:HEM:O1A	2.03	0.59
1:B:97:THR:CG2	1:B:100:GLY:H	2.09	0.58
1:C:66:THR:HG22	1:C:234:GLY:HA3	1.84	0.58
1:D:20:VAL:H	1:D:113:THR:HB	1.68	0.58
1:H:94:PHE:O	1:H:97:THR:HB	2.03	0.58
1:T:174:THR:HG22	1:T:211:LEU:CD1	2.33	0.58
1:A:145:ILE:CD1	1:A:233:LEU:HD13	2.33	0.58
1:J:174:THR:HB	2:J:1000:HEM:CBB	2.33	0.58
1:S:41:ARG:O	1:S:44:ALA:HB3	2.03	0.58
1:C:183:ARG:NH2	3:C:2000:NO2:O2	2.36	0.58
1:D:116:LEU:HA	2:D:1000:HEM:O1A	2.03	0.58
1:H:212:MET:HG3	1:I:190:GLY:HA2	1.84	0.58
1:K:11:ARG:NH2	1:K:62:ASP:OD1	2.35	0.58
1:C:116:LEU:HA	2:C:1000:HEM:O1A	2.04	0.58
1:N:55:HIS:CD2	1:N:58:ASN:HD22	2.22	0.58
1:P:235:THR:HG23	1:P:237:HIS:NE2	2.18	0.57
1:D:174:THR:HG22	1:D:211:LEU:CD1	2.34	0.57
1:L:212:MET:HG3	1:M:190:GLY:HA3	1.86	0.57
1:P:66:THR:HG22	1:P:234:GLY:CA	2.34	0.57
1:Q:118:TYR:HE2	2:Q:1000:HEM:O1D	1.87	0.57
1:T:211:LEU:CD1	2:T:1000:HEM:HBB2	2.32	0.57
1:A:65:LEU:HB3	1:A:235:THR:HG22	1.87	0.57
1:E:145:ILE:HD13	1:E:233:LEU:HD13	1.86	0.57
1:O:221:ASN:HA	1:O:224:HIS:CD2	2.39	0.57
1:F:118:TYR:CD2	1:F:167:MET:HG3	2.39	0.57
1:A:219:LYS:O	1:A:222:LYS:HB2	2.04	0.57
1:B:166:GLU:OE1	1:B:166:GLU:HA	2.05	0.57
1:G:235:THR:CG2	1:G:237:HIS:NE2	2.67	0.57
1:T:159:SER:OG	1:T:162:GLU:HG3	2.05	0.57
1:H:11:ARG:NH2	1:H:62:ASP:OD1	2.36	0.57
1:M:235:THR:HG23	1:M:237:HIS:NE2	2.19	0.57
1:R:221:ASN:HA	1:R:224:HIS:CD2	2.40	0.57
1:K:118:TYR:CD2	1:K:167:MET:HG3	2.40	0.57
1:M:20:VAL:H	1:M:113:THR:HB	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:27:PHE:CD2	1:P:75:PHE:CE2	2.93	0.57
1:R:97:THR:HG22	1:R:100:GLY:H	1.70	0.57
1:G:221:ASN:HA	1:G:224:HIS:CD2	2.40	0.57
2:K:1000:HEM:HBB2	2:K:1000:HEM:HHC	1.86	0.56
1:Q:109:LEU:HB3	1:Q:197:ILE:CD1	2.34	0.56
1:D:97:THR:HG22	1:D:100:GLY:N	2.10	0.56
1:J:167:MET:CE	2:J:1000:HEM:HBD1	2.35	0.56
1:E:174:THR:HB	2:E:1000:HEM:CBB	2.35	0.56
1:F:94:PHE:O	1:F:97:THR:HG22	2.03	0.56
1:K:235:THR:CG2	1:K:237:HIS:NE2	2.68	0.56
1:M:212:MET:HG3	1:N:190:GLY:CA	2.35	0.56
1:T:23:VAL:HG22	1:T:110:VAL:HG22	1.87	0.56
1:E:20:VAL:H	1:E:113:THR:HB	1.71	0.56
1:N:38:VAL:O	1:N:39:ALA:CB	2.52	0.56
1:R:65:LEU:HB3	1:R:235:THR:HG22	1.87	0.56
1:R:117:ASN:N	2:R:1000:HEM:O1A	2.39	0.56
1:T:150:LYS:HB3	1:T:226:ARG:HB3	1.87	0.56
1:I:11:ARG:NH2	1:I:62:ASP:OD1	2.39	0.56
1:P:195:ASP:HB3	1:P:196:PHE:CE2	2.40	0.56
1:R:26:MET:HG3	1:R:76:PHE:HB3	1.88	0.56
1:K:190:GLY:HA3	1:O:212:MET:HG3	1.88	0.56
1:M:145:ILE:CD1	1:M:233:LEU:HD13	2.35	0.56
1:O:20:VAL:H	1:O:113:THR:HB	1.71	0.56
1:O:145:ILE:HD13	1:O:233:LEU:HD13	1.88	0.56
1:E:235:THR:CG2	1:E:237:HIS:NE2	2.68	0.55
1:G:66:THR:HG22	1:G:234:GLY:HA3	1.88	0.55
1:H:65:LEU:HB3	1:H:235:THR:HG22	1.87	0.55
1:T:118:TYR:CD2	1:T:167:MET:HG3	2.41	0.55
1:J:180:ASN:HB3	1:J:181:VAL:HG23	1.88	0.55
1:H:224:HIS:CE1	5:H:3000:HOH:O	2.59	0.55
1:C:38:VAL:HB	1:C:41:ARG:HH12	1.71	0.55
1:D:174:THR:HG22	1:D:211:LEU:HD11	1.88	0.55
1:E:59:VAL:HG12	1:E:81:ALA:HB2	1.88	0.55
1:E:116:LEU:HA	2:E:1000:HEM:O1A	2.07	0.55
1:K:212:MET:HG3	1:L:190:GLY:HA3	1.87	0.55
1:L:182:LYS:O	1:L:200:PHE:HA	2.07	0.55
1:P:41:ARG:NH2	1:P:247:ALA:O	2.37	0.55
1:S:30:ARG:O	1:S:33:TRP:HB3	2.06	0.55
1:C:222:LYS:HE3	1:E:154:GLU:OE1	2.05	0.55
2:H:1000:HEM:HBB2	2:H:1000:HEM:CHC	2.19	0.55
1:I:38:VAL:O	1:I:39:ALA:CB	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:THR:CG2	1:G:100:GLY:H	2.10	0.55
1:G:196:PHE:HZ	2:G:1000:HEM:O2D	1.85	0.55
1:C:211:LEU:CD1	2:C:1000:HEM:HBB2	2.36	0.55
1:J:26:MET:SD	1:J:26:MET:N	2.80	0.54
1:L:221:ASN:HA	1:L:224:HIS:CD2	2.42	0.54
1:P:174:THR:HG22	1:P:211:LEU:HD11	1.88	0.54
1:Q:18:PRO:HA	1:Q:113:THR:CG2	2.36	0.54
1:C:221:ASN:ND2	1:C:224:HIS:CD2	2.52	0.54
1:P:27:PHE:CB	1:P:75:PHE:CZ	2.88	0.54
1:P:154:GLU:OE1	1:S:222:LYS:HE2	2.07	0.54
1:Q:158:MET:O	1:Q:163:ARG:NH1	2.41	0.54
1:B:182:LYS:O	1:B:200:PHE:HA	2.08	0.54
1:C:20:VAL:H	1:C:113:THR:HB	1.72	0.54
1:H:145:ILE:CD1	1:H:233:LEU:HD13	2.36	0.54
1:B:88:GLN:HG3	1:D:69:LEU:HG	1.90	0.54
1:L:196:PHE:CE1	2:L:1000:HEM:O2D	2.60	0.54
2:L:1000:HEM:HHC	2:L:1000:HEM:CBB	2.31	0.54
1:K:97:THR:HG22	1:K:100:GLY:N	2.21	0.54
1:B:154:GLU:OE1	1:D:222:LYS:HE3	2.08	0.54
1:F:92:ARG:NH1	1:J:245:ALA:HB1	2.23	0.54
1:F:116:LEU:HA	2:F:1000:HEM:O1A	2.07	0.54
1:I:235:THR:CG2	1:I:237:HIS:NE2	2.71	0.54
1:M:94:PHE:O	1:M:97:THR:HB	2.07	0.54
1:A:11:ARG:NH2	1:A:62:ASP:OD1	2.40	0.53
1:A:33:TRP:CZ2	1:A:41:ARG:HG2	2.43	0.53
1:F:97:THR:CG2	1:F:100:GLY:H	2.21	0.53
1:C:158:MET:O	1:C:163:ARG:NH1	2.41	0.53
1:D:221:ASN:HA	1:D:224:HIS:CD2	2.43	0.53
1:S:41:ARG:NH2	1:S:247:ALA:O	2.36	0.53
1:Q:221:ASN:HD22	1:Q:224:HIS:HD2	1.54	0.53
1:S:235:THR:HG23	1:S:237:HIS:CD2	2.43	0.53
1:H:118:TYR:HE2	2:H:1000:HEM:O1D	1.91	0.53
1:L:21:PHE:O	1:L:80:ASN:HA	2.09	0.53
1:F:119:ILE:HG13	2:F:1000:HEM:HMA2	1.91	0.53
1:F:177:TYR:HB2	2:F:1000:HEM:HBB1	1.88	0.53
1:K:97:THR:CG2	1:K:100:GLY:H	2.17	0.53
1:T:17:GLN:O	1:T:113:THR:HG21	2.08	0.53
1:E:211:LEU:O	1:E:214:SER:HB2	2.07	0.53
1:I:65:LEU:HB3	1:I:235:THR:HG22	1.91	0.53
1:T:174:THR:HG22	1:T:211:LEU:HD11	1.89	0.53
1:G:182:LYS:O	1:G:200:PHE:HA	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:TYR:CD2	1:H:167:MET:HG3	2.43	0.53
1:K:38:VAL:O	1:K:39:ALA:CB	2.56	0.53
1:A:127:LEU:HD23	1:A:175:LEU:HD11	1.91	0.53
1:F:26:MET:HB2	1:F:107:GLU:HB2	1.91	0.53
1:G:158:MET:O	1:G:163:ARG:NH1	2.41	0.53
1:I:116:LEU:HA	2:I:1000:HEM:O1A	2.08	0.53
1:R:99:VAL:HG21	1:R:243:ILE:HD12	1.90	0.53
1:D:182:LYS:O	1:D:200:PHE:HA	2.09	0.52
1:D:235:THR:CG2	1:D:237:HIS:NE2	2.72	0.52
1:C:75:PHE:CD1	1:C:246:LEU:HD11	2.44	0.52
1:N:167:MET:CE	2:N:1000:HEM:HBD1	2.39	0.52
1:P:88:GLN:OE1	1:S:235:THR:HG21	2.08	0.52
1:B:67:ARG:HG2	1:C:92:ARG:HG3	1.91	0.52
1:M:235:THR:CG2	1:M:237:HIS:NE2	2.72	0.52
1:N:150:LYS:HB3	1:N:226:ARG:HB3	1.91	0.52
1:M:211:LEU:HD11	2:M:1000:HEM:HBB2	1.90	0.52
1:S:63:LEU:HB3	1:S:239:PRO:HA	1.92	0.52
1:A:94:PHE:O	1:A:97:THR:HB	2.10	0.52
1:E:221:ASN:ND2	1:E:224:HIS:CD2	2.55	0.52
1:G:221:ASN:ND2	1:G:224:HIS:CD2	2.51	0.52
1:J:70:GLU:HA	1:J:70:GLU:OE1	2.10	0.52
1:Q:118:TYR:CD2	1:Q:167:MET:HG3	2.44	0.52
1:T:22:GLY:HA2	1:T:79:ILE:O	2.09	0.52
1:T:66:THR:HG22	1:T:234:GLY:HA3	1.91	0.52
1:D:11:ARG:NH2	1:D:62:ASP:OD1	2.43	0.52
1:H:224:HIS:HE1	5:H:3000:HOH:O	1.92	0.52
1:R:119:ILE:HG13	2:R:1000:HEM:HMA2	1.92	0.52
1:M:38:VAL:O	1:M:39:ALA:HB2	2.09	0.52
1:G:118:TYR:HE2	2:G:1000:HEM:O1D	1.91	0.52
1:G:235:THR:HG23	1:G:237:HIS:CD2	2.45	0.52
1:J:118:TYR:HE2	2:J:1000:HEM:O1D	1.93	0.52
1:N:150:LYS:HG2	1:N:225:VAL:CG2	2.40	0.52
1:A:27:PHE:CE1	1:A:95:ARG:HD2	2.45	0.52
1:E:150:LYS:HA	1:E:195:ASP:HB2	1.92	0.52
1:G:180:ASN:HB3	1:G:181:VAL:HG23	1.92	0.52
1:O:196:PHE:CE2	2:O:1000:HEM:O2D	2.63	0.52
1:T:66:THR:HG22	1:T:234:GLY:CA	2.40	0.52
1:F:105:VAL:HG12	1:J:71:THR:HG23	1.92	0.51
1:O:11:ARG:NH2	1:O:62:ASP:OD1	2.43	0.51
1:H:159:SER:OG	1:H:162:GLU:HG3	2.10	0.51
1:I:119:ILE:CG1	2:I:1000:HEM:HMA2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:221:ASN:HA	1:J:224:HIS:CD2	2.45	0.51
1:F:212:MET:HG3	1:G:190:GLY:HA2	1.91	0.51
1:Q:235:THR:HG23	1:Q:237:HIS:NE2	2.25	0.51
1:S:44:ALA:HB1	1:S:99:VAL:HG22	1.92	0.51
2:B:1000:HEM:CBB	2:B:1000:HEM:HHC	2.41	0.51
1:C:18:PRO:HA	1:C:113:THR:HG21	1.89	0.51
1:I:222:LYS:HE2	1:J:154:GLU:OE1	2.10	0.51
1:Q:117:ASN:N	2:Q:1000:HEM:O1A	2.41	0.51
1:A:212:MET:HG3	1:D:190:GLY:HA3	1.93	0.51
1:F:67:ARG:HG2	1:G:92:ARG:HG3	1.93	0.51
2:B:1000:HEM:HHC	2:B:1000:HEM:HBB2	1.93	0.51
1:R:41:ARG:NH2	1:R:247:ALA:O	2.43	0.51
1:S:33:TRP:HB2	1:S:102:ASN:HB3	1.91	0.51
1:D:65:LEU:HB3	1:D:235:THR:HG22	1.93	0.51
1:E:9:ILE:HG22	1:E:9:ILE:O	2.11	0.51
1:M:118:TYR:CD2	1:M:167:MET:HG3	2.46	0.51
1:M:145:ILE:HD13	1:M:233:LEU:HD13	1.93	0.51
1:L:145:ILE:HD13	1:L:233:LEU:HD13	1.93	0.51
1:Q:221:ASN:ND2	1:Q:224:HIS:HD2	2.09	0.51
1:R:92:ARG:HG2	1:R:92:ARG:HH11	1.75	0.51
1:O:38:VAL:O	1:O:39:ALA:HB2	2.10	0.51
1:S:29:LEU:HD21	1:S:99:VAL:HG12	1.93	0.51
1:B:154:GLU:OE1	1:D:222:LYS:CE	2.59	0.50
1:E:70:GLU:OE2	1:E:232:THR:HA	2.11	0.50
1:E:195:ASP:HB3	1:E:196:PHE:CE2	2.47	0.50
1:L:66:THR:HG22	1:L:234:GLY:HA3	1.93	0.50
1:G:11:ARG:NH2	1:G:62:ASP:OD1	2.44	0.50
1:L:235:THR:CG2	1:L:237:HIS:NE2	2.71	0.50
1:R:145:ILE:HD13	1:R:233:LEU:HD13	1.93	0.50
1:C:174:THR:HG22	1:C:211:LEU:CD1	2.41	0.50
1:E:36:VAL:O	1:E:41:ARG:HD3	2.12	0.50
1:G:118:TYR:CD2	1:G:167:MET:HG3	2.46	0.50
1:S:66:THR:HG22	1:S:234:GLY:CA	2.40	0.50
1:T:142:ARG:NE	1:T:203:ASP:OD1	2.40	0.50
1:C:11:ARG:NH2	1:C:62:ASP:OD1	2.45	0.50
1:P:67:ARG:HG2	1:T:92:ARG:HG3	1.93	0.50
1:F:196:PHE:HZ	2:F:1000:HEM:O2D	1.87	0.50
1:O:180:ASN:HB3	1:O:181:VAL:HG23	1.93	0.50
1:S:116:LEU:HA	2:S:1000:HEM:O1A	2.12	0.50
1:G:71:THR:HG23	1:H:105:VAL:HG12	1.94	0.50
1:I:28:LYS:NZ	1:I:72:ASN:HD22	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:235:THR:CG2	1:J:237:HIS:NE2	2.74	0.50
1:N:116:LEU:HD22	2:N:1000:HEM:HBA2	1.94	0.50
1:Q:224:HIS:CD2	1:Q:227:TRP:CD1	3.00	0.50
1:D:175:LEU:HD12	1:K:126:GLY:HA2	1.94	0.50
1:B:235:THR:HG23	1:B:237:HIS:CD2	2.46	0.50
1:N:75:PHE:CD1	1:N:246:LEU:HD11	2.46	0.50
1:J:18:PRO:CA	1:J:113:THR:HG22	2.19	0.49
1:L:183:ARG:NH2	3:L:2000:NO2:O2	2.41	0.49
1:Q:31:PRO:HB3	1:R:30:ARG:NH2	2.27	0.49
1:Q:212:MET:HG3	1:R:190:GLY:CA	2.37	0.49
1:M:119:ILE:O	1:M:119:ILE:HG22	2.12	0.49
1:I:38:VAL:O	1:I:39:ALA:HB2	2.13	0.49
1:J:97:THR:HG22	1:J:100:GLY:N	2.24	0.49
1:C:180:ASN:HB3	1:C:181:VAL:HG23	1.94	0.49
1:F:148:PRO:HG2	1:F:228:GLY:O	2.12	0.49
1:C:67:ARG:HG2	1:E:92:ARG:HG3	1.93	0.49
1:E:63:LEU:HD13	1:E:77:PHE:CE1	2.46	0.49
1:E:119:ILE:HG13	2:E:1000:HEM:HMA3	1.95	0.49
1:G:55:HIS:CD2	1:G:58:ASN:HD22	2.30	0.49
1:N:44:ALA:HB1	1:N:99:VAL:HG22	1.93	0.49
1:L:44:ALA:HB1	1:L:99:VAL:CG2	2.42	0.49
1:S:38:VAL:O	1:S:39:ALA:HB2	2.12	0.49
1:L:92:ARG:HH11	1:L:92:ARG:HG2	1.78	0.49
1:Q:105:VAL:HG12	1:T:71:THR:HG23	1.94	0.49
1:S:33:TRP:CH2	1:S:41:ARG:HG2	2.47	0.49
1:J:95:ARG:HA	1:J:100:GLY:HA3	1.95	0.49
1:S:119:ILE:HB	2:S:1000:HEM:HMA2	1.95	0.49
1:A:237:HIS:HB2	1:A:242:VAL:HG23	1.94	0.48
1:B:13:THR:O	1:B:16:THR:HB	2.13	0.48
1:E:186:TYR:HB2	1:E:197:ILE:HB	1.94	0.48
1:G:211:LEU:HD21	2:G:1000:HEM:CBB	2.43	0.48
1:I:20:VAL:H	1:I:113:THR:HB	1.77	0.48
1:Q:118:TYR:CE2	2:Q:1000:HEM:O1D	2.66	0.48
1:R:38:VAL:O	1:R:39:ALA:HB2	2.13	0.48
1:C:118:TYR:CD2	1:C:167:MET:HG3	2.48	0.48
1:G:147:ILE:HG21	2:G:1000:HEM:HBC1	1.95	0.48
1:O:211:LEU:CD1	2:O:1000:HEM:HBB2	2.44	0.48
1:J:38:VAL:O	1:J:39:ALA:HB2	2.13	0.48
1:B:158:MET:O	1:B:163:ARG:NH1	2.44	0.48
1:G:44:ALA:HB1	1:G:99:VAL:CG2	2.42	0.48
1:Q:27:PHE:CE1	1:Q:105:VAL:HG22	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD13	1:A:119:ILE:O	2.14	0.48
1:E:211:LEU:HD11	2:E:1000:HEM:CBB	2.43	0.48
1:P:27:PHE:CD2	1:P:75:PHE:HE2	2.31	0.48
1:D:196:PHE:CE1	2:D:1000:HEM:O2D	2.64	0.48
1:G:38:VAL:O	1:G:39:ALA:HB2	2.14	0.48
1:Q:26:MET:SD	1:Q:26:MET:N	2.87	0.48
1:Q:196:PHE:HZ	2:Q:1000:HEM:O2D	1.93	0.48
1:R:10:GLU:HB2	1:R:13:THR:HB	1.96	0.48
1:S:27:PHE:CE1	1:S:105:VAL:HG22	2.48	0.48
1:T:11:ARG:NH1	1:T:60:LEU:HD11	2.28	0.48
1:D:195:ASP:HB3	1:D:196:PHE:CE2	2.48	0.48
1:I:159:SER:OG	1:I:162:GLU:HG3	2.14	0.48
1:P:62:ASP:HB2	1:P:78:ARG:HB3	1.96	0.48
1:Q:180:ASN:HB3	1:Q:181:VAL:HG23	1.95	0.48
1:Q:183:ARG:HD2	2:Q:1000:HEM:HMB2	1.95	0.48
1:S:147:ILE:HG12	1:S:231:THR:HG23	1.96	0.48
1:B:145:ILE:CD1	1:B:233:LEU:HD13	2.43	0.48
1:K:88:GLN:O	1:K:92:ARG:HB2	2.14	0.48
1:A:44:ALA:HB1	1:A:99:VAL:CG2	2.44	0.48
1:E:235:THR:HG23	1:E:237:HIS:CD2	2.48	0.48
1:F:180:ASN:CB	1:F:181:VAL:HG23	2.43	0.48
1:P:30:ARG:NH2	1:S:31:PRO:HB3	2.28	0.48
1:S:53:GLU:HB3	1:S:56:LYS:HZ3	1.79	0.48
1:L:24:PHE:HB2	1:L:109:LEU:HB2	1.96	0.47
1:R:116:LEU:CD2	2:R:1000:HEM:HBA2	2.44	0.47
1:T:26:MET:HG3	1:T:76:PHE:CB	2.44	0.47
1:C:150:LYS:HA	1:C:195:ASP:HB2	1.96	0.47
1:M:38:VAL:O	1:M:39:ALA:CB	2.61	0.47
1:N:21:PHE:O	1:N:80:ASN:HA	2.14	0.47
1:P:145:ILE:HD13	1:P:233:LEU:HD13	1.95	0.47
1:E:64:TYR:CD1	1:E:144:VAL:HG11	2.49	0.47
1:L:235:THR:HG23	1:L:237:HIS:CD2	2.49	0.47
1:P:27:PHE:CE1	1:P:105:VAL:HG22	2.50	0.47
1:B:59:VAL:HB	1:B:79:ILE:HG23	1.95	0.47
1:Q:97:THR:CG2	1:Q:100:GLY:H	2.15	0.47
1:I:97:THR:HG22	1:I:100:GLY:N	2.09	0.47
1:J:118:TYR:CD2	1:J:167:MET:HG3	2.50	0.47
1:P:180:ASN:HB3	1:P:181:VAL:HG23	1.96	0.47
1:A:63:LEU:HG	1:A:242:VAL:HG11	1.95	0.47
1:G:183:ARG:NH2	3:G:2000:NO2:O2	2.44	0.47
1:Q:41:ARG:NE	1:Q:247:ALA:O	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:38:VAL:O	1:R:39:ALA:CB	2.62	0.47
1:D:26:MET:HB3	1:D:73:SER:HB3	1.97	0.47
1:J:211:LEU:HD11	2:J:1000:HEM:HBB2	1.96	0.47
1:K:169:VAL:O	1:K:173:PRO:HD3	2.14	0.47
1:L:119:ILE:HG13	2:L:1000:HEM:HMA3	1.96	0.47
1:R:145:ILE:CD1	1:R:233:LEU:HD13	2.45	0.47
1:R:211:LEU:HD11	2:R:1000:HEM:CBB	2.42	0.47
1:C:55:HIS:CD2	1:C:58:ASN:HD22	2.32	0.47
1:G:211:LEU:CD1	2:G:1000:HEM:HBB2	2.33	0.47
1:L:38:VAL:O	1:L:39:ALA:CB	2.62	0.47
1:Q:128:ASN:O	1:Q:131:LEU:HB3	2.15	0.47
1:C:145:ILE:HD13	1:C:233:LEU:HD13	1.97	0.47
1:E:28:LYS:HD2	1:E:106:PHE:CE1	2.50	0.47
1:F:211:LEU:CD1	2:F:1000:HEM:HBB2	2.44	0.47
1:S:55:HIS:CD2	1:S:58:ASN:HD22	2.33	0.47
1:S:174:THR:HB	2:S:1000:HEM:CBB	2.45	0.47
1:S:186:TYR:HB2	1:S:197:ILE:HB	1.97	0.47
1:T:45:ALA:CB	1:T:244:LYS:HG3	2.45	0.47
1:B:150:LYS:HA	1:B:195:ASP:HB2	1.95	0.47
1:H:24:PHE:HB2	1:H:109:LEU:HB2	1.97	0.47
1:Q:217:GLN:HA	1:R:156:TRP:O	2.15	0.47
1:R:53:GLU:O	1:R:56:LYS:HG3	2.15	0.47
1:A:157:ASN:HD21	1:E:218:VAL:C	2.18	0.46
1:D:177:TYR:HB2	2:D:1000:HEM:HBB1	1.98	0.46
1:F:118:TYR:CE2	2:F:1000:HEM:O1D	2.65	0.46
1:N:150:LYS:HG2	1:N:225:VAL:HG23	1.96	0.46
1:I:97:THR:HG23	1:I:98:THR:N	2.30	0.46
1:K:35:LYS:HB2	1:K:35:LYS:HE3	1.73	0.46
1:O:182:LYS:O	1:O:200:PHE:HA	2.15	0.46
1:I:212:MET:CG	1:J:190:GLY:HA3	2.43	0.46
1:N:65:LEU:HB3	1:N:235:THR:HG22	1.97	0.46
1:Q:151:LYS:NZ	2:Q:1000:HEM:HBD2	2.31	0.46
1:F:65:LEU:HB3	1:F:235:THR:HG22	1.97	0.46
1:L:94:PHE:O	1:L:97:THR:HB	2.14	0.46
1:O:147:ILE:HG12	1:O:231:THR:HG23	1.97	0.46
1:S:211:LEU:O	1:S:214:SER:HB2	2.16	0.46
1:G:196:PHE:CZ	2:G:1000:HEM:HAD1	2.50	0.46
1:I:29:LEU:N	1:I:74:ASP:OD2	2.45	0.46
1:N:26:MET:HB3	1:N:73:SER:HB3	1.97	0.46
1:N:221:ASN:ND2	1:N:224:HIS:CD2	2.55	0.46
1:F:154:GLU:OE1	1:J:222:LYS:HE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:ARG:HG2	1:H:92:ARG:HH11	1.80	0.46
1:S:118:TYR:CE2	2:S:1000:HEM:O1D	2.69	0.46
1:T:33:TRP:CH2	1:T:99:VAL:HG13	2.51	0.46
1:K:36:VAL:O	1:K:41:ARG:HD3	2.16	0.46
1:L:22:GLY:HA2	1:L:79:ILE:O	2.15	0.46
1:P:63:LEU:HD23	1:P:239:PRO:O	2.16	0.46
1:N:195:ASP:HB3	1:N:196:PHE:CE2	2.51	0.46
1:B:211:LEU:HD11	2:B:1000:HEM:HBB2	1.97	0.46
1:I:215:LEU:HD12	1:I:215:LEU:HA	1.81	0.46
1:M:218:VAL:C	1:N:157:ASN:HD21	2.18	0.46
1:Q:44:ALA:HB1	1:Q:99:VAL:HG22	1.97	0.46
1:Q:177:TYR:CD2	1:Q:211:LEU:HD13	2.51	0.46
1:C:159:SER:OG	1:C:162:GLU:HG3	2.15	0.46
1:H:221:ASN:HA	1:H:224:HIS:CD2	2.51	0.46
1:N:116:LEU:CD2	2:N:1000:HEM:HBA2	2.46	0.46
1:J:11:ARG:NH2	1:J:62:ASP:OD1	2.49	0.45
1:K:159:SER:O	1:K:163:ARG:HG3	2.16	0.45
1:L:215:LEU:O	1:L:218:VAL:HG22	2.16	0.45
1:M:222:LYS:HE2	1:N:154:GLU:OE1	2.16	0.45
1:S:33:TRP:CZ2	1:S:99:VAL:HG13	2.51	0.45
1:G:38:VAL:O	1:G:38:VAL:HG13	2.16	0.45
1:G:70:GLU:HA	1:G:70:GLU:OE1	2.15	0.45
1:R:159:SER:OG	1:R:162:GLU:HG3	2.16	0.45
1:R:177:TYR:CD2	1:R:211:LEU:HD13	2.51	0.45
1:T:77:PHE:HE2	1:T:94:PHE:CE2	2.34	0.45
1:T:145:ILE:HD13	1:T:233:LEU:HD13	1.98	0.45
1:T:146:VAL:O	1:T:146:VAL:HG12	2.16	0.45
1:A:212:MET:HG3	1:D:190:GLY:CA	2.47	0.45
1:T:70:GLU:OE2	1:T:232:THR:HA	2.17	0.45
1:B:219:LYS:O	1:B:222:LYS:HB2	2.16	0.45
1:G:211:LEU:O	1:G:214:SER:HB2	2.16	0.45
1:Q:151:LYS:HZ2	2:Q:1000:HEM:HBD2	1.81	0.45
1:J:177:TYR:HB2	2:J:1000:HEM:HBB1	1.99	0.45
1:N:159:SER:HG	1:N:162:GLU:HG3	1.78	0.45
1:P:119:ILE:O	1:P:119:ILE:HG22	2.17	0.45
1:P:196:PHE:CE1	2:P:1000:HEM:O2D	2.69	0.45
1:B:217:GLN:HG2	1:C:156:TRP:O	2.17	0.45
2:B:1000:HEM:HBB2	2:B:1000:HEM:CHC	2.47	0.45
1:F:8:LYS:HB3	1:F:8:LYS:HE2	1.76	0.45
1:M:219:LYS:N	1:N:157:ASN:HD21	2.14	0.45
1:Q:52:ILE:HG12	1:Q:61:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:118:TYR:CE2	2:R:1000:HEM:O1D	2.62	0.45
1:S:117:ASN:N	2:S:1000:HEM:O1A	2.40	0.45
1:E:145:ILE:CD1	1:E:233:LEU:HD13	2.46	0.45
1:F:242:VAL:O	1:F:246:LEU:HG	2.17	0.45
1:L:169:VAL:O	1:L:173:PRO:HD3	2.15	0.45
1:T:27:PHE:O	1:T:73:SER:HA	2.16	0.45
1:B:92:ARG:HG3	1:D:67:ARG:HG2	1.98	0.45
1:J:182:LYS:HB2	1:J:201:GLU:HB2	1.99	0.45
1:E:37:PRO:O	1:E:39:ALA:N	2.50	0.44
1:J:188:SER:O	1:J:189:THR:C	2.55	0.44
1:K:24:PHE:O	1:K:108:THR:HA	2.18	0.44
1:K:92:ARG:HG3	1:O:67:ARG:HG2	1.99	0.44
1:S:24:PHE:HB2	1:S:109:LEU:HB2	1.99	0.44
1:C:212:MET:HG3	1:E:190:GLY:HA2	2.00	0.44
1:F:117:ASN:N	2:F:1000:HEM:O1A	2.47	0.44
1:H:167:MET:O	1:H:170:HIS:HB3	2.16	0.44
1:I:221:ASN:HA	1:I:224:HIS:CD2	2.52	0.44
1:J:167:MET:HE2	2:J:1000:HEM:HBD1	1.99	0.44
1:M:62:ASP:HB2	1:M:78:ARG:HB3	1.99	0.44
1:D:211:LEU:HD21	2:D:1000:HEM:HMC2	1.98	0.44
1:E:8:LYS:HE2	1:E:8:LYS:HB2	1.45	0.44
1:F:174:THR:HB	2:F:1000:HEM:CBB	2.48	0.44
1:Q:95:ARG:HB3	1:T:67:ARG:NH2	2.32	0.44
1:R:47:GLU:OE2	1:R:97:THR:HA	2.17	0.44
1:R:215:LEU:O	1:R:218:VAL:HG22	2.17	0.44
1:T:62:ASP:HB3	1:T:64:TYR:CZ	2.52	0.44
1:C:196:PHE:HZ	2:C:1000:HEM:O2D	1.94	0.44
1:E:95:ARG:HA	1:E:100:GLY:HA3	1.98	0.44
1:E:174:THR:HB	2:E:1000:HEM:HBB2	2.00	0.44
1:G:88:GLN:O	1:G:92:ARG:HB2	2.18	0.44
1:Q:30:ARG:O	1:Q:33:TRP:HB3	2.17	0.44
1:S:11:ARG:NH2	1:S:62:ASP:OD1	2.30	0.44
1:T:38:VAL:O	1:T:39:ALA:CB	2.66	0.44
1:E:117:ASN:N	2:E:1000:HEM:O1A	2.43	0.44
1:J:28:LYS:NZ	1:J:72:ASN:HD22	2.16	0.44
1:P:97:THR:CG2	1:P:100:GLY:H	2.29	0.44
1:T:27:PHE:CE1	1:T:105:VAL:HG22	2.53	0.44
1:B:233:LEU:HD12	1:B:234:GLY:N	2.32	0.44
1:C:75:PHE:CD1	1:C:246:LEU:CD1	3.01	0.44
1:C:211:LEU:CD1	2:C:1000:HEM:CBB	2.95	0.44
1:H:235:THR:HG23	1:H:237:HIS:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:LYS:HB3	1:I:226:ARG:HB3	2.00	0.44
1:L:83:ASP:HB3	1:L:86:LYS:HD2	1.98	0.44
1:Q:94:PHE:O	1:Q:97:THR:CB	2.64	0.44
1:T:65:LEU:HB3	1:T:235:THR:HG22	2.00	0.44
1:C:211:LEU:HD11	2:C:1000:HEM:CBB	2.47	0.44
1:F:150:LYS:HB3	1:F:226:ARG:HB3	2.00	0.44
1:H:26:MET:HB3	1:H:73:SER:HB3	2.00	0.44
1:I:26:MET:HB2	1:I:107:GLU:HB2	2.00	0.44
1:T:235:THR:HG23	1:T:237:HIS:CD2	2.52	0.44
1:A:182:LYS:HB2	1:A:201:GLU:HB2	1.99	0.44
1:G:62:ASP:HB3	1:G:64:TYR:CZ	2.53	0.44
1:J:94:PHE:O	1:J:97:THR:HG22	2.18	0.44
1:O:110:VAL:CG1	1:O:111:GLY:N	2.81	0.44
1:P:66:THR:CG2	1:P:234:GLY:HA3	2.44	0.44
1:Q:25:THR:HB	1:Q:27:PHE:HE2	1.83	0.44
1:R:69:LEU:HG	1:S:88:GLN:HB2	1.99	0.44
1:C:166:GLU:HA	1:C:166:GLU:OE1	2.17	0.44
1:F:97:THR:HG22	1:F:100:GLY:H	1.82	0.44
1:G:61:VAL:HG22	1:G:79:ILE:HD12	2.00	0.44
1:H:42:LYS:HD3	1:H:247:ALA:HB1	2.00	0.44
1:K:21:PHE:O	1:K:80:ASN:HA	2.18	0.44
1:L:166:GLU:OE1	1:L:166:GLU:HA	2.17	0.44
1:T:184:LYS:HG2	1:T:186:TYR:CE2	2.53	0.44
1:I:211:LEU:CD1	2:I:1000:HEM:HBB2	2.42	0.43
1:M:150:LYS:HB3	1:M:226:ARG:HB3	2.00	0.43
1:O:195:ASP:HB3	1:O:196:PHE:CE2	2.53	0.43
1:P:27:PHE:HD2	1:P:75:PHE:CE2	2.34	0.43
1:P:145:ILE:CD1	1:P:233:LEU:HD13	2.48	0.43
1:P:158:MET:O	1:P:163:ARG:NH1	2.51	0.43
1:T:240:GLU:O	1:T:244:LYS:HB2	2.18	0.43
1:E:180:ASN:HB3	1:E:181:VAL:HG23	2.00	0.43
1:F:145:ILE:CD1	1:F:233:LEU:HD13	2.43	0.43
1:G:118:TYR:CE2	2:G:1000:HEM:O1D	2.70	0.43
1:P:237:HIS:HB2	1:P:242:VAL:HG23	1.99	0.43
1:A:235:THR:HG23	1:A:237:HIS:CD2	2.50	0.43
1:D:196:PHE:CE2	2:D:1000:HEM:O2D	2.70	0.43
1:F:237:HIS:HB2	1:F:242:VAL:HG23	2.00	0.43
1:G:33:TRP:CZ2	1:G:41:ARG:HG2	2.53	0.43
1:R:55:HIS:CD2	1:R:58:ASN:HD22	2.37	0.43
1:T:136:TYR:CD2	1:T:182:LYS:HE3	2.53	0.43
1:F:141:PRO:HA	1:F:203:ASP:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ASN:HB3	1:D:181:VAL:HG23	2.01	0.43
1:N:211:LEU:HD11	2:N:1000:HEM:HBB2	2.00	0.43
1:R:52:ILE:HG12	1:R:61:VAL:HG11	1.99	0.43
1:G:211:LEU:CD1	2:G:1000:HEM:CBB	2.94	0.43
1:P:44:ALA:HB1	1:P:99:VAL:CG2	2.46	0.43
1:R:38:VAL:HB	1:R:41:ARG:NH1	2.33	0.43
1:R:95:ARG:HA	1:R:100:GLY:HA3	2.00	0.43
1:A:36:VAL:O	1:A:41:ARG:HD3	2.19	0.43
2:H:1000:HEM:CBB	2:H:1000:HEM:CHC	2.90	0.43
1:L:215:LEU:HD12	1:L:215:LEU:HA	1.80	0.43
1:T:64:TYR:CD2	1:T:76:PHE:CE2	3.06	0.43
1:T:188:SER:HB2	1:T:194:THR:HG23	2.00	0.43
1:T:221:ASN:HA	1:T:224:HIS:CD2	2.53	0.43
1:B:224:HIS:HE1	5:B:3000:HOH:O	2.01	0.43
1:G:235:THR:CG2	1:G:237:HIS:CD2	3.02	0.43
1:L:182:LYS:HB2	1:L:201:GLU:HB2	2.00	0.43
1:N:66:THR:HG22	1:N:234:GLY:HA3	2.00	0.43
1:P:38:VAL:O	1:P:39:ALA:CB	2.65	0.43
1:T:52:ILE:HG12	1:T:61:VAL:HG21	2.01	0.43
1:T:196:PHE:CE1	2:T:1000:HEM:O2D	2.68	0.43
1:H:69:LEU:HD23	1:H:69:LEU:HA	1.84	0.43
1:Q:72:ASN:O	1:Q:73:SER:HB3	2.19	0.43
1:R:163:ARG:O	1:R:167:MET:HG2	2.19	0.43
1:D:38:VAL:O	1:D:39:ALA:HB2	2.17	0.43
1:D:145:ILE:HA	1:D:232:THR:O	2.19	0.43
1:J:62:ASP:HB3	1:J:64:TYR:CZ	2.54	0.43
1:J:97:THR:HG23	1:J:99:VAL:N	2.34	0.43
1:P:33:TRP:CH2	1:P:99:VAL:HG13	2.54	0.43
1:Q:63:LEU:HB3	1:Q:239:PRO:HA	2.01	0.43
1:B:20:VAL:H	1:B:113:THR:HB	1.83	0.42
1:C:221:ASN:HA	1:C:224:HIS:CD2	2.53	0.42
1:I:145:ILE:HD13	1:I:233:LEU:HD13	1.99	0.42
1:L:64:TYR:CD1	1:L:144:VAL:HG11	2.54	0.42
1:Q:183:ARG:HD2	2:Q:1000:HEM:CMB	2.49	0.42
1:R:235:THR:HG23	1:R:237:HIS:CD2	2.53	0.42
1:S:18:PRO:HA	1:S:113:THR:CG2	2.36	0.42
1:A:118:TYR:CD2	1:A:167:MET:HG3	2.53	0.42
1:B:149:VAL:HA	1:B:226:ARG:O	2.19	0.42
1:F:224:HIS:HE1	5:F:3000:HOH:O	2.02	0.42
1:P:88:GLN:HB2	1:S:69:LEU:HD21	2.01	0.42
1:T:97:THR:CG2	1:T:99:VAL:HG23	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ARG:HD2	1:C:74:ASP:OD1	2.20	0.42
1:I:182:LYS:HB2	1:I:201:GLU:HB2	2.00	0.42
1:I:196:PHE:CE1	2:I:1000:HEM:O2D	2.73	0.42
1:J:38:VAL:O	1:J:39:ALA:CB	2.66	0.42
1:K:20:VAL:H	1:K:113:THR:HB	1.84	0.42
1:K:127:LEU:HD22	1:K:171:THR:HG22	2.02	0.42
1:K:167:MET:O	1:K:170:HIS:HB3	2.18	0.42
1:M:11:ARG:HH22	1:M:62:ASP:CG	2.20	0.42
2:M:1000:HEM:HBB2	2:M:1000:HEM:HHC	2.02	0.42
1:T:36:VAL:O	1:T:37:PRO:C	2.56	0.42
1:M:117:ASN:N	2:M:1000:HEM:O1A	2.51	0.42
1:N:182:LYS:O	1:N:200:PHE:HA	2.19	0.42
1:N:221:ASN:HA	1:N:224:HIS:CD2	2.55	0.42
1:P:127:LEU:HD23	1:P:127:LEU:HA	1.86	0.42
1:R:118:TYR:CD2	1:R:167:MET:HG3	2.55	0.42
1:G:182:LYS:HB2	1:G:201:GLU:HB2	2.01	0.42
1:I:169:VAL:O	1:I:173:PRO:HD2	2.19	0.42
1:Q:31:PRO:C	1:Q:33:TRP:H	2.23	0.42
1:C:224:HIS:HE1	5:C:3000:HOH:O	2.03	0.42
1:O:110:VAL:HG12	1:O:111:GLY:N	2.35	0.42
1:R:196:PHE:HZ	2:R:1000:HEM:O2D	1.96	0.42
1:A:221:ASN:HA	1:A:224:HIS:CD2	2.55	0.42
1:D:38:VAL:O	1:D:39:ALA:HB3	2.20	0.42
1:E:221:ASN:HA	1:E:224:HIS:CD2	2.55	0.42
1:I:64:TYR:CD2	1:I:76:PHE:CE2	3.08	0.42
1:M:8:LYS:HE3	1:M:10:GLU:OE2	2.20	0.42
2:M:1000:HEM:HHC	2:M:1000:HEM:CBB	2.49	0.42
1:N:183:ARG:HD2	2:N:1000:HEM:C3B	2.55	0.42
1:O:21:PHE:O	1:O:80:ASN:HA	2.20	0.42
1:A:64:TYR:CD1	1:A:144:VAL:HG11	2.55	0.42
1:A:117:ASN:N	2:A:1000:HEM:O1A	2.52	0.42
1:A:176:ALA:O	1:A:179:VAL:HG22	2.19	0.42
1:B:224:HIS:CE1	5:B:3000:HOH:O	2.73	0.42
1:C:229:SER:HA	1:C:230:PRO:HA	1.76	0.42
1:D:182:LYS:HB2	1:D:201:GLU:HB2	2.01	0.42
1:D:219:LYS:O	1:D:222:LYS:HB2	2.19	0.42
1:E:36:VAL:HG12	1:E:41:ARG:HG3	2.02	0.42
1:E:66:THR:HG22	1:E:234:GLY:HA3	2.02	0.42
1:G:198:THR:HG21	2:G:1000:HEM:CHD	2.49	0.42
1:H:196:PHE:HZ	2:H:1000:HEM:O2D	1.93	0.42
1:M:70:GLU:OE2	1:M:232:THR:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:63:LEU:HG	1:Q:242:VAL:HG11	2.02	0.42
1:R:119:ILE:CG1	2:R:1000:HEM:HMA2	2.49	0.42
1:T:166:GLU:OE1	1:T:166:GLU:HA	2.20	0.42
1:A:188:SER:HB2	1:A:194:THR:O	2.20	0.42
1:E:33:TRP:O	1:E:41:ARG:HD2	2.20	0.42
1:H:97:THR:HG23	1:H:98:THR:N	2.33	0.42
1:M:67:ARG:HG2	1:N:92:ARG:HG3	2.01	0.42
1:M:166:GLU:OE1	1:M:166:GLU:HA	2.20	0.42
1:S:174:THR:HB	2:S:1000:HEM:HBB2	2.02	0.42
1:Q:20:VAL:O	1:Q:113:THR:HB	2.20	0.42
1:Q:97:THR:HG22	1:Q:100:GLY:N	2.12	0.42
1:D:188:SER:O	1:D:189:THR:C	2.58	0.41
1:G:150:LYS:HA	1:G:195:ASP:HB2	2.01	0.41
1:I:150:LYS:HA	1:I:195:ASP:HB2	2.01	0.41
1:I:182:LYS:O	1:I:200:PHE:HA	2.20	0.41
1:J:196:PHE:HZ	2:J:1000:HEM:O2D	1.91	0.41
1:K:196:PHE:HZ	2:K:1000:HEM:O2D	1.89	0.41
1:N:235:THR:CG2	1:N:237:HIS:NE2	2.83	0.41
1:O:17:GLN:O	1:O:113:THR:CG2	2.50	0.41
1:O:18:PRO:CA	1:O:113:THR:HG22	2.41	0.41
1:Q:18:PRO:CA	1:Q:113:THR:HG22	2.50	0.41
1:Q:235:THR:CG2	1:Q:237:HIS:NE2	2.83	0.41
1:S:20:VAL:H	1:S:113:THR:HB	1.85	0.41
1:T:196:PHE:HZ	2:T:1000:HEM:O2D	1.93	0.41
1:D:174:THR:HB	2:D:1000:HEM:CBB	2.49	0.41
1:J:92:ARG:HG2	1:J:92:ARG:HH11	1.84	0.41
1:N:116:LEU:HA	2:N:1000:HEM:O1A	2.20	0.41
1:S:38:VAL:O	1:S:39:ALA:CB	2.68	0.41
1:D:55:HIS:HE1	1:D:93:GLU:OE1	2.03	0.41
1:Q:33:TRP:HB2	1:Q:102:ASN:HB3	2.02	0.41
1:S:145:ILE:HD13	1:S:233:LEU:HD13	2.02	0.41
1:S:196:PHE:CE1	2:S:1000:HEM:O2D	2.72	0.41
1:S:170:HIS:HE1	2:S:1000:HEM:C4C	2.38	0.41
1:C:188:SER:O	1:C:189:THR:C	2.58	0.41
1:D:211:LEU:HD11	2:D:1000:HEM:HBB2	2.02	0.41
1:G:188:SER:HB2	1:G:194:THR:HG23	2.01	0.41
1:H:222:LYS:HE2	1:I:154:GLU:OE1	2.20	0.41
1:M:11:ARG:NH2	1:M:62:ASP:OD1	2.38	0.41
1:N:63:LEU:HD21	1:N:243:ILE:HD11	2.03	0.41
1:N:167:MET:HE2	2:N:1000:HEM:HBD1	2.02	0.41
1:R:170:HIS:O	1:R:173:PRO:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:LEU:HA	1:H:15:LEU:HD23	1.83	0.41
1:A:157:ASN:HD21	1:E:219:LYS:N	2.19	0.41
1:C:28:LYS:NZ	1:C:72:ASN:HD22	2.19	0.41
1:F:170:HIS:O	1:F:173:PRO:HD2	2.20	0.41
1:H:70:GLU:OE2	1:H:232:THR:HA	2.20	0.41
1:H:198:THR:HG21	2:H:1000:HEM:HBC2	2.02	0.41
1:P:118:TYR:CD2	1:P:167:MET:HG3	2.56	0.41
1:B:88:GLN:O	1:B:92:ARG:HB2	2.21	0.41
1:G:26:MET:HB2	1:G:107:GLU:HB2	2.03	0.41
1:I:30:ARG:O	1:I:33:TRP:HB3	2.21	0.41
1:J:145:ILE:HD13	1:J:233:LEU:HD13	2.02	0.41
1:S:62:ASP:HB3	1:S:64:TYR:CZ	2.55	0.41
1:A:33:TRP:CH2	1:A:41:ARG:HG2	2.55	0.41
1:B:229:SER:HA	1:B:230:PRO:HA	1.85	0.41
1:D:24:PHE:N	1:D:24:PHE:CD2	2.88	0.41
1:D:88:GLN:O	1:D:92:ARG:HB2	2.21	0.41
1:H:29:LEU:HD13	1:H:33:TRP:CD1	2.56	0.41
1:O:219:LYS:O	1:O:222:LYS:HB2	2.21	0.41
1:R:25:THR:HG22	1:R:105:VAL:HG13	2.02	0.41
1:S:53:GLU:HB3	1:S:56:LYS:NZ	2.36	0.41
1:T:97:THR:HG23	1:T:99:VAL:HG23	2.02	0.41
1:T:99:VAL:HG11	1:T:243:ILE:HG23	2.03	0.41
1:T:145:ILE:CD1	1:T:233:LEU:HD13	2.51	0.41
1:T:242:VAL:O	1:T:246:LEU:HG	2.20	0.41
1:C:53:GLU:O	1:C:56:LYS:HB2	2.21	0.41
1:G:24:PHE:HB2	1:G:109:LEU:HB2	2.03	0.41
1:G:116:LEU:CA	2:G:1000:HEM:O1A	2.67	0.41
1:H:71:THR:HG23	1:I:105:VAL:HG12	2.03	0.41
1:M:150:LYS:HG2	1:M:225:VAL:HG23	2.01	0.41
1:N:17:GLN:O	1:N:113:THR:CG2	2.54	0.41
1:N:196:PHE:HZ	2:N:1000:HEM:O2D	2.00	0.41
1:O:158:MET:O	1:O:163:ARG:NH1	2.53	0.41
1:R:116:LEU:CA	2:R:1000:HEM:O1A	2.69	0.41
1:D:33:TRP:CZ2	1:D:41:ARG:HG2	2.57	0.40
1:J:33:TRP:HB2	1:J:102:ASN:HB3	2.03	0.40
1:L:119:ILE:HG22	1:L:119:ILE:O	2.21	0.40
1:P:59:VAL:HG11	1:P:87:ALA:HA	2.03	0.40
1:P:157:ASN:HD21	1:S:219:LYS:N	2.19	0.40
1:R:9:ILE:O	1:R:9:ILE:HG22	2.20	0.40
1:B:38:VAL:O	1:B:39:ALA:HB2	2.21	0.40
1:K:28:LYS:NZ	1:K:72:ASN:HD22	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:30:ARG:NH2	1:T:101:LYS:O	2.36	0.40
1:E:42:LYS:HD3	1:E:247:ALA:HB1	2.04	0.40
1:H:53:GLU:O	1:H:56:LYS:HG3	2.22	0.40
1:J:229:SER:HA	1:J:230:PRO:HA	1.84	0.40
1:P:127:LEU:CD1	1:P:168:GLU:HG2	2.47	0.40
1:Q:95:ARG:HA	1:Q:100:GLY:HA3	2.03	0.40
1:R:27:PHE:HB2	1:R:75:PHE:CZ	2.57	0.40
1:R:119:ILE:HG12	2:R:1000:HEM:HAA1	2.02	0.40
1:S:158:MET:O	1:S:163:ARG:NH1	2.54	0.40
1:A:174:THR:O	2:A:1000:HEM:CBB	2.70	0.40
1:B:55:HIS:CD2	1:B:58:ASN:HD22	2.40	0.40
1:B:195:ASP:HB3	1:B:196:PHE:CE2	2.56	0.40
1:F:24:PHE:HA	1:F:77:PHE:O	2.21	0.40
1:G:196:PHE:CE1	2:G:1000:HEM:HAD1	2.57	0.40
1:J:97:THR:HG23	1:J:99:VAL:H	1.86	0.40
1:M:186:TYR:HB2	1:M:197:ILE:HB	2.04	0.40
1:P:51:LEU:HD11	1:P:93:GLU:HB3	2.04	0.40
1:Q:8:LYS:HB3	1:Q:8:LYS:HE2	1.78	0.40
1:R:97:THR:HG23	1:R:100:GLY:H	1.86	0.40
1:S:38:VAL:O	1:S:38:VAL:HG13	2.22	0.40
1:S:65:LEU:HB3	1:S:235:THR:HG22	2.03	0.40
1:T:72:ASN:O	1:T:73:SER:HB3	2.21	0.40
1:A:20:VAL:H	1:A:113:THR:HB	1.87	0.40
1:B:18:PRO:CA	1:B:113:THR:HG22	2.39	0.40
1:N:94:PHE:O	1:N:97:THR:HB	2.22	0.40
1:R:183:ARG:HD2	2:R:1000:HEM:C2B	2.56	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	239/248 (96%)	230 (96%)	8 (3%)	1 (0%)	34	72
1	B	239/248 (96%)	228 (95%)	8 (3%)	3 (1%)	12	45
1	C	239/248 (96%)	231 (97%)	5 (2%)	3 (1%)	12	45
1	D	239/248 (96%)	232 (97%)	6 (2%)	1 (0%)	34	72
1	E	239/248 (96%)	228 (95%)	8 (3%)	3 (1%)	12	45
1	F	239/248 (96%)	226 (95%)	11 (5%)	2 (1%)	19	57
1	G	239/248 (96%)	228 (95%)	9 (4%)	2 (1%)	19	57
1	H	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	34	72
1	I	239/248 (96%)	226 (95%)	12 (5%)	1 (0%)	34	72
1	J	239/248 (96%)	229 (96%)	9 (4%)	1 (0%)	34	72
1	K	239/248 (96%)	228 (95%)	10 (4%)	1 (0%)	34	72
1	L	239/248 (96%)	231 (97%)	7 (3%)	1 (0%)	34	72
1	M	239/248 (96%)	228 (95%)	9 (4%)	2 (1%)	19	57
1	N	239/248 (96%)	225 (94%)	11 (5%)	3 (1%)	12	45
1	O	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	34	72
1	P	239/248 (96%)	223 (93%)	13 (5%)	3 (1%)	12	45
1	Q	239/248 (96%)	223 (93%)	12 (5%)	4 (2%)	9	39
1	R	239/248 (96%)	225 (94%)	11 (5%)	3 (1%)	12	45
1	S	239/248 (96%)	226 (95%)	9 (4%)	4 (2%)	9	39
1	T	239/248 (96%)	225 (94%)	12 (5%)	2 (1%)	19	57
All	All	4780/4960 (96%)	4546 (95%)	192 (4%)	42 (1%)	17	55

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ALA
1	C	39	ALA
1	E	39	ALA
1	F	38	VAL
1	F	39	ALA
1	G	39	ALA
1	H	39	ALA
1	J	39	ALA
1	K	39	ALA
1	M	39	ALA
1	M	56	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	39	ALA
1	P	39	ALA
1	Q	39	ALA
1	S	39	ALA
1	A	39	ALA
1	B	56	LYS
1	C	56	LYS
1	D	39	ALA
1	E	38	VAL
1	I	39	ALA
1	L	39	ALA
1	N	39	ALA
1	Q	38	VAL
1	R	39	ALA
1	S	38	VAL
1	S	56	LYS
1	T	39	ALA
1	C	38	VAL
1	E	56	LYS
1	Q	134	ALA
1	P	189	THR
1	Q	32	ASP
1	R	134	ALA
1	N	176	ALA
1	R	37	PRO
1	S	75	PHE
1	G	38	VAL
1	T	37	PRO
1	B	119	ILE
1	N	119	ILE
1	P	119	ILE

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/219 (97%)	197 (93%)	15 (7%)	14	46
1	B	212/219 (97%)	200 (94%)	12 (6%)	20	56
1	C	212/219 (97%)	200 (94%)	12 (6%)	20	56
1	D	212/219 (97%)	199 (94%)	13 (6%)	18	53
1	E	212/219 (97%)	199 (94%)	13 (6%)	18	53
1	F	212/219 (97%)	197 (93%)	15 (7%)	14	46
1	G	212/219 (97%)	200 (94%)	12 (6%)	20	56
1	H	212/219 (97%)	199 (94%)	13 (6%)	18	53
1	I	212/219 (97%)	201 (95%)	11 (5%)	23	59
1	J	212/219 (97%)	196 (92%)	16 (8%)	13	43
1	K	212/219 (97%)	200 (94%)	12 (6%)	20	56
1	L	212/219 (97%)	199 (94%)	13 (6%)	18	53
1	M	212/219 (97%)	200 (94%)	12 (6%)	20	56
1	N	212/219 (97%)	198 (93%)	14 (7%)	16	49
1	O	212/219 (97%)	201 (95%)	11 (5%)	23	59
1	P	212/219 (97%)	203 (96%)	9 (4%)	30	66
1	Q	212/219 (97%)	193 (91%)	19 (9%)	9	35
1	R	212/219 (97%)	202 (95%)	10 (5%)	26	63
1	S	212/219 (97%)	201 (95%)	11 (5%)	23	59
1	T	212/219 (97%)	195 (92%)	17 (8%)	12	40
All	All	4240/4380 (97%)	3980 (94%)	260 (6%)	18	53

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	16	THR
1	A	25	THR
1	A	32	ASP
1	A	38	VAL
1	A	97	THR
1	A	107	GLU
1	A	135	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	145	ILE
1	A	192	ASP
1	A	214	SER
1	A	215	LEU
1	A	229	SER
1	A	235	THR
1	A	240	GLU
1	B	11	ARG
1	B	16	THR
1	B	26	MET
1	B	56	LYS
1	B	97	THR
1	B	107	GLU
1	B	131	LEU
1	B	135	THR
1	B	215	LEU
1	B	229	SER
1	B	235	THR
1	B	248	ASP
1	C	11	ARG
1	C	16	THR
1	C	25	THR
1	C	92	ARG
1	C	97	THR
1	C	135	THR
1	C	192	ASP
1	C	214	SER
1	C	215	LEU
1	C	229	SER
1	C	233	LEU
1	C	235	THR
1	D	11	ARG
1	D	16	THR
1	D	25	THR
1	D	26	MET
1	D	97	THR
1	D	124	SER
1	D	135	THR
1	D	139	PRO
1	D	145	ILE
1	D	192	ASP
1	D	233	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	235	THR
1	D	248	ASP
1	E	8	LYS
1	E	16	THR
1	E	56	LYS
1	E	97	THR
1	E	99	VAL
1	E	135	THR
1	E	137	SER
1	E	145	ILE
1	E	215	LEU
1	E	229	SER
1	E	233	LEU
1	E	235	THR
1	E	248	ASP
1	F	10	GLU
1	F	11	ARG
1	F	13	THR
1	F	25	THR
1	F	26	MET
1	F	99	VAL
1	F	135	THR
1	F	137	SER
1	F	145	ILE
1	F	192	ASP
1	F	214	SER
1	F	215	LEU
1	F	229	SER
1	F	235	THR
1	F	248	ASP
1	G	11	ARG
1	G	26	MET
1	G	42	LYS
1	G	96	SER
1	G	97	THR
1	G	98	THR
1	G	145	ILE
1	G	165	LYS
1	G	192	ASP
1	G	215	LEU
1	G	229	SER
1	G	235	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	11	ARG
1	H	16	THR
1	H	26	MET
1	H	92	ARG
1	H	97	THR
1	H	99	VAL
1	H	145	ILE
1	H	192	ASP
1	H	214	SER
1	H	215	LEU
1	H	229	SER
1	H	235	THR
1	H	248	ASP
1	I	11	ARG
1	I	25	THR
1	I	26	MET
1	I	96	SER
1	I	97	THR
1	I	113	THR
1	I	135	THR
1	I	145	ILE
1	I	192	ASP
1	I	215	LEU
1	I	235	THR
1	J	11	ARG
1	J	16	THR
1	J	26	MET
1	J	56	LYS
1	J	92	ARG
1	J	97	THR
1	J	113	THR
1	J	135	THR
1	J	145	ILE
1	J	192	ASP
1	J	214	SER
1	J	215	LEU
1	J	229	SER
1	J	233	LEU
1	J	235	THR
1	J	248	ASP
1	K	8	LYS
1	K	16	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	25	THR
1	K	97	THR
1	K	99	VAL
1	K	107	GLU
1	K	137	SER
1	K	145	ILE
1	K	192	ASP
1	K	214	SER
1	K	215	LEU
1	K	235	THR
1	L	16	THR
1	L	92	ARG
1	L	97	THR
1	L	135	THR
1	L	137	SER
1	L	145	ILE
1	L	165	LYS
1	L	192	ASP
1	L	214	SER
1	L	215	LEU
1	L	233	LEU
1	L	235	THR
1	L	248	ASP
1	M	16	THR
1	M	25	THR
1	M	92	ARG
1	M	97	THR
1	M	99	VAL
1	M	150	LYS
1	M	165	LYS
1	M	183	ARG
1	M	192	ASP
1	M	215	LEU
1	M	235	THR
1	M	248	ASP
1	N	11	ARG
1	N	26	MET
1	N	97	THR
1	N	99	VAL
1	N	113	THR
1	N	145	ILE
1	N	189	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	192	ASP
1	N	215	LEU
1	N	229	SER
1	N	233	LEU
1	N	235	THR
1	N	240	GLU
1	N	248	ASP
1	O	11	ARG
1	O	16	THR
1	O	26	MET
1	O	56	LYS
1	O	97	THR
1	O	99	VAL
1	O	145	ILE
1	O	192	ASP
1	O	215	LEU
1	O	235	THR
1	O	240	GLU
1	P	16	THR
1	P	26	MET
1	P	50	LYS
1	P	92	ARG
1	P	99	VAL
1	P	145	ILE
1	P	192	ASP
1	P	215	LEU
1	P	235	THR
1	Q	8	LYS
1	Q	11	ARG
1	Q	16	THR
1	Q	25	THR
1	Q	26	MET
1	Q	56	LYS
1	Q	71	THR
1	Q	96	SER
1	Q	97	THR
1	Q	99	VAL
1	Q	113	THR
1	Q	135	THR
1	Q	137	SER
1	Q	145	ILE
1	Q	165	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	183	ARG
1	Q	192	ASP
1	Q	215	LEU
1	Q	235	THR
1	R	25	THR
1	R	92	ARG
1	R	121	LYS
1	R	135	THR
1	R	145	ILE
1	R	189	THR
1	R	192	ASP
1	R	215	LEU
1	R	235	THR
1	R	248	ASP
1	S	16	THR
1	S	25	THR
1	S	26	MET
1	S	97	THR
1	S	99	VAL
1	S	183	ARG
1	S	192	ASP
1	S	215	LEU
1	S	227	TRP
1	S	229	SER
1	S	240	GLU
1	T	8	LYS
1	T	11	ARG
1	T	16	THR
1	T	92	ARG
1	T	96	SER
1	T	97	THR
1	T	99	VAL
1	T	135	THR
1	T	145	ILE
1	T	165	LYS
1	T	192	ASP
1	T	215	LEU
1	T	232	THR
1	T	233	LEU
1	T	235	THR
1	T	240	GLU
1	T	248	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	72	ASN
1	A	157	ASN
1	A	180	ASN
1	A	221	ASN
1	A	224	HIS
1	B	55	HIS
1	B	72	ASN
1	B	157	ASN
1	B	221	ASN
1	B	224	HIS
1	C	55	HIS
1	C	72	ASN
1	C	102	ASN
1	C	157	ASN
1	C	217	GLN
1	C	221	ASN
1	C	224	HIS
1	D	55	HIS
1	D	72	ASN
1	D	80	ASN
1	D	157	ASN
1	D	217	GLN
1	D	221	ASN
1	D	224	HIS
1	E	55	HIS
1	E	72	ASN
1	E	80	ASN
1	E	157	ASN
1	E	221	ASN
1	E	224	HIS
1	F	55	HIS
1	F	72	ASN
1	F	157	ASN
1	F	224	HIS
1	G	55	HIS
1	G	72	ASN
1	G	157	ASN
1	G	217	GLN
1	G	221	ASN
1	G	224	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	72	ASN
1	H	102	ASN
1	H	157	ASN
1	H	221	ASN
1	H	224	HIS
1	I	58	ASN
1	I	72	ASN
1	I	157	ASN
1	I	221	ASN
1	I	224	HIS
1	J	72	ASN
1	J	157	ASN
1	J	217	GLN
1	J	221	ASN
1	J	224	HIS
1	K	58	ASN
1	K	72	ASN
1	K	157	ASN
1	K	221	ASN
1	K	224	HIS
1	L	55	HIS
1	L	72	ASN
1	L	157	ASN
1	L	221	ASN
1	L	224	HIS
1	M	55	HIS
1	M	72	ASN
1	M	157	ASN
1	M	217	GLN
1	M	221	ASN
1	M	224	HIS
1	N	55	HIS
1	N	72	ASN
1	N	157	ASN
1	N	217	GLN
1	N	221	ASN
1	N	224	HIS
1	O	157	ASN
1	O	221	ASN
1	O	224	HIS
1	P	157	ASN
1	P	224	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	55	HIS
1	Q	157	ASN
1	Q	217	GLN
1	Q	221	ASN
1	Q	224	HIS
1	R	55	HIS
1	R	157	ASN
1	R	224	HIS
1	S	55	HIS
1	S	157	ASN
1	S	217	GLN
1	S	221	ASN
1	S	224	HIS
1	T	72	ASN
1	T	157	ASN
1	T	221	ASN
1	T	224	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 60 ligands modelled in this entry, 20 are monoatomic - leaving 40 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	$\#\|Z\|>2$
3	NO2	L	2000	2	1,2,2	4.65	1 (100%)	0,1,1	-	-
3	NO2	P	2000	2	1,2,2	4.72	1 (100%)	0,1,1	-	-
2	HEM	I	1000	1,3	41,50,50	2.25	9 (21%)	45,82,82	2.09	10 (22%)
3	NO2	G	2000	2	1,2,2	4.76	1 (100%)	0,1,1	-	-
2	HEM	L	1000	1,3	41,50,50	2.04	8 (19%)	45,82,82	2.07	14 (31%)
3	NO2	C	2000	2	1,2,2	4.53	1 (100%)	0,1,1	-	-
2	HEM	P	1000	1,3	41,50,50	2.25	10 (24%)	45,82,82	1.99	13 (28%)
3	NO2	S	2000	2	1,2,2	4.65	1 (100%)	0,1,1	-	-
2	HEM	Q	1000	1,3	41,50,50	2.56	12 (29%)	45,82,82	2.19	15 (33%)
3	NO2	E	2000	2	1,2,2	3.93	1 (100%)	0,1,1	-	-
2	HEM	F	1000	1,3	41,50,50	1.90	8 (19%)	45,82,82	2.18	14 (31%)
3	NO2	R	2000	2	1,2,2	4.80	1 (100%)	0,1,1	-	-
3	NO2	D	2000	2	1,2,2	4.50	1 (100%)	0,1,1	-	-
3	NO2	K	2000	2	1,2,2	4.74	1 (100%)	0,1,1	-	-
2	HEM	A	1000	1,3	41,50,50	2.19	9 (21%)	45,82,82	1.99	12 (26%)
3	NO2	N	2000	2	1,2,2	4.39	1 (100%)	0,1,1	-	-
3	NO2	T	2000	2	1,2,2	4.30	1 (100%)	0,1,1	-	-
3	NO2	H	2000	2	1,2,2	4.61	1 (100%)	0,1,1	-	-
3	NO2	B	2000	2	1,2,2	4.33	1 (100%)	0,1,1	-	-
2	HEM	R	1000	1,3	41,50,50	1.96	7 (17%)	45,82,82	2.12	14 (31%)
2	HEM	N	1000	1,3	41,50,50	2.19	10 (24%)	45,82,82	1.98	10 (22%)
3	NO2	M	2000	2	1,2,2	6.20	1 (100%)	0,1,1	-	-
2	HEM	C	1000	1,3	41,50,50	2.31	9 (21%)	45,82,82	2.41	16 (35%)
3	NO2	J	2000	2	1,2,2	4.49	1 (100%)	0,1,1	-	-
2	HEM	B	1000	1,3	41,50,50	2.22	9 (21%)	45,82,82	2.40	12 (26%)
3	NO2	I	2000	2	1,2,2	3.85	1 (100%)	0,1,1	-	-
2	HEM	M	1000	1,3	41,50,50	2.09	9 (21%)	45,82,82	2.28	17 (37%)
3	NO2	O	2000	2	1,2,2	4.43	1 (100%)	0,1,1	-	-
2	HEM	H	1000	1,3	41,50,50	2.11	9 (21%)	45,82,82	2.18	13 (28%)
2	HEM	E	1000	1,3	41,50,50	2.03	9 (21%)	45,82,82	1.95	15 (33%)
2	HEM	G	1000	1,3	41,50,50	2.27	10 (24%)	45,82,82	2.49	19 (42%)
2	HEM	S	1000	1,3	41,50,50	2.26	10 (24%)	45,82,82	1.92	8 (17%)
3	NO2	F	2000	2	1,2,2	4.51	1 (100%)	0,1,1	-	-
3	NO2	A	2000	2	1,2,2	3.88	1 (100%)	0,1,1	-	-
2	HEM	O	1000	1,3	41,50,50	2.03	9 (21%)	45,82,82	1.73	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	D	1000	1,3	41,50,50	2.14	11 (26%)	45,82,82	1.90	10 (22%)
2	HEM	T	1000	1,3	41,50,50	2.03	10 (24%)	45,82,82	1.95	13 (28%)
2	HEM	K	1000	1,3	41,50,50	2.12	11 (26%)	45,82,82	2.05	12 (26%)
2	HEM	J	1000	1,3	41,50,50	2.23	7 (17%)	45,82,82	2.38	18 (40%)
3	NO2	Q	2000	2	1,2,2	4.73	1 (100%)	0,1,1	-	-

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	I	1000	1,3	-	1/12/54/54	-
2	HEM	L	1000	1,3	-	3/12/54/54	-
2	HEM	P	1000	1,3	-	2/12/54/54	-
2	HEM	Q	1000	1,3	-	2/12/54/54	-
2	HEM	F	1000	1,3	-	6/12/54/54	-
2	HEM	A	1000	1,3	-	6/12/54/54	-
2	HEM	R	1000	1,3	-	4/12/54/54	-
2	HEM	N	1000	1,3	-	6/12/54/54	-
2	HEM	C	1000	1,3	-	6/12/54/54	-
2	HEM	B	1000	1,3	-	0/12/54/54	-
2	HEM	M	1000	1,3	-	3/12/54/54	-
2	HEM	H	1000	1,3	-	2/12/54/54	-
2	HEM	E	1000	1,3	-	4/12/54/54	-
2	HEM	G	1000	1,3	-	3/12/54/54	-
2	HEM	S	1000	1,3	-	3/12/54/54	-
2	HEM	O	1000	1,3	-	5/12/54/54	-
2	HEM	D	1000	1,3	-	6/12/54/54	-
2	HEM	T	1000	1,3	-	5/12/54/54	-
2	HEM	K	1000	1,3	-	2/12/54/54	-
2	HEM	J	1000	1,3	-	6/12/54/54	-

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1000	HEM	C3D-C2D	9.24	1.56	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	1000	HEM	C3D-C2D	9.18	1.56	1.36
2	P	1000	HEM	C3D-C2D	9.10	1.56	1.36
2	J	1000	HEM	C3D-C2D	8.98	1.55	1.36
2	K	1000	HEM	C3D-C2D	8.63	1.55	1.36
2	G	1000	HEM	C3D-C2D	8.63	1.55	1.36
2	I	1000	HEM	C3D-C2D	8.53	1.54	1.36
2	M	1000	HEM	C3D-C2D	8.33	1.54	1.36
2	B	1000	HEM	C3D-C2D	8.27	1.54	1.36
2	T	1000	HEM	C3D-C2D	8.19	1.54	1.36
2	L	1000	HEM	C3D-C2D	8.15	1.54	1.36
2	C	1000	HEM	C3D-C2D	8.09	1.53	1.36
2	H	1000	HEM	C3D-C2D	8.04	1.53	1.36
2	O	1000	HEM	C3D-C2D	7.95	1.53	1.36
2	N	1000	HEM	C3D-C2D	7.94	1.53	1.36
2	D	1000	HEM	C3D-C2D	7.84	1.53	1.36
2	A	1000	HEM	C3D-C2D	7.65	1.53	1.36
2	R	1000	HEM	C3D-C2D	7.58	1.52	1.36
2	E	1000	HEM	C3D-C2D	7.45	1.52	1.36
2	F	1000	HEM	C3D-C2D	6.69	1.51	1.36
2	C	1000	HEM	C3C-C2C	-6.37	1.31	1.40
3	M	2000	NO2	O1-N	6.20	1.53	1.22
2	A	1000	HEM	C3C-C2C	-6.01	1.32	1.40
2	D	1000	HEM	C3C-C2C	-5.94	1.32	1.40
2	E	1000	HEM	C3C-C2C	-5.74	1.32	1.40
2	P	1000	HEM	C3C-C2C	-5.62	1.32	1.40
2	H	1000	HEM	C3C-C2C	-5.39	1.32	1.40
2	Q	1000	HEM	C3C-C2C	-5.35	1.32	1.40
2	A	1000	HEM	FE-ND	5.33	2.23	1.96
2	B	1000	HEM	FE-ND	5.23	2.22	1.96
2	B	1000	HEM	C3C-C2C	-5.22	1.33	1.40
2	I	1000	HEM	FE-ND	5.13	2.22	1.96
2	J	1000	HEM	FE-ND	5.05	2.21	1.96
2	G	1000	HEM	C3C-C2C	-5.05	1.33	1.40
2	T	1000	HEM	C3C-C2C	-5.00	1.33	1.40
2	N	1000	HEM	C3C-C2C	-4.96	1.33	1.40
3	R	2000	NO2	O1-N	4.80	1.46	1.22
3	G	2000	NO2	O1-N	4.76	1.46	1.22
3	K	2000	NO2	O1-N	4.74	1.46	1.22
3	Q	2000	NO2	O1-N	4.73	1.46	1.22
3	P	2000	NO2	O1-N	4.72	1.46	1.22
2	I	1000	HEM	C3C-C2C	-4.72	1.33	1.40
2	C	1000	HEM	C3C-CAC	4.70	1.57	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2000	NO2	O1-N	4.65	1.45	1.22
3	S	2000	NO2	O1-N	4.65	1.45	1.22
3	H	2000	NO2	O1-N	4.61	1.45	1.22
3	C	2000	NO2	O1-N	4.53	1.45	1.22
3	F	2000	NO2	O1-N	4.51	1.45	1.22
3	D	2000	NO2	O1-N	4.50	1.45	1.22
3	J	2000	NO2	O1-N	4.49	1.44	1.22
3	O	2000	NO2	O1-N	4.43	1.44	1.22
2	J	1000	HEM	C3C-C2C	-4.42	1.34	1.40
2	Q	1000	HEM	FE-ND	4.41	2.18	1.96
2	M	1000	HEM	C3C-C2C	-4.40	1.34	1.40
3	N	2000	NO2	O1-N	4.39	1.44	1.22
2	L	1000	HEM	C3C-C2C	-4.34	1.34	1.40
3	B	2000	NO2	O1-N	4.33	1.44	1.22
3	T	2000	NO2	O1-N	4.30	1.44	1.22
2	Q	1000	HEM	CAA-C2A	4.24	1.58	1.52
2	G	1000	HEM	FE-ND	4.23	2.17	1.96
2	Q	1000	HEM	CAB-C3B	4.21	1.58	1.47
2	O	1000	HEM	C3C-CAC	4.19	1.56	1.47
2	C	1000	HEM	FE-ND	4.11	2.17	1.96
2	R	1000	HEM	C3C-C2C	-4.09	1.34	1.40
2	A	1000	HEM	C3C-CAC	4.05	1.56	1.47
2	S	1000	HEM	C3C-CAC	4.01	1.56	1.47
2	K	1000	HEM	C3C-C2C	-4.00	1.34	1.40
2	N	1000	HEM	FE-ND	4.00	2.16	1.96
2	I	1000	HEM	C3C-CAC	4.00	1.56	1.47
2	S	1000	HEM	FE-ND	3.96	2.16	1.96
3	E	2000	NO2	O1-N	3.93	1.42	1.22
2	L	1000	HEM	CAB-C3B	3.93	1.58	1.47
2	R	1000	HEM	C3C-CAC	3.92	1.55	1.47
3	A	2000	NO2	O1-N	3.88	1.41	1.22
2	F	1000	HEM	C3C-CAC	3.86	1.55	1.47
3	I	2000	NO2	O1-N	3.85	1.41	1.22
2	D	1000	HEM	C3C-CAC	3.68	1.55	1.47
2	G	1000	HEM	CAB-C3B	3.67	1.57	1.47
2	J	1000	HEM	C3C-CAC	3.64	1.55	1.47
2	Q	1000	HEM	C1B-C2B	3.63	1.51	1.44
2	F	1000	HEM	FE-ND	3.61	2.14	1.96
2	N	1000	HEM	O2D-CGD	-3.59	1.18	1.30
2	G	1000	HEM	C3C-CAC	3.58	1.55	1.47
2	R	1000	HEM	FE-NB	3.54	2.14	1.96
2	H	1000	HEM	C3C-CAC	3.54	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	HEM	C3C-CAC	3.51	1.55	1.47
2	M	1000	HEM	C3C-CAC	3.51	1.55	1.47
2	P	1000	HEM	CAB-C3B	3.49	1.56	1.47
2	E	1000	HEM	C3C-CAC	3.43	1.54	1.47
2	K	1000	HEM	C3C-CAC	3.41	1.54	1.47
2	C	1000	HEM	C3B-C2B	-3.37	1.30	1.37
2	Q	1000	HEM	O2D-CGD	-3.36	1.19	1.30
2	S	1000	HEM	C3C-C2C	-3.34	1.35	1.40
2	O	1000	HEM	C3C-C2C	-3.32	1.35	1.40
2	B	1000	HEM	C3B-C2B	-3.27	1.30	1.37
2	K	1000	HEM	CAB-C3B	3.23	1.56	1.47
2	S	1000	HEM	CAB-C3B	3.15	1.56	1.47
2	L	1000	HEM	FE-ND	3.10	2.12	1.96
2	Q	1000	HEM	C3C-CAC	3.07	1.54	1.47
2	G	1000	HEM	CMD-C2D	3.06	1.57	1.50
2	O	1000	HEM	FE-ND	3.03	2.11	1.96
2	N	1000	HEM	C3C-CAC	3.02	1.54	1.47
2	F	1000	HEM	C3C-C2C	-2.97	1.36	1.40
2	C	1000	HEM	O2D-CGD	-2.93	1.20	1.30
2	Q	1000	HEM	C1A-NA	2.93	1.42	1.36
2	M	1000	HEM	CAB-C3B	2.91	1.55	1.47
2	P	1000	HEM	O1D-CGD	2.90	1.31	1.22
2	O	1000	HEM	CAB-C3B	2.89	1.55	1.47
2	T	1000	HEM	C3C-CAC	2.88	1.53	1.47
2	H	1000	HEM	CMD-C2D	2.87	1.56	1.50
2	E	1000	HEM	O2D-CGD	-2.85	1.21	1.30
2	F	1000	HEM	C3B-C2B	-2.81	1.31	1.37
2	R	1000	HEM	CAB-C3B	2.80	1.55	1.47
2	G	1000	HEM	C3B-C2B	-2.80	1.31	1.37
2	S	1000	HEM	CMB-C2B	2.79	1.56	1.50
2	N	1000	HEM	CMB-C2B	2.78	1.56	1.50
2	Q	1000	HEM	CAD-C3D	2.78	1.58	1.51
2	M	1000	HEM	FE-ND	2.77	2.10	1.96
2	Q	1000	HEM	CMB-C2B	2.76	1.56	1.50
2	F	1000	HEM	CAB-C3B	2.75	1.54	1.47
2	S	1000	HEM	O1D-CGD	2.74	1.31	1.22
2	B	1000	HEM	O2D-CGD	-2.70	1.21	1.30
2	D	1000	HEM	FE-ND	2.69	2.10	1.96
2	P	1000	HEM	C3C-CAC	2.68	1.53	1.47
2	K	1000	HEM	CBD-CAD	2.65	1.60	1.52
2	D	1000	HEM	CAA-C2A	2.64	1.55	1.52
2	N	1000	HEM	CAB-C3B	2.63	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1000	HEM	C1A-NA	2.61	1.41	1.36
2	H	1000	HEM	C4A-CHB	-2.59	1.33	1.41
2	G	1000	HEM	C4D-ND	-2.58	1.35	1.40
2	O	1000	HEM	CAA-C2A	2.57	1.55	1.52
2	P	1000	HEM	C3B-C4B	2.57	1.50	1.44
2	S	1000	HEM	CMC-C2C	2.55	1.57	1.51
2	L	1000	HEM	C3C-CAC	2.55	1.53	1.47
2	P	1000	HEM	CMB-C2B	2.51	1.56	1.50
2	I	1000	HEM	CAB-C3B	2.49	1.54	1.47
2	A	1000	HEM	CAA-C2A	2.49	1.55	1.52
2	O	1000	HEM	O2D-CGD	-2.48	1.22	1.30
2	S	1000	HEM	CAA-C2A	2.47	1.55	1.52
2	C	1000	HEM	CMD-C2D	2.47	1.56	1.50
2	R	1000	HEM	O2D-CGD	-2.44	1.22	1.30
2	K	1000	HEM	O2A-CGA	-2.43	1.22	1.30
2	B	1000	HEM	CAB-C3B	2.42	1.54	1.47
2	I	1000	HEM	C3B-C2B	-2.41	1.32	1.37
2	J	1000	HEM	CAB-C3B	2.41	1.54	1.47
2	C	1000	HEM	O2A-CGA	-2.40	1.22	1.30
2	M	1000	HEM	CBD-CAD	2.40	1.59	1.52
2	K	1000	HEM	C1A-NA	2.39	1.41	1.36
2	H	1000	HEM	CAB-C3B	2.38	1.53	1.47
2	C	1000	HEM	CAB-C3B	2.38	1.53	1.47
2	T	1000	HEM	FE-ND	2.38	2.08	1.96
2	E	1000	HEM	CAB-C3B	2.36	1.53	1.47
2	O	1000	HEM	C3B-C2B	-2.35	1.32	1.37
2	E	1000	HEM	O2A-CGA	-2.35	1.22	1.30
2	I	1000	HEM	CMA-C3A	2.34	1.56	1.51
2	A	1000	HEM	C3B-C2B	-2.33	1.32	1.37
2	N	1000	HEM	O2A-CGA	-2.32	1.22	1.30
2	T	1000	HEM	CAB-C3B	2.32	1.53	1.47
2	D	1000	HEM	C3B-C2B	-2.32	1.32	1.37
2	R	1000	HEM	FE-ND	2.32	2.08	1.96
2	L	1000	HEM	CMB-C2B	2.31	1.55	1.50
2	P	1000	HEM	O2A-CGA	-2.31	1.23	1.30
2	H	1000	HEM	C3B-C2B	-2.30	1.32	1.37
2	D	1000	HEM	CMA-C3A	2.29	1.56	1.51
2	N	1000	HEM	C3B-C2B	-2.29	1.32	1.37
2	L	1000	HEM	C3B-C2B	-2.29	1.32	1.37
2	H	1000	HEM	CMB-C2B	2.27	1.55	1.50
2	T	1000	HEM	C3B-C2B	-2.26	1.32	1.37
2	D	1000	HEM	CAB-C3B	2.26	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1000	HEM	O2D-CGD	-2.25	1.23	1.30
2	M	1000	HEM	C1A-NA	2.24	1.40	1.36
2	J	1000	HEM	O2D-CGD	-2.23	1.23	1.30
2	D	1000	HEM	O2A-CGA	-2.23	1.23	1.30
2	K	1000	HEM	C3B-C2B	-2.21	1.32	1.37
2	A	1000	HEM	O2D-CGD	-2.21	1.23	1.30
2	P	1000	HEM	CAD-C3D	2.21	1.57	1.51
2	A	1000	HEM	CAB-C3B	2.18	1.53	1.47
2	A	1000	HEM	O2A-CGA	-2.18	1.23	1.30
2	D	1000	HEM	CHC-C4B	-2.18	1.34	1.41
2	G	1000	HEM	C1A-NA	2.18	1.40	1.36
2	Q	1000	HEM	CMC-C2C	2.15	1.56	1.51
2	F	1000	HEM	C1A-NA	2.15	1.40	1.36
2	D	1000	HEM	CBD-CAD	2.15	1.58	1.52
2	N	1000	HEM	CAA-C2A	2.13	1.55	1.52
2	O	1000	HEM	CMC-C2C	2.12	1.56	1.51
2	P	1000	HEM	FE-ND	2.12	2.07	1.96
2	H	1000	HEM	CHC-C4B	-2.11	1.34	1.41
2	T	1000	HEM	FE-NB	2.11	2.07	1.96
2	K	1000	HEM	FE-ND	2.11	2.07	1.96
2	E	1000	HEM	C4A-CHB	-2.10	1.35	1.41
2	I	1000	HEM	C2C-C1C	2.10	1.47	1.42
2	E	1000	HEM	FE-ND	2.09	2.07	1.96
2	K	1000	HEM	CMB-C2B	2.07	1.55	1.50
2	B	1000	HEM	CMD-C2D	2.06	1.55	1.50
2	L	1000	HEM	O2D-CGD	-2.06	1.23	1.30
2	E	1000	HEM	CMB-C2B	2.06	1.55	1.50
2	S	1000	HEM	CHA-C4D	2.06	1.40	1.35
2	J	1000	HEM	C3B-C2B	-2.05	1.33	1.37
2	T	1000	HEM	CMB-C2B	2.05	1.55	1.50
2	M	1000	HEM	CMD-C2D	2.04	1.55	1.50
2	B	1000	HEM	CAA-C2A	2.03	1.55	1.52
2	K	1000	HEM	CMD-C2D	2.03	1.55	1.50
2	G	1000	HEM	CAD-C3D	2.03	1.56	1.51
2	M	1000	HEM	C1B-C2B	2.01	1.48	1.44
2	T	1000	HEM	C2C-C1C	2.01	1.47	1.42
2	T	1000	HEM	CAA-C2A	2.00	1.55	1.52

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1000	HEM	C4D-ND-C1D	8.59	113.94	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1000	HEM	C4D-ND-C1D	8.15	113.50	105.07
2	I	1000	HEM	C4D-ND-C1D	7.91	113.24	105.07
2	R	1000	HEM	C4D-ND-C1D	7.65	112.97	105.07
2	B	1000	HEM	C4D-ND-C1D	7.53	112.85	105.07
2	M	1000	HEM	C4D-ND-C1D	7.46	112.78	105.07
2	C	1000	HEM	C4D-ND-C1D	7.39	112.70	105.07
2	B	1000	HEM	C4C-CHD-C1D	7.33	132.23	122.56
2	A	1000	HEM	C4D-ND-C1D	7.15	112.46	105.07
2	Q	1000	HEM	C4D-ND-C1D	6.98	112.28	105.07
2	L	1000	HEM	C4D-ND-C1D	6.83	112.13	105.07
2	S	1000	HEM	C4D-ND-C1D	6.60	111.89	105.07
2	N	1000	HEM	C4D-ND-C1D	6.56	111.84	105.07
2	K	1000	HEM	C4D-ND-C1D	6.48	111.77	105.07
2	C	1000	HEM	C4C-CHD-C1D	6.44	131.05	122.56
2	F	1000	HEM	C4D-ND-C1D	6.34	111.62	105.07
2	F	1000	HEM	C4C-CHD-C1D	6.19	130.73	122.56
2	D	1000	HEM	C4D-ND-C1D	5.99	111.26	105.07
2	P	1000	HEM	C4D-ND-C1D	5.87	111.13	105.07
2	T	1000	HEM	C4D-ND-C1D	5.79	111.05	105.07
2	K	1000	HEM	C4C-CHD-C1D	5.72	130.11	122.56
2	M	1000	HEM	C4C-CHD-C1D	5.55	129.88	122.56
2	H	1000	HEM	CMA-C3A-C4A	-5.49	120.02	128.46
2	G	1000	HEM	C4C-CHD-C1D	5.45	129.76	122.56
2	J	1000	HEM	C4C-CHD-C1D	5.35	129.62	122.56
2	Q	1000	HEM	C2C-C3C-C4C	5.14	110.49	106.90
2	P	1000	HEM	C4C-CHD-C1D	5.09	129.28	122.56
2	N	1000	HEM	C4C-CHD-C1D	5.04	129.20	122.56
2	O	1000	HEM	C4D-ND-C1D	5.03	110.27	105.07
2	B	1000	HEM	CMA-C3A-C4A	-4.96	120.84	128.46
2	G	1000	HEM	CMA-C3A-C4A	-4.92	120.90	128.46
2	H	1000	HEM	O2D-CGD-O1D	-4.88	111.13	123.30
2	E	1000	HEM	C4D-ND-C1D	4.81	110.04	105.07
2	S	1000	HEM	CMA-C3A-C4A	-4.75	121.16	128.46
2	H	1000	HEM	C4C-CHD-C1D	4.71	128.77	122.56
2	T	1000	HEM	C4C-CHD-C1D	4.70	128.76	122.56
2	I	1000	HEM	C4C-CHD-C1D	4.61	128.64	122.56
2	J	1000	HEM	O2D-CGD-O1D	-4.53	112.01	123.30
2	A	1000	HEM	C4C-CHD-C1D	4.50	128.50	122.56
2	E	1000	HEM	CMA-C3A-C4A	-4.46	121.61	128.46
2	Q	1000	HEM	C4C-CHD-C1D	4.45	128.43	122.56
2	C	1000	HEM	O2D-CGD-O1D	-4.23	112.76	123.30
2	L	1000	HEM	C4B-CHC-C1C	4.17	128.06	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1000	HEM	CAD-CBD-CGD	-4.10	104.77	113.60
2	P	1000	HEM	C2C-C3C-C4C	4.04	109.72	106.90
2	N	1000	HEM	O2D-CGD-O1D	-4.01	113.31	123.30
2	C	1000	HEM	CMA-C3A-C4A	-3.91	122.45	128.46
2	R	1000	HEM	C4C-CHD-C1D	3.89	127.70	122.56
2	B	1000	HEM	O2D-CGD-O1D	-3.89	113.61	123.30
2	Q	1000	HEM	C4A-C3A-C2A	3.88	109.69	107.00
2	F	1000	HEM	O2D-CGD-O1D	-3.87	113.65	123.30
2	G	1000	HEM	O2D-CGD-O1D	-3.82	113.78	123.30
2	J	1000	HEM	C2C-C3C-C4C	3.80	109.55	106.90
2	D	1000	HEM	C4C-CHD-C1D	3.72	127.47	122.56
2	C	1000	HEM	O2A-CGA-O1A	-3.71	114.05	123.30
2	M	1000	HEM	CMA-C3A-C4A	-3.71	122.76	128.46
2	R	1000	HEM	O2D-CGD-O1D	-3.69	114.09	123.30
2	K	1000	HEM	CMA-C3A-C4A	-3.69	122.80	128.46
2	H	1000	HEM	O2A-CGA-CBA	3.68	125.86	114.03
2	H	1000	HEM	CMA-C3A-C2A	3.64	131.81	124.94
2	G	1000	HEM	O2A-CGA-O1A	-3.63	114.26	123.30
2	B	1000	HEM	CMB-C2B-C1B	3.63	130.56	125.04
2	L	1000	HEM	O2A-CGA-CBA	3.62	125.65	114.03
2	H	1000	HEM	O2A-CGA-O1A	-3.61	114.31	123.30
2	E	1000	HEM	C4C-CHD-C1D	3.57	127.28	122.56
2	O	1000	HEM	O2D-CGD-O1D	-3.57	114.40	123.30
2	O	1000	HEM	C4C-CHD-C1D	3.57	127.27	122.56
2	G	1000	HEM	O2A-CGA-CBA	3.55	125.45	114.03
2	M	1000	HEM	CBB-CAB-C3B	-3.54	110.03	127.62
2	I	1000	HEM	O2D-CGD-O1D	-3.53	114.51	123.30
2	F	1000	HEM	C4A-C3A-C2A	3.52	109.44	107.00
2	H	1000	HEM	C4D-ND-C1D	3.51	108.69	105.07
2	B	1000	HEM	O2A-CGA-CBA	3.50	125.28	114.03
2	Q	1000	HEM	CBB-CAB-C3B	-3.49	110.23	127.62
2	A	1000	HEM	O2D-CGD-O1D	-3.49	114.61	123.30
2	J	1000	HEM	O2A-CGA-CBA	3.47	125.18	114.03
2	T	1000	HEM	C2C-C3C-C4C	3.47	109.32	106.90
2	E	1000	HEM	CBA-CAA-C2A	-3.45	106.73	112.62
2	I	1000	HEM	O2A-CGA-O1A	-3.44	114.72	123.30
2	P	1000	HEM	CAA-CBA-CGA	-3.44	104.11	113.76
2	J	1000	HEM	CMA-C3A-C4A	-3.42	123.21	128.46
2	C	1000	HEM	CMA-C3A-C2A	3.41	131.38	124.94
2	S	1000	HEM	CMA-C3A-C2A	3.39	131.33	124.94
2	F	1000	HEM	CMA-C3A-C4A	-3.35	123.31	128.46
2	L	1000	HEM	O2D-CGD-O1D	-3.33	115.01	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1000	HEM	C1B-NB-C4B	-3.31	101.65	105.07
2	K	1000	HEM	O2A-CGA-O1A	-3.30	115.07	123.30
2	K	1000	HEM	O2D-CGD-O1D	-3.30	115.07	123.30
2	R	1000	HEM	CMA-C3A-C4A	-3.29	123.40	128.46
2	B	1000	HEM	CBB-CAB-C3B	-3.28	111.28	127.62
2	M	1000	HEM	O2D-CGD-O1D	-3.28	115.12	123.30
2	L	1000	HEM	CMA-C3A-C4A	-3.28	123.43	128.46
2	R	1000	HEM	C2C-C3C-C4C	3.27	109.18	106.90
2	E	1000	HEM	O2D-CGD-O1D	-3.26	115.17	123.30
2	G	1000	HEM	C2C-C3C-C4C	3.25	109.17	106.90
2	T	1000	HEM	O2A-CGA-CBA	3.23	124.40	114.03
2	H	1000	HEM	C1D-C2D-C3D	-3.22	103.57	106.96
2	Q	1000	HEM	CMB-C2B-C1B	3.21	129.93	125.04
2	C	1000	HEM	CMB-C2B-C1B	3.18	129.88	125.04
2	D	1000	HEM	C2C-C3C-C4C	3.18	109.12	106.90
2	H	1000	HEM	C4B-C3B-C2B	3.16	109.62	107.11
2	T	1000	HEM	O2D-CGD-O1D	-3.14	115.47	123.30
2	B	1000	HEM	CMA-C3A-C2A	3.13	130.85	124.94
2	C	1000	HEM	O2A-CGA-CBA	3.13	124.09	114.03
2	P	1000	HEM	C4D-C3D-C2D	-3.09	102.39	106.90
2	B	1000	HEM	O2A-CGA-O1A	-3.08	115.62	123.30
2	F	1000	HEM	C2C-C3C-C4C	3.04	109.02	106.90
2	S	1000	HEM	O2A-CGA-CBA	3.03	123.77	114.03
2	L	1000	HEM	CMB-C2B-C1B	3.03	129.66	125.04
2	N	1000	HEM	O2A-CGA-O1A	-3.01	115.80	123.30
2	D	1000	HEM	CMD-C2D-C1D	2.99	129.60	125.04
2	R	1000	HEM	C4B-CHC-C1C	2.99	126.50	122.56
2	I	1000	HEM	CAD-CBD-CGD	-2.96	107.22	113.60
2	Q	1000	HEM	O2D-CGD-O1D	-2.95	115.94	123.30
2	S	1000	HEM	CAA-CBA-CGA	-2.94	105.52	113.76
2	J	1000	HEM	C3C-C4C-NC	-2.93	105.41	110.94
2	C	1000	HEM	C2C-C3C-C4C	2.93	108.94	106.90
2	I	1000	HEM	O2A-CGA-CBA	2.92	123.42	114.03
2	K	1000	HEM	O2A-CGA-CBA	2.92	123.42	114.03
2	H	1000	HEM	CMB-C2B-C1B	2.91	129.47	125.04
2	Q	1000	HEM	O2A-CGA-O1A	-2.89	116.10	123.30
2	A	1000	HEM	O2A-CGA-O1A	-2.88	116.12	123.30
2	O	1000	HEM	C4D-C3D-C2D	-2.88	102.71	106.90
2	T	1000	HEM	CHC-C4B-C3B	2.86	128.94	124.57
2	S	1000	HEM	CBD-CAD-C3D	-2.85	104.70	112.63
2	G	1000	HEM	CMA-C3A-C2A	2.85	130.31	124.94
2	A	1000	HEM	C2C-C3C-C4C	2.85	108.89	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1000	HEM	C3C-C4C-NC	-2.82	105.62	110.94
2	E	1000	HEM	CBD-CAD-C3D	-2.82	104.80	112.63
2	Q	1000	HEM	O2A-CGA-CBA	2.81	123.06	114.03
2	O	1000	HEM	C4A-C3A-C2A	2.79	108.94	107.00
2	E	1000	HEM	CMA-C3A-C2A	2.79	130.20	124.94
2	G	1000	HEM	O2D-CGD-CBD	2.78	122.95	114.03
2	O	1000	HEM	CMA-C3A-C4A	-2.76	124.23	128.46
2	G	1000	HEM	CAD-CBD-CGD	-2.75	107.67	113.60
2	Q	1000	HEM	CMA-C3A-C4A	-2.75	124.24	128.46
2	A	1000	HEM	CAD-CBD-CGD	-2.75	107.69	113.60
2	S	1000	HEM	C4B-CHC-C1C	2.73	126.16	122.56
2	M	1000	HEM	O2A-CGA-CBA	2.72	122.77	114.03
2	D	1000	HEM	O2A-CGA-CBA	2.70	122.70	114.03
2	E	1000	HEM	O2A-CGA-O1A	-2.69	116.58	123.30
2	L	1000	HEM	C2C-C3C-C4C	2.69	108.78	106.90
2	M	1000	HEM	CMB-C2B-C1B	2.69	129.13	125.04
2	J	1000	HEM	C2D-C1D-ND	-2.68	106.67	109.88
2	J	1000	HEM	O2A-CGA-O1A	-2.67	116.63	123.30
2	B	1000	HEM	C2C-C3C-C4C	2.67	108.76	106.90
2	I	1000	HEM	C2C-C3C-C4C	2.66	108.75	106.90
2	G	1000	HEM	CHB-C1B-NB	2.65	127.66	124.38
2	E	1000	HEM	CAD-C3D-C4D	2.64	129.28	124.66
2	H	1000	HEM	CBB-CAB-C3B	-2.64	114.48	127.62
2	E	1000	HEM	O2A-CGA-CBA	2.64	122.51	114.03
2	I	1000	HEM	CAA-CBA-CGA	-2.63	106.40	113.76
2	M	1000	HEM	C4A-C3A-C2A	2.63	108.82	107.00
2	M	1000	HEM	C2C-C3C-C4C	2.61	108.72	106.90
2	R	1000	HEM	CAD-C3D-C4D	2.61	129.22	124.66
2	A	1000	HEM	CMB-C2B-C1B	2.60	129.01	125.04
2	F	1000	HEM	C3C-C4C-NC	-2.60	106.04	110.94
2	P	1000	HEM	C4B-CHC-C1C	2.58	125.96	122.56
2	N	1000	HEM	CAA-CBA-CGA	-2.58	106.53	113.76
2	T	1000	HEM	C3B-C2B-C1B	2.57	108.39	106.49
2	S	1000	HEM	C2C-C3C-C4C	2.57	108.69	106.90
2	G	1000	HEM	C4A-C3A-C2A	2.57	108.78	107.00
2	F	1000	HEM	C3B-C2B-C1B	2.56	108.39	106.49
2	P	1000	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
2	R	1000	HEM	CAA-CBA-CGA	-2.55	106.61	113.76
2	F	1000	HEM	O2A-CGA-O1A	-2.53	117.00	123.30
2	F	1000	HEM	O2A-CGA-CBA	2.53	122.15	114.03
2	K	1000	HEM	C4D-C3D-C2D	-2.53	103.21	106.90
2	N	1000	HEM	CMB-C2B-C1B	2.52	128.87	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1000	HEM	CMA-C3A-C4A	-2.50	124.62	128.46
2	C	1000	HEM	C3C-C4C-NC	-2.50	106.23	110.94
2	A	1000	HEM	O2A-CGA-CBA	2.49	122.03	114.03
2	J	1000	HEM	O2D-CGD-CBD	2.48	122.00	114.03
2	E	1000	HEM	CMD-C2D-C1D	2.46	128.78	125.04
2	P	1000	HEM	O2A-CGA-O1A	-2.45	117.19	123.30
2	G	1000	HEM	CAB-C3B-C2B	-2.45	120.54	128.60
2	P	1000	HEM	CAB-C3B-C2B	-2.45	120.54	128.60
2	N	1000	HEM	O2A-CGA-CBA	2.44	121.87	114.03
2	B	1000	HEM	CMB-C2B-C3B	-2.43	122.35	128.30
2	M	1000	HEM	CBD-CAD-C3D	-2.43	105.88	112.63
2	L	1000	HEM	CBB-CAB-C3B	-2.42	115.58	127.62
2	M	1000	HEM	CBA-CAA-C2A	-2.42	108.50	112.62
2	D	1000	HEM	CHA-C4D-ND	2.41	127.36	124.38
2	R	1000	HEM	C3C-C4C-NC	-2.41	106.40	110.94
2	F	1000	HEM	CMB-C2B-C1B	2.41	128.70	125.04
2	G	1000	HEM	CHB-C1B-C2B	-2.40	120.09	126.72
2	Q	1000	HEM	CHC-C4B-NB	2.39	127.03	124.43
2	Q	1000	HEM	C4D-C3D-C2D	-2.39	103.41	106.90
2	K	1000	HEM	C4A-C3A-C2A	2.38	108.65	107.00
2	A	1000	HEM	C3C-C4C-NC	-2.37	106.47	110.94
2	Q	1000	HEM	C3C-C4C-NC	-2.36	106.48	110.94
2	N	1000	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
2	M	1000	HEM	O2A-CGA-O1A	-2.35	117.44	123.30
2	J	1000	HEM	CAD-C3D-C2D	2.35	132.26	127.88
2	J	1000	HEM	CMB-C2B-C1B	2.33	128.59	125.04
2	F	1000	HEM	CHB-C1B-NB	2.32	127.25	124.38
2	T	1000	HEM	CHB-C1B-NB	2.32	127.24	124.38
2	E	1000	HEM	CHB-C1B-NB	2.31	127.24	124.38
2	R	1000	HEM	O2A-CGA-O1A	-2.30	117.56	123.30
2	P	1000	HEM	C3C-C4C-NC	-2.29	106.61	110.94
2	L	1000	HEM	O2A-CGA-O1A	-2.29	117.59	123.30
2	Q	1000	HEM	CMB-C2B-C3B	-2.29	122.70	128.30
2	H	1000	HEM	CHB-C1B-NB	2.28	127.20	124.38
2	R	1000	HEM	C3D-C4D-ND	-2.28	107.62	110.17
2	Q	1000	HEM	CBD-CAD-C3D	-2.27	106.33	112.63
2	E	1000	HEM	C4B-C3B-C2B	2.26	108.91	107.11
2	C	1000	HEM	CBD-CAD-C3D	-2.24	106.39	112.63
2	L	1000	HEM	CMA-C3A-C2A	2.24	129.17	124.94
2	E	1000	HEM	C2C-C3C-C4C	2.23	108.45	106.90
2	A	1000	HEM	CMA-C3A-C4A	-2.22	125.05	128.46
2	C	1000	HEM	C2B-C1B-NB	2.22	112.47	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1000	HEM	CMA-C3A-C2A	2.22	129.13	124.94
2	J	1000	HEM	CHD-C1D-C2D	2.22	128.45	124.98
2	L	1000	HEM	CAA-CBA-CGA	-2.22	107.53	113.76
2	K	1000	HEM	CHD-C1D-ND	2.22	126.84	124.43
2	T	1000	HEM	CMA-C3A-C4A	-2.22	125.06	128.46
2	C	1000	HEM	CMD-C2D-C1D	2.21	128.41	125.04
2	M	1000	HEM	CMB-C2B-C3B	-2.21	122.89	128.30
2	A	1000	HEM	CAA-CBA-CGA	-2.21	107.56	113.76
2	F	1000	HEM	CMB-C2B-C3B	-2.20	122.91	128.30
2	M	1000	HEM	C4B-C3B-C2B	2.20	108.86	107.11
2	F	1000	HEM	C4D-C3D-C2D	-2.20	103.69	106.90
2	J	1000	HEM	C4B-C3B-C2B	2.19	108.86	107.11
2	I	1000	HEM	C2D-C1D-ND	-2.19	107.26	109.88
2	C	1000	HEM	CAD-CBD-CGD	-2.18	108.92	113.60
2	I	1000	HEM	CMA-C3A-C4A	-2.17	125.12	128.46
2	K	1000	HEM	CMB-C2B-C1B	2.16	128.33	125.04
2	G	1000	HEM	C4B-C3B-C2B	2.14	108.81	107.11
2	E	1000	HEM	CMB-C2B-C1B	2.13	128.29	125.04
2	P	1000	HEM	O2A-CGA-CBA	2.13	120.88	114.03
2	T	1000	HEM	CAA-CBA-CGA	-2.13	107.78	113.76
2	K	1000	HEM	CAD-C3D-C4D	2.11	128.35	124.66
2	L	1000	HEM	CHB-C1B-NB	2.11	126.99	124.38
2	P	1000	HEM	CAD-C3D-C2D	2.10	131.79	127.88
2	T	1000	HEM	C4D-C3D-C2D	-2.10	103.84	106.90
2	H	1000	HEM	O2D-CGD-CBD	2.10	120.76	114.03
2	R	1000	HEM	CMA-C3A-C2A	2.09	128.89	124.94
2	T	1000	HEM	C1B-NB-C4B	2.09	107.24	105.07
2	O	1000	HEM	O2A-CGA-CBA	2.09	120.74	114.03
2	K	1000	HEM	CMC-C2C-C3C	2.08	128.57	124.68
2	G	1000	HEM	C1D-C2D-C3D	-2.08	104.77	106.96
2	J	1000	HEM	CHA-C4D-ND	2.07	126.94	124.38
2	R	1000	HEM	C1B-NB-C4B	2.07	107.21	105.07
2	L	1000	HEM	CHA-C4D-ND	2.07	126.94	124.38
2	C	1000	HEM	CHD-C1D-C2D	2.05	128.19	124.98
2	D	1000	HEM	CHC-C4B-NB	2.05	126.66	124.43
2	D	1000	HEM	O2A-CGA-O1A	-2.05	118.20	123.30
2	B	1000	HEM	C3C-C4C-NC	-2.05	107.08	110.94
2	O	1000	HEM	C3B-C2B-C1B	2.04	108.00	106.49
2	O	1000	HEM	CBA-CAA-C2A	-2.04	109.13	112.62
2	A	1000	HEM	C4D-C3D-C2D	-2.04	103.92	106.90
2	L	1000	HEM	C2D-C1D-ND	-2.04	107.44	109.88
2	G	1000	HEM	C2B-C1B-NB	2.03	112.25	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1000	HEM	CHB-C1B-NB	2.03	126.89	124.38
2	T	1000	HEM	C4B-CHC-C1C	2.03	125.23	122.56
2	R	1000	HEM	O2D-CGD-CBD	2.02	120.53	114.03
2	J	1000	HEM	CBB-CAB-C3B	-2.02	117.58	127.62
2	M	1000	HEM	C3C-C4C-NC	-2.02	107.13	110.94
2	N	1000	HEM	CBB-CAB-C3B	-2.02	117.59	127.62
2	J	1000	HEM	C4D-C3D-C2D	-2.02	103.96	106.90
2	G	1000	HEM	C4D-C3D-C2D	-2.01	103.97	106.90
2	N	1000	HEM	CAD-C3D-C4D	2.01	128.16	124.66
2	M	1000	HEM	C1B-NB-C4B	2.00	107.14	105.07
2	P	1000	HEM	O2D-CGD-O1D	-2.00	118.31	123.30
2	M	1000	HEM	C3B-C2B-C1B	2.00	107.97	106.49

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	HEM	C2B-C3B-CAB-CBB
2	A	1000	HEM	C4B-C3B-CAB-CBB
2	D	1000	HEM	C2B-C3B-CAB-CBB
2	D	1000	HEM	C4B-C3B-CAB-CBB
2	J	1000	HEM	C2B-C3B-CAB-CBB
2	J	1000	HEM	C4B-C3B-CAB-CBB
2	Q	1000	HEM	C2B-C3B-CAB-CBB
2	Q	1000	HEM	C4B-C3B-CAB-CBB
2	C	1000	HEM	C2B-C3B-CAB-CBB
2	F	1000	HEM	C2B-C3B-CAB-CBB
2	G	1000	HEM	C2B-C3B-CAB-CBB
2	N	1000	HEM	C2B-C3B-CAB-CBB
2	O	1000	HEM	C2B-C3B-CAB-CBB
2	R	1000	HEM	C2B-C3B-CAB-CBB
2	S	1000	HEM	C2B-C3B-CAB-CBB
2	C	1000	HEM	C4B-C3B-CAB-CBB
2	F	1000	HEM	C4B-C3B-CAB-CBB
2	G	1000	HEM	C4B-C3B-CAB-CBB
2	N	1000	HEM	C4B-C3B-CAB-CBB
2	O	1000	HEM	C4B-C3B-CAB-CBB
2	S	1000	HEM	C4B-C3B-CAB-CBB
2	E	1000	HEM	C2B-C3B-CAB-CBB
2	T	1000	HEM	C2B-C3B-CAB-CBB
2	L	1000	HEM	C4B-C3B-CAB-CBB
2	E	1000	HEM	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	R	1000	HEM	C4B-C3B-CAB-CBB
2	T	1000	HEM	C4B-C3B-CAB-CBB
2	F	1000	HEM	CAA-CBA-CGA-O1A
2	L	1000	HEM	CAD-CBD-CGD-O1D
2	N	1000	HEM	CAD-CBD-CGD-O1D
2	N	1000	HEM	CAD-CBD-CGD-O2D
2	D	1000	HEM	CAA-CBA-CGA-O2A
2	T	1000	HEM	CAA-CBA-CGA-O1A
2	F	1000	HEM	CAA-CBA-CGA-O2A
2	H	1000	HEM	CAD-CBD-CGD-O1D
2	R	1000	HEM	CAD-CBD-CGD-O1D
2	E	1000	HEM	CAD-CBD-CGD-O1D
2	J	1000	HEM	CAD-CBD-CGD-O1D
2	O	1000	HEM	CAD-CBD-CGD-O1D
2	L	1000	HEM	CAD-CBD-CGD-O2D
2	D	1000	HEM	CAD-CBD-CGD-O1D
2	R	1000	HEM	CAD-CBD-CGD-O2D
2	C	1000	HEM	CAD-CBD-CGD-O1D
2	D	1000	HEM	CAA-CBA-CGA-O1A
2	T	1000	HEM	CAA-CBA-CGA-O2A
2	E	1000	HEM	CAD-CBD-CGD-O2D
2	O	1000	HEM	CAD-CBD-CGD-O2D
2	C	1000	HEM	CAD-CBD-CGD-O2D
2	D	1000	HEM	CAD-CBD-CGD-O2D
2	A	1000	HEM	CAD-CBD-CGD-O1D
2	H	1000	HEM	CAD-CBD-CGD-O2D
2	F	1000	HEM	CAD-CBD-CGD-O1D
2	J	1000	HEM	CAD-CBD-CGD-O2D
2	A	1000	HEM	CAA-CBA-CGA-O2A
2	I	1000	HEM	CAA-CBA-CGA-O2A
2	C	1000	HEM	CAA-CBA-CGA-O2A
2	M	1000	HEM	CAA-CBA-CGA-O2A
2	P	1000	HEM	CAD-CBD-CGD-O2D
2	G	1000	HEM	CAD-CBD-CGD-O2D
2	O	1000	HEM	CAA-CBA-CGA-O2A
2	A	1000	HEM	CAD-CBD-CGD-O2D
2	J	1000	HEM	CAA-CBA-CGA-O1A
2	K	1000	HEM	CAA-CBA-CGA-O2A
2	T	1000	HEM	CAD-CBD-CGD-O2D
2	K	1000	HEM	CAA-CBA-CGA-O1A
2	M	1000	HEM	CAA-CBA-CGA-O1A
2	S	1000	HEM	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1000	HEM	CAA-CBA-CGA-O1A
2	J	1000	HEM	CAA-CBA-CGA-O2A
2	C	1000	HEM	CAA-CBA-CGA-O1A
2	M	1000	HEM	CAD-CBD-CGD-O2D
2	F	1000	HEM	CAD-CBD-CGD-O2D
2	N	1000	HEM	CAA-CBA-CGA-O1A
2	N	1000	HEM	CAA-CBA-CGA-O2A
2	P	1000	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

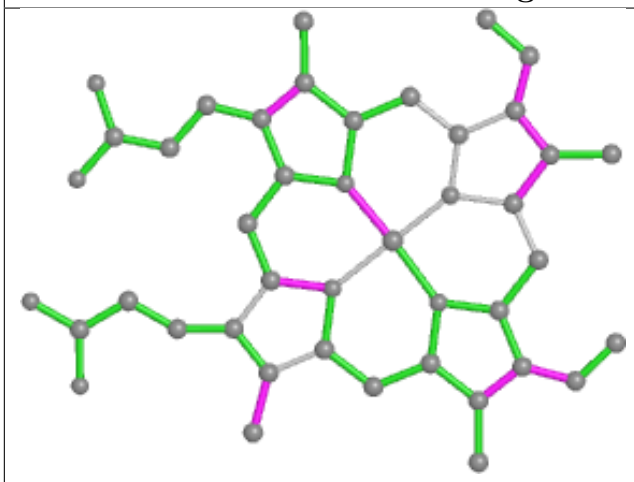
23 monomers are involved in 168 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	2000	NO2	1	0
2	I	1000	HEM	7	0
3	G	2000	NO2	1	0
2	L	1000	HEM	7	0
3	C	2000	NO2	1	0
2	P	1000	HEM	3	0
2	Q	1000	HEM	10	0
2	F	1000	HEM	11	0
2	A	1000	HEM	8	0
2	R	1000	HEM	14	0
2	N	1000	HEM	10	0
2	C	1000	HEM	7	0
2	B	1000	HEM	6	0
2	M	1000	HEM	6	0
2	H	1000	HEM	9	0
2	E	1000	HEM	8	0
2	G	1000	HEM	15	0
2	S	1000	HEM	9	0
2	O	1000	HEM	5	0
2	D	1000	HEM	9	0
2	T	1000	HEM	6	0
2	K	1000	HEM	5	0
2	J	1000	HEM	10	0

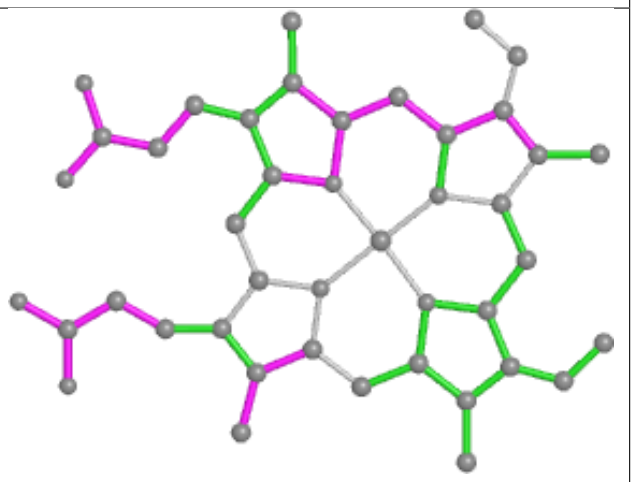
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

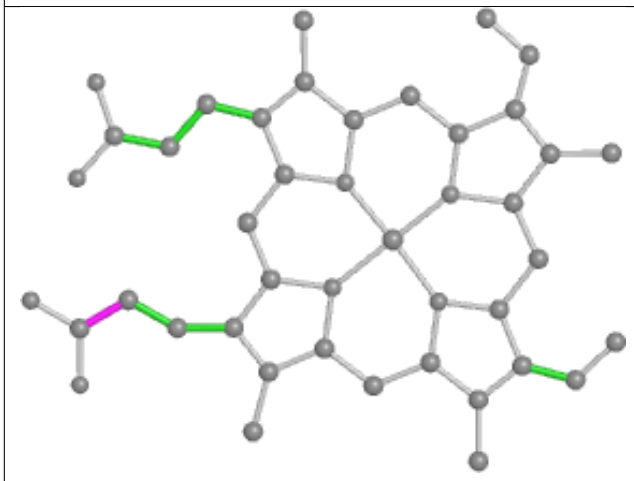
Ligand HEM I 1000



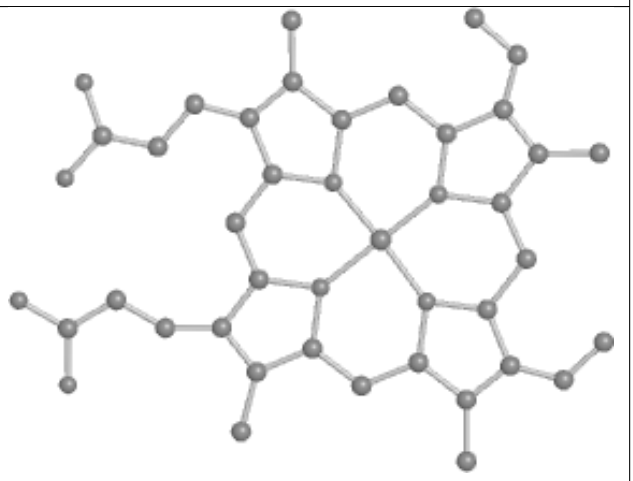
Bond lengths



Bond angles

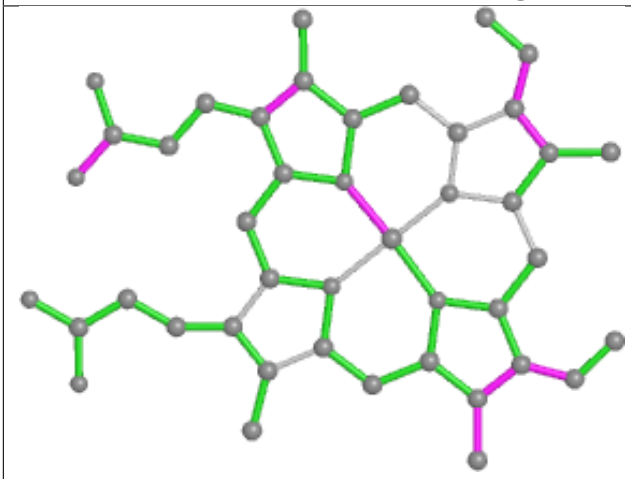


Torsions

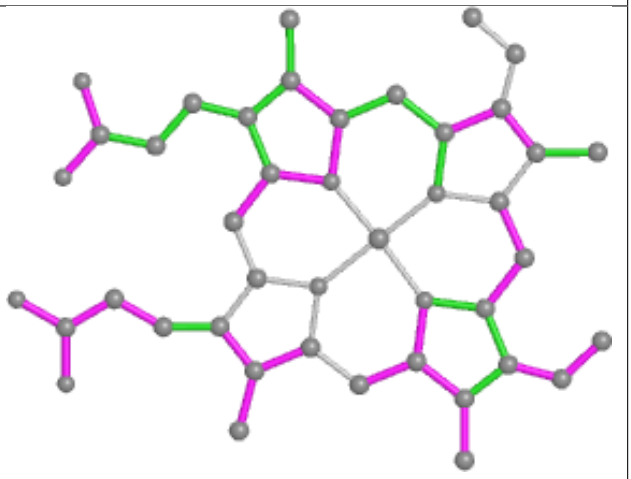


Rings

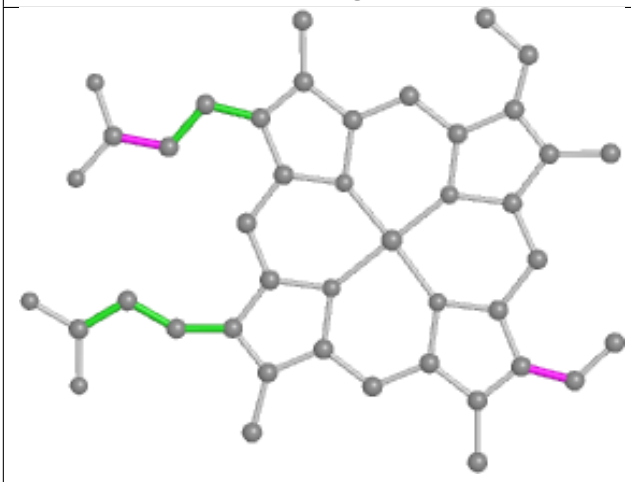
Ligand HEM L 1000



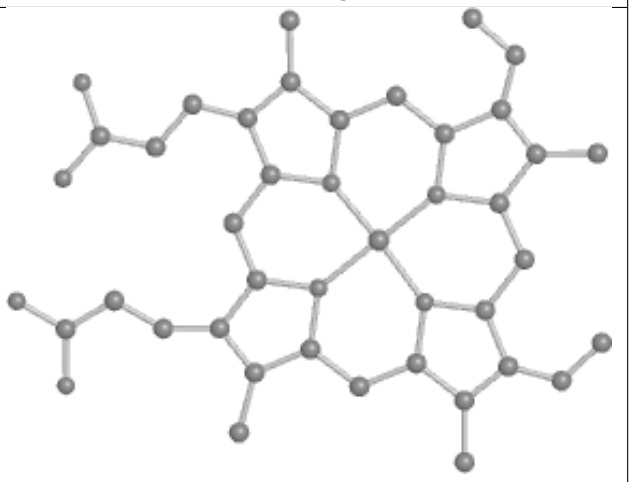
Bond lengths



Bond angles

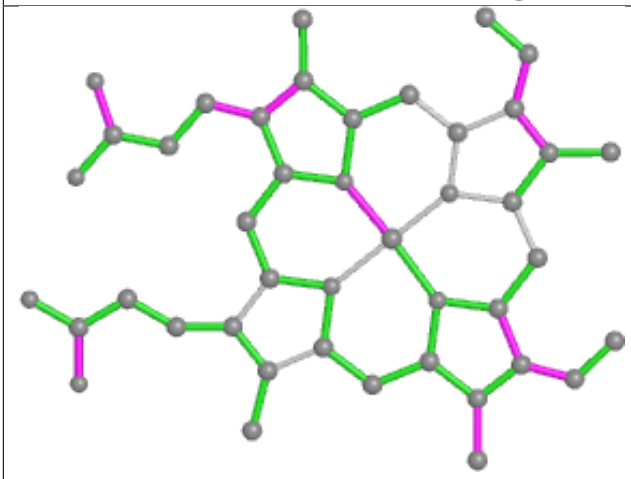


Torsions

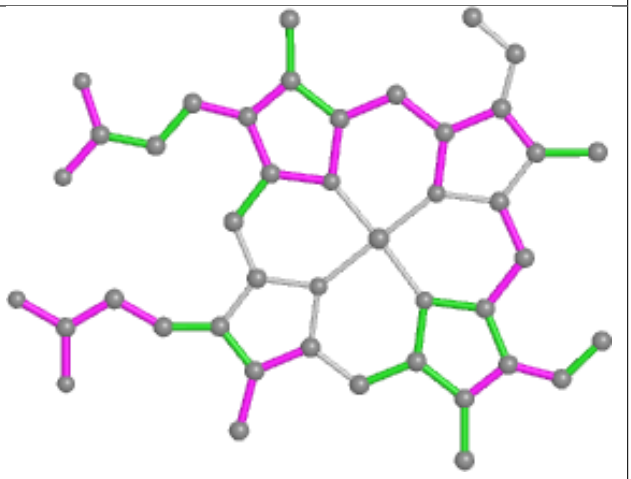


Rings

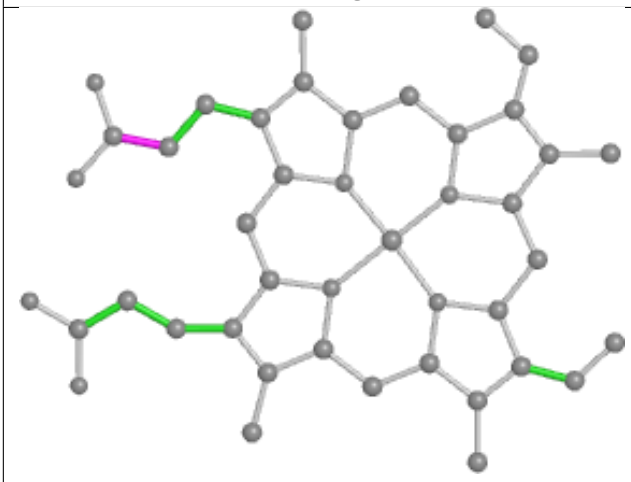
Ligand HEM P 1000



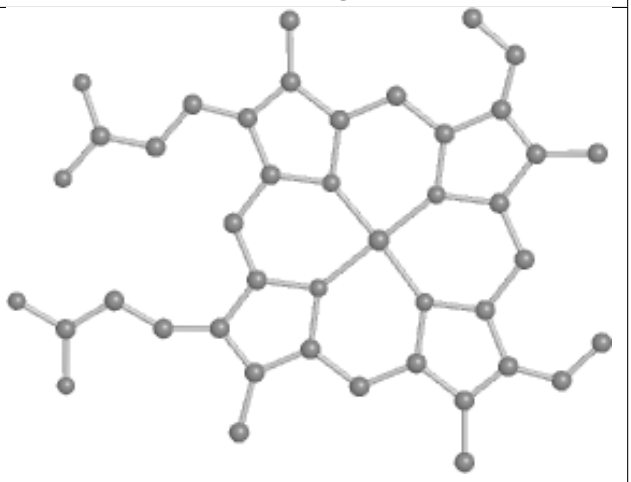
Bond lengths



Bond angles

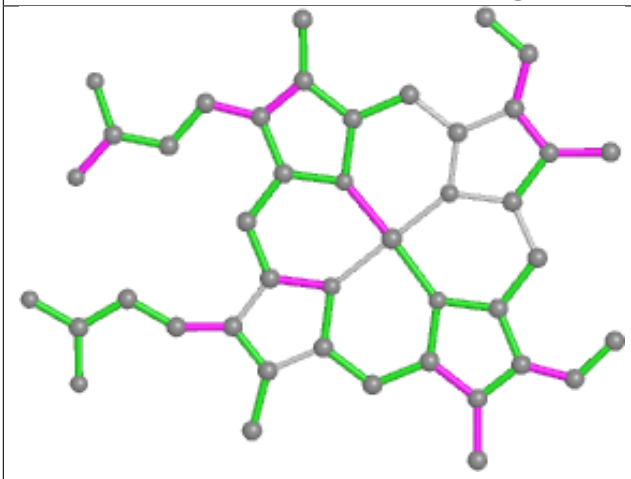


Torsions

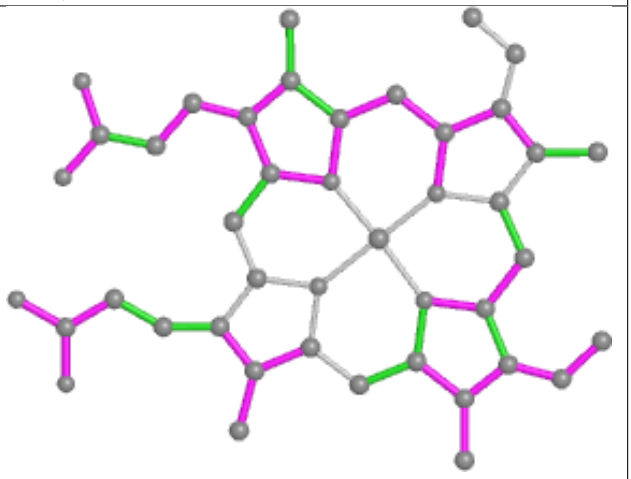


Rings

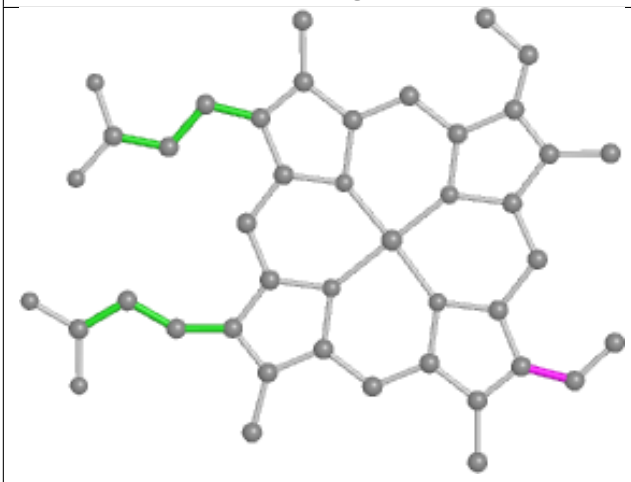
Ligand HEM Q 1000



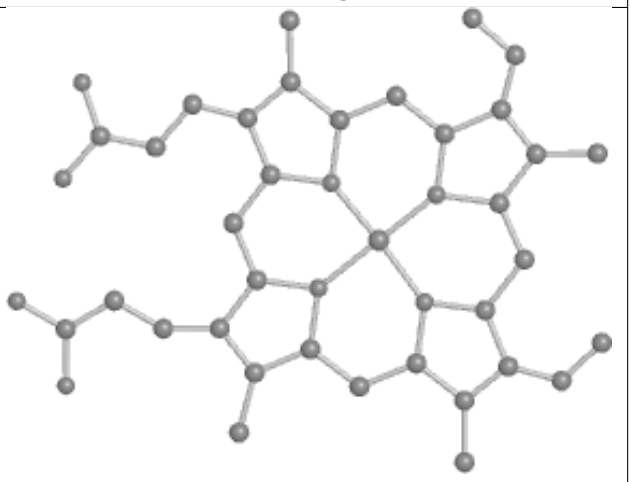
Bond lengths



Bond angles

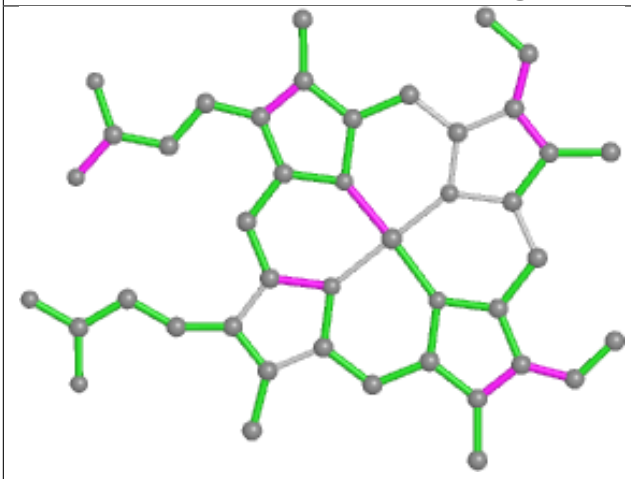


Torsions

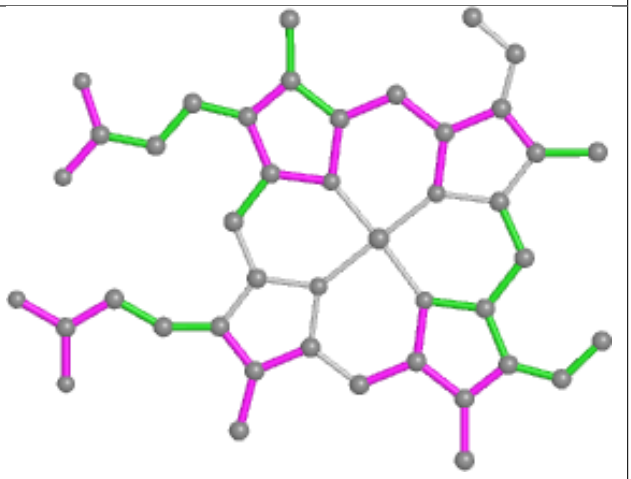


Rings

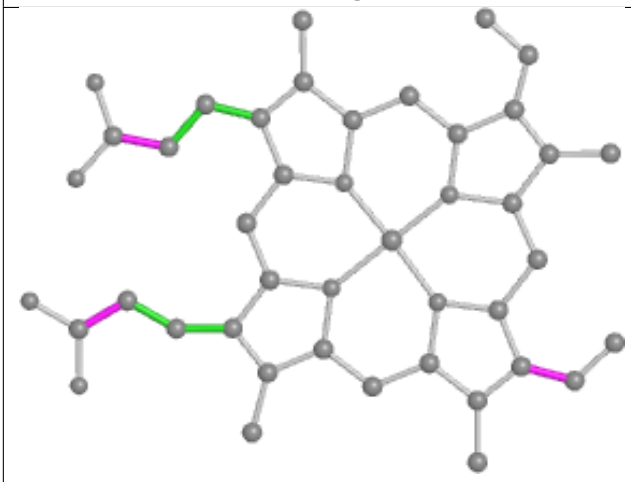
Ligand HEM F 1000



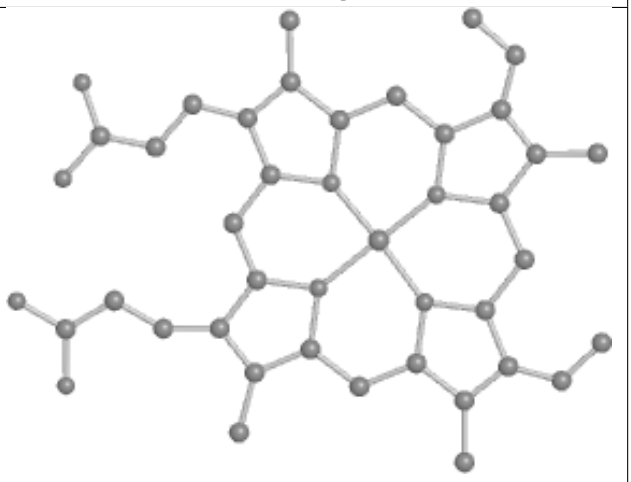
Bond lengths



Bond angles

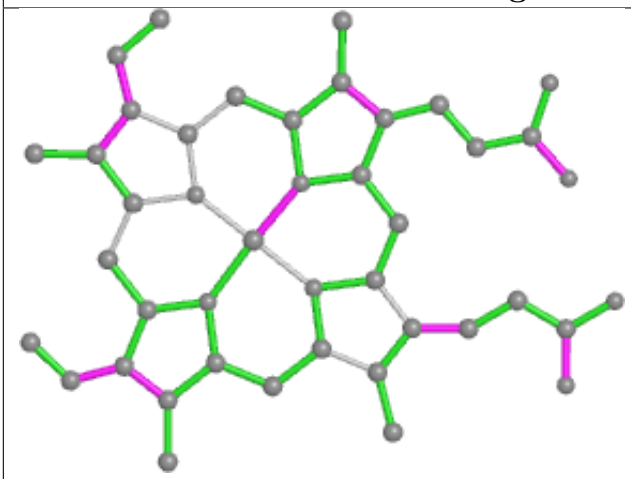


Torsions

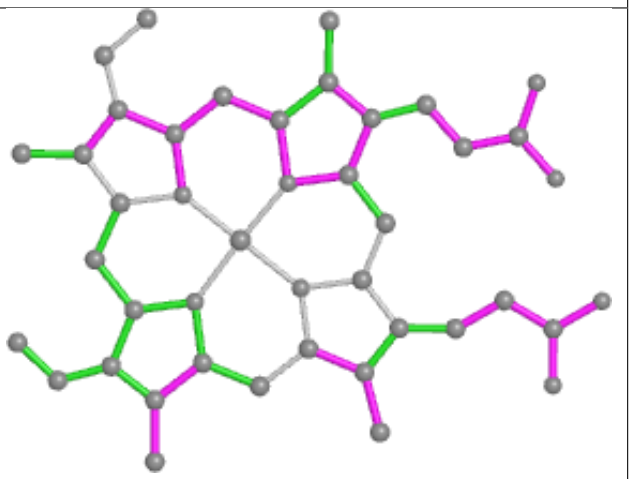


Rings

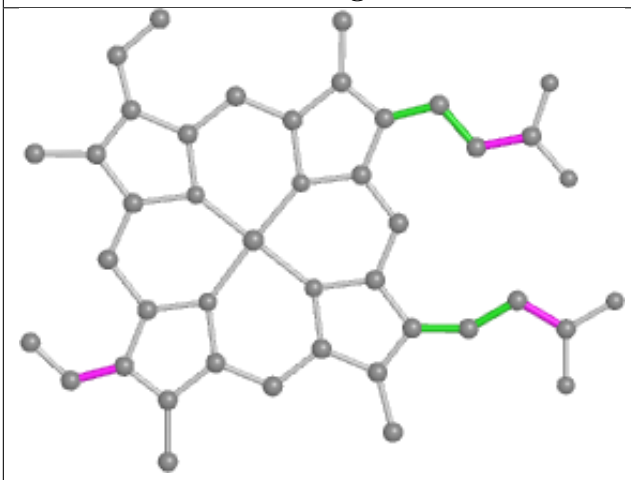
Ligand HEM A 1000



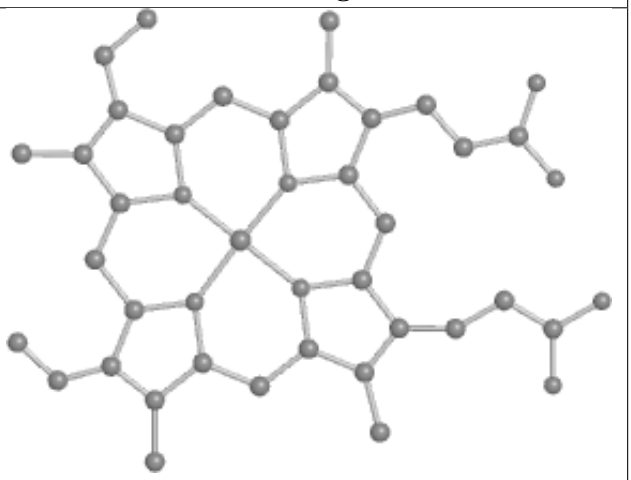
Bond lengths



Bond angles

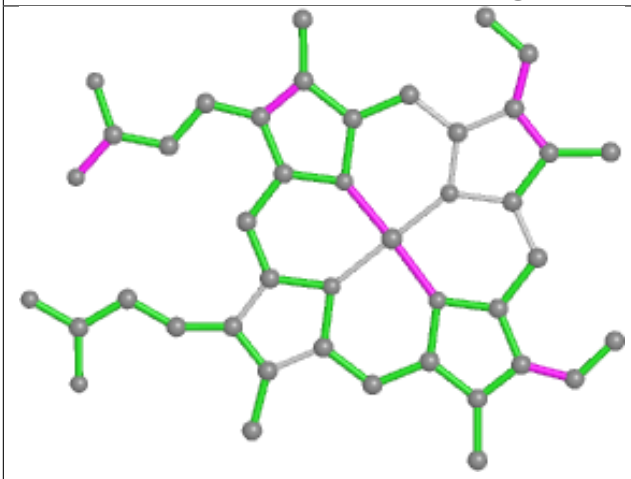


Torsions

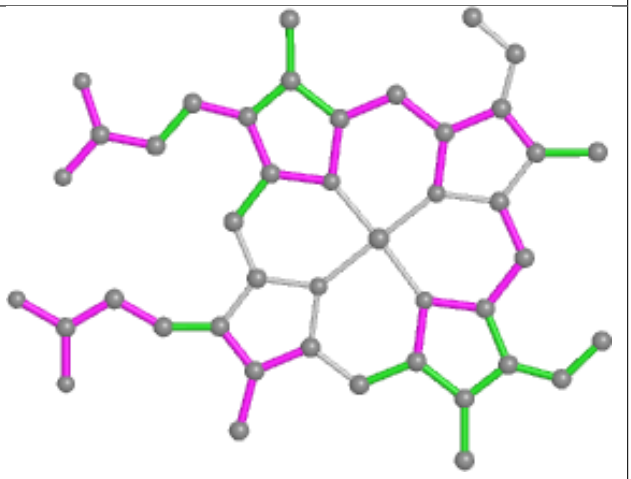


Rings

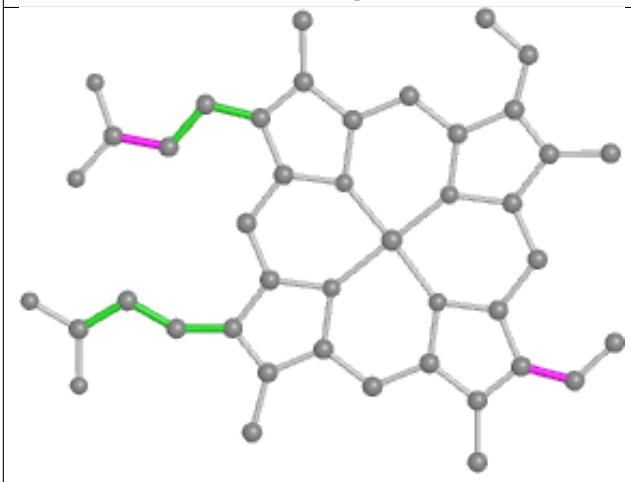
Ligand HEM R 1000



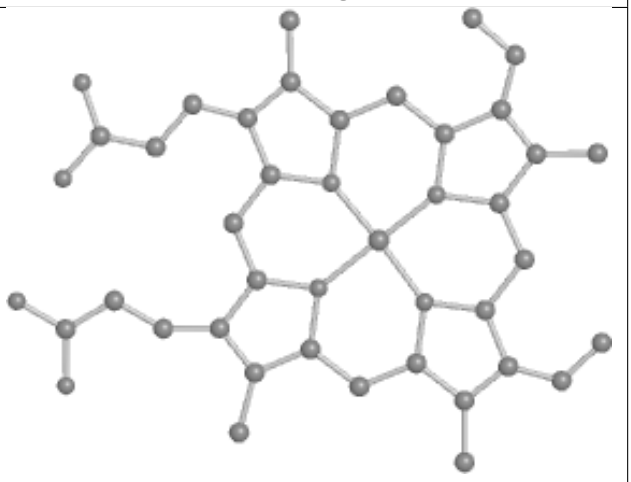
Bond lengths



Bond angles

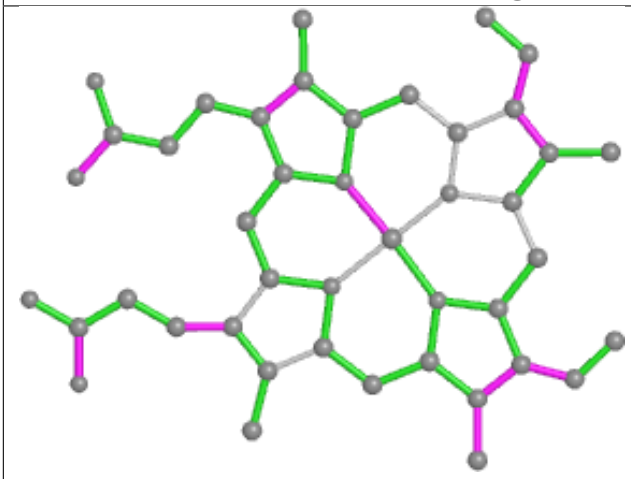


Torsions

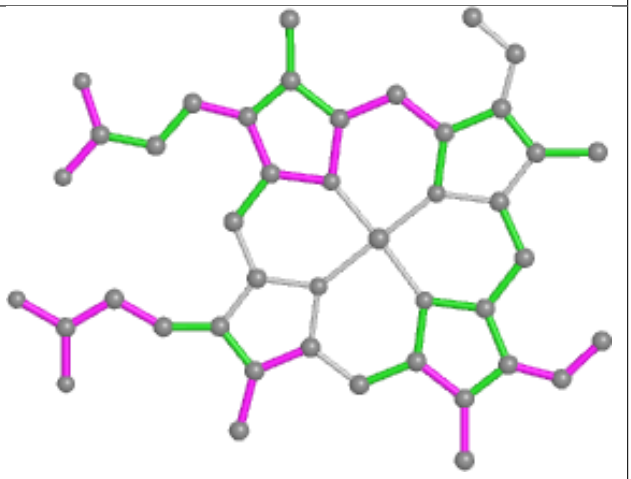


Rings

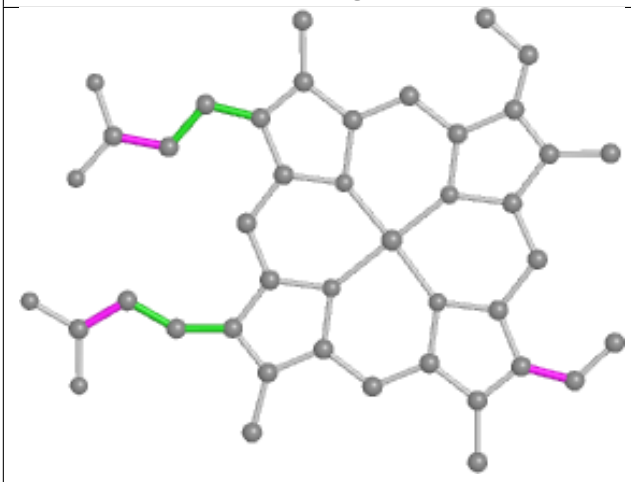
Ligand HEM N 1000



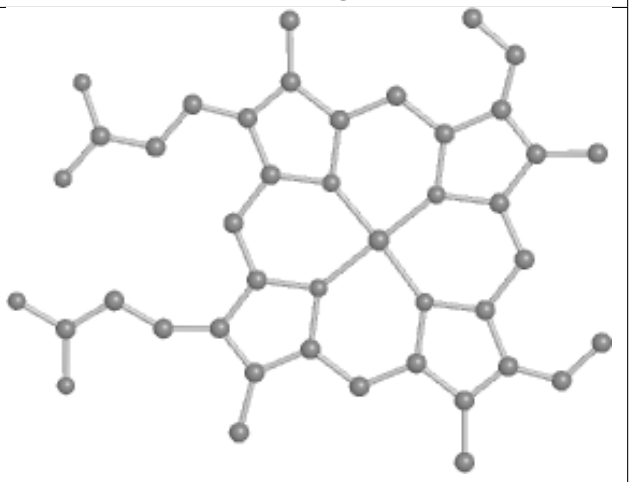
Bond lengths



Bond angles

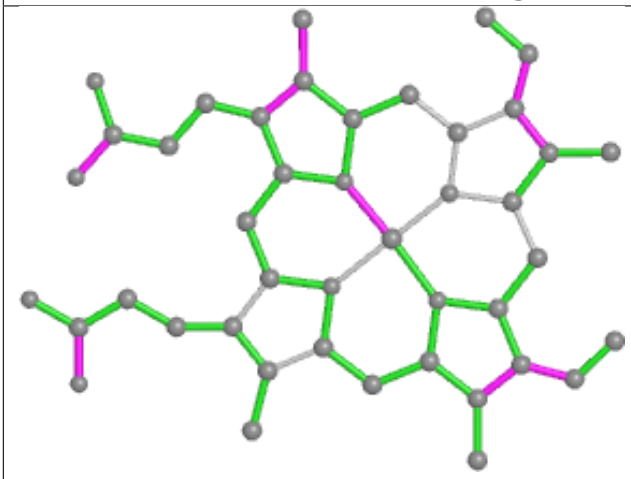


Torsions

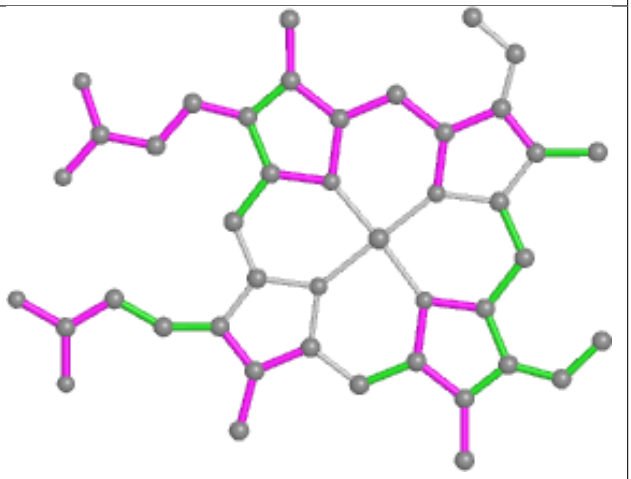


Rings

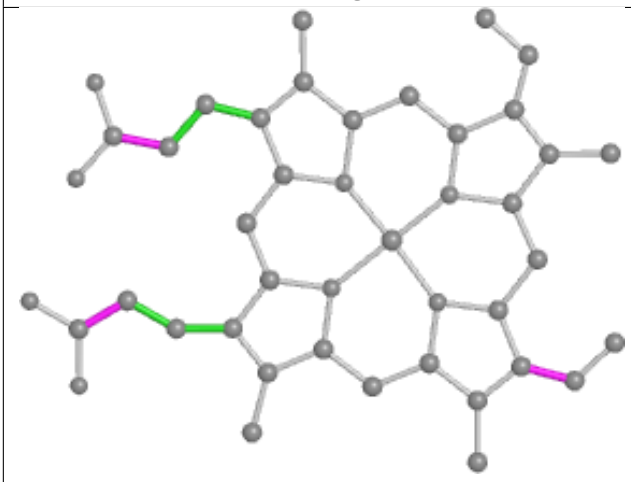
Ligand HEM C 1000



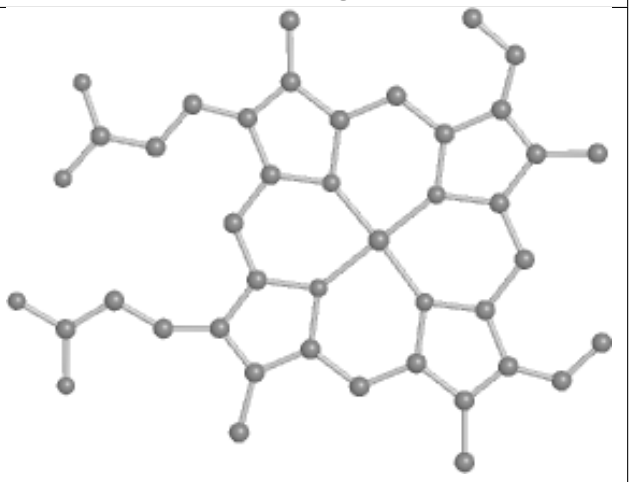
Bond lengths



Bond angles

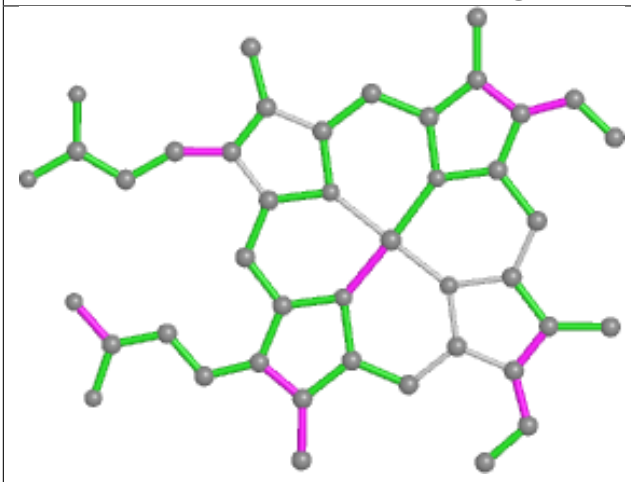


Torsions

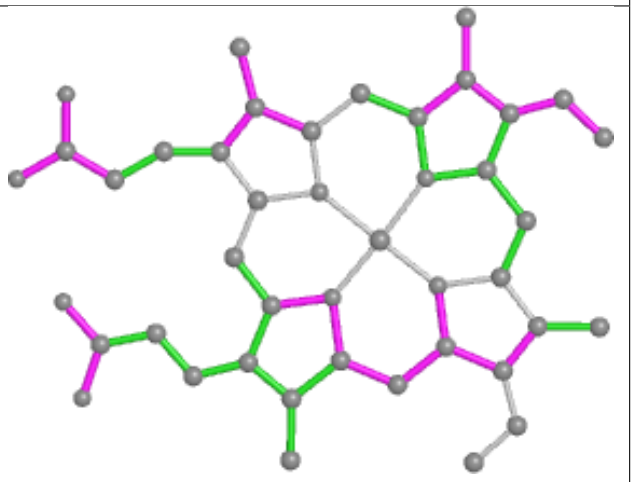


Rings

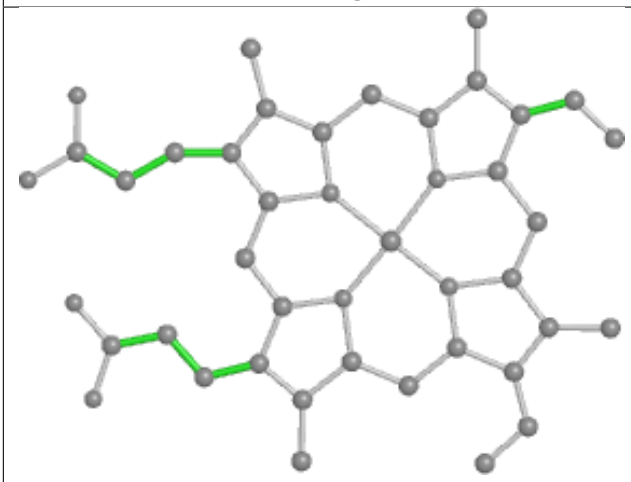
Ligand HEM B 1000



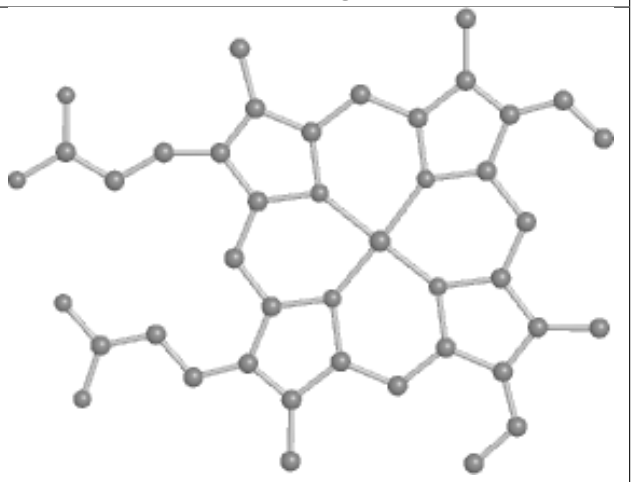
Bond lengths



Bond angles

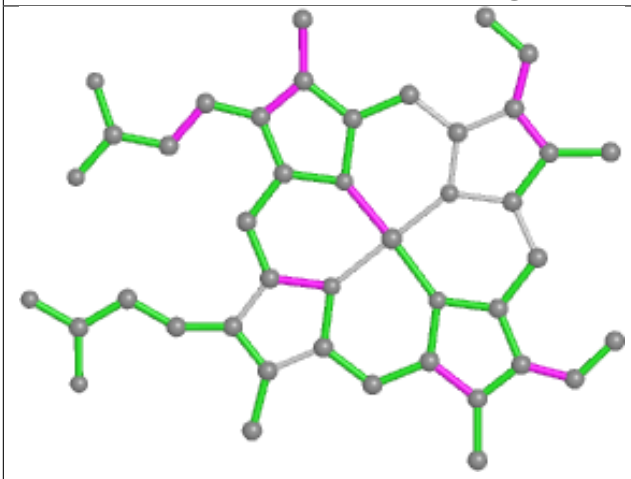


Torsions

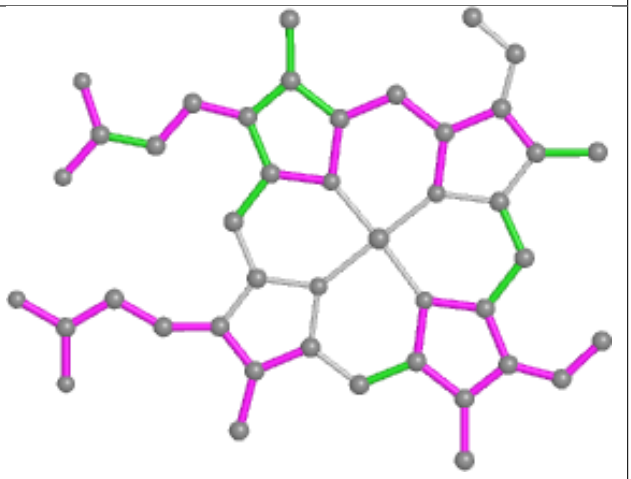


Rings

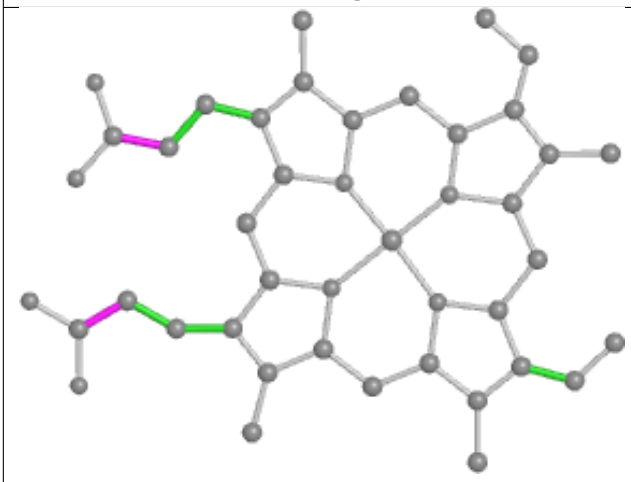
Ligand HEM M 1000



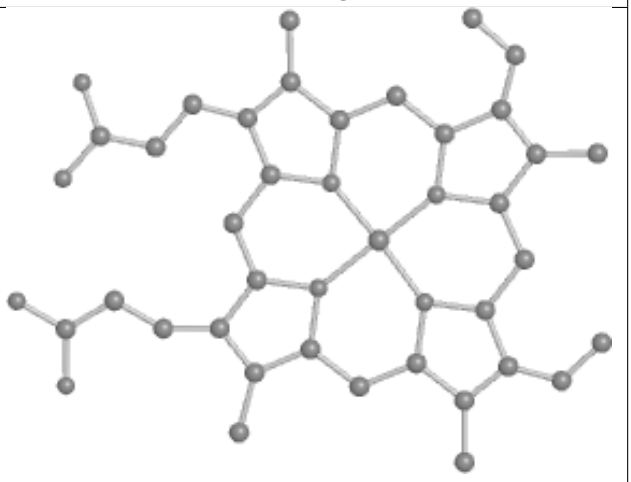
Bond lengths



Bond angles

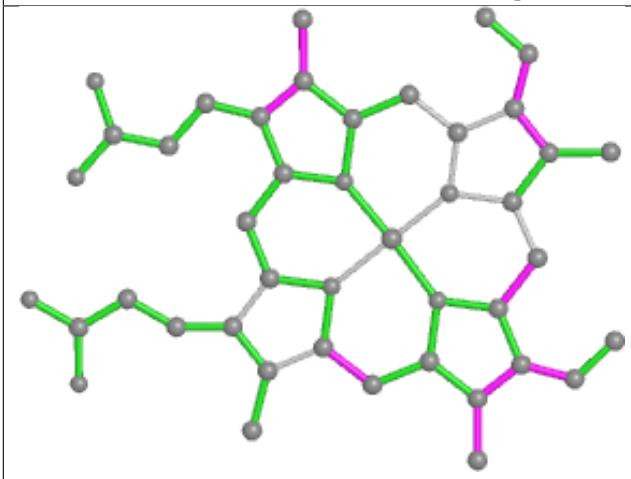


Torsions

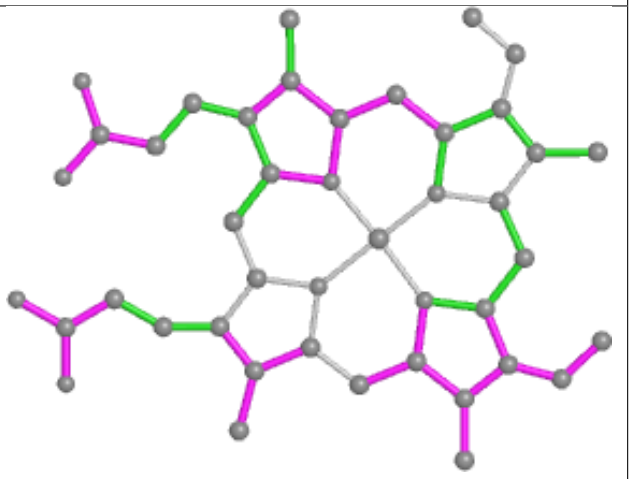


Rings

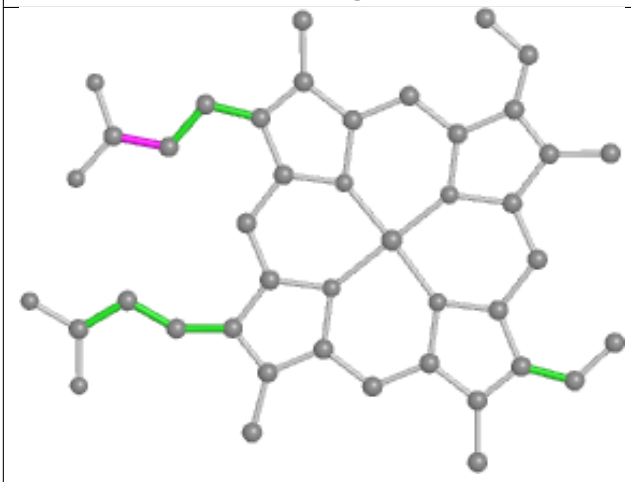
Ligand HEM H 1000



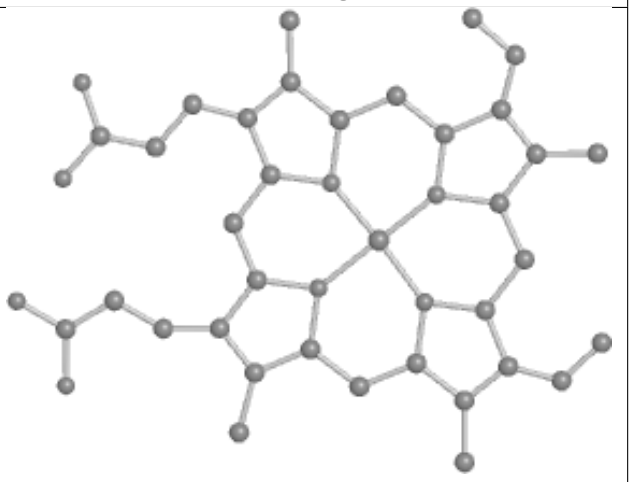
Bond lengths



Bond angles

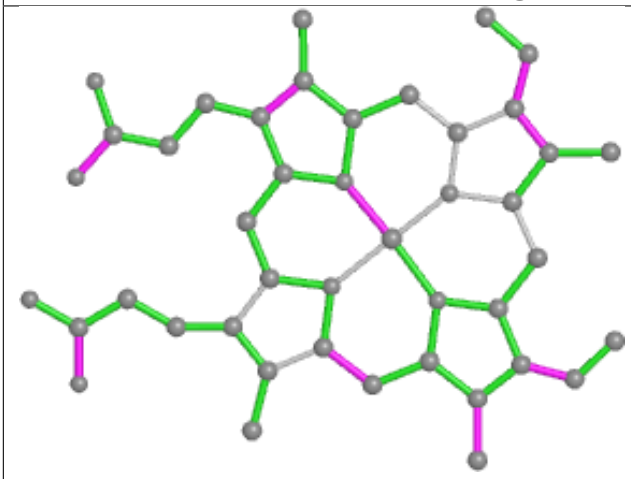


Torsions

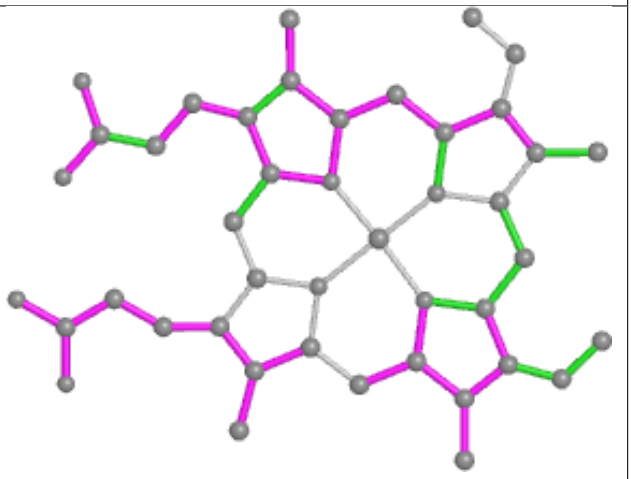


Rings

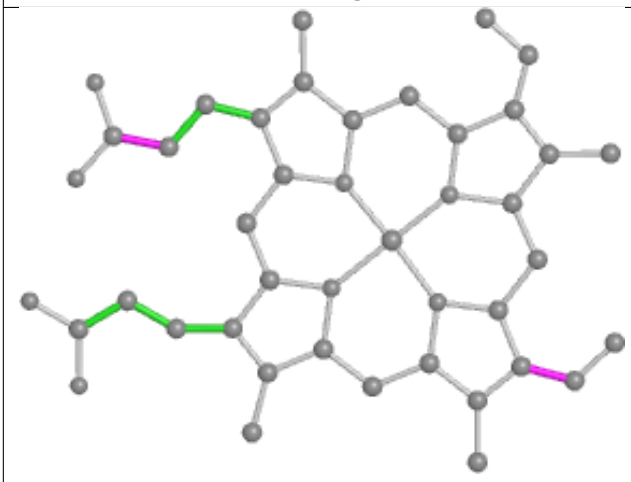
Ligand HEM E 1000



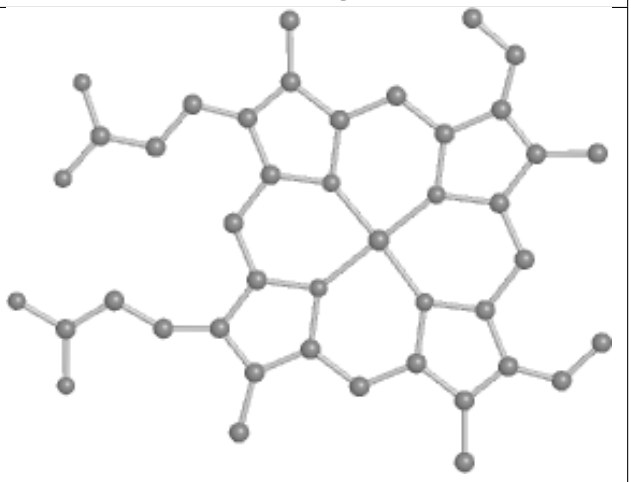
Bond lengths



Bond angles

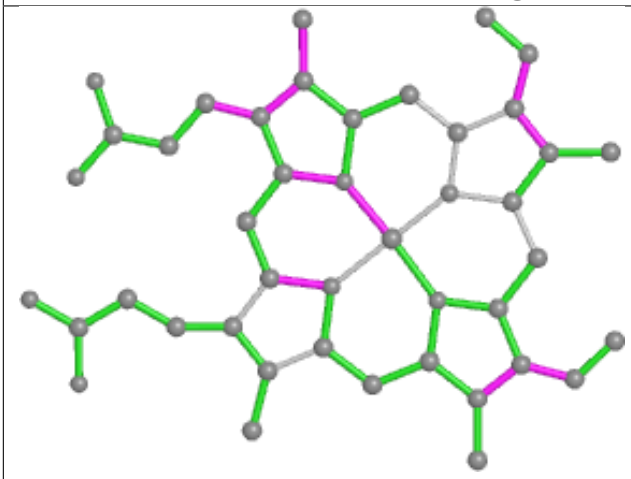


Torsions

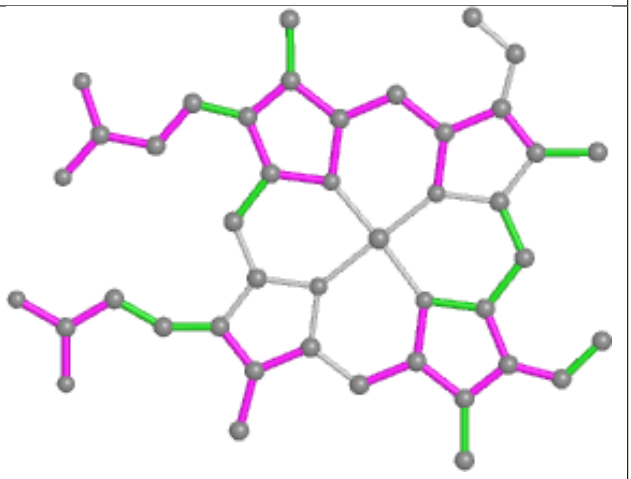


Rings

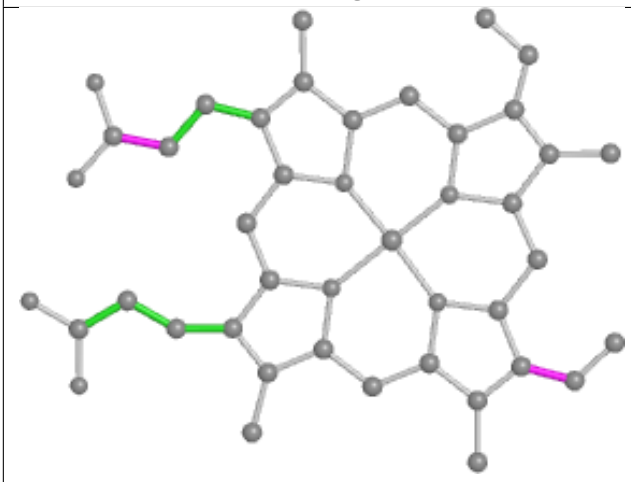
Ligand HEM G 1000



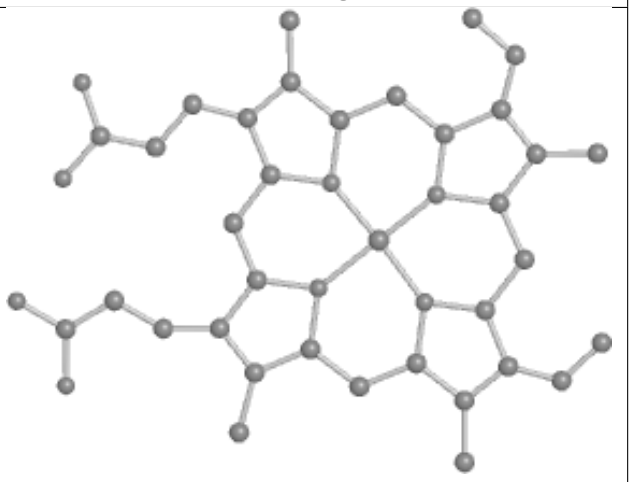
Bond lengths



Bond angles

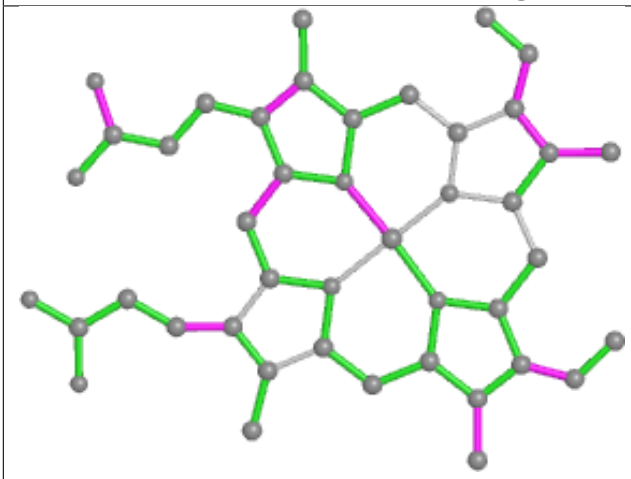


Torsions

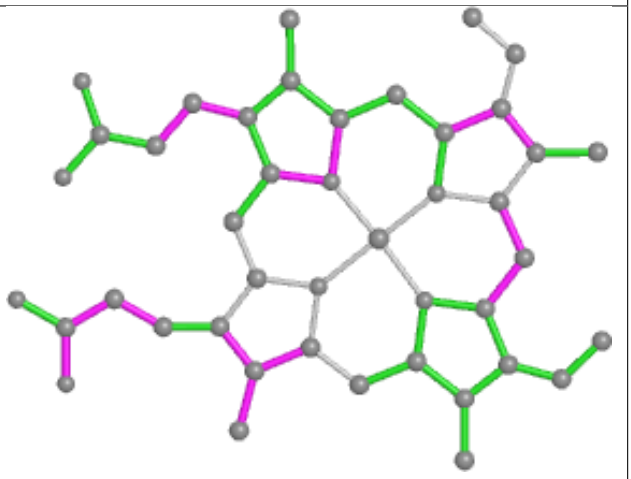


Rings

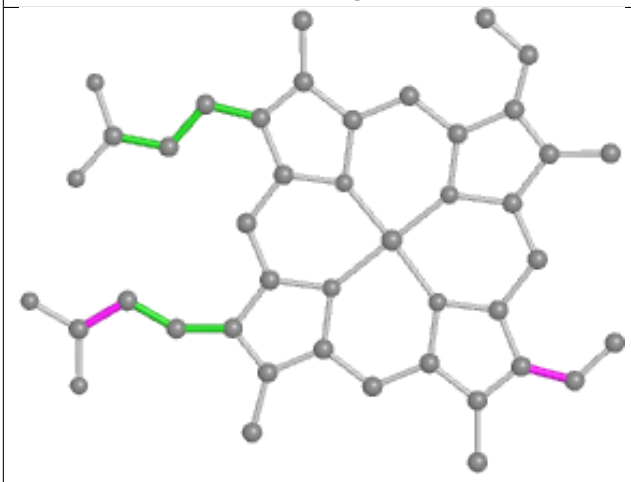
Ligand HEM S 1000



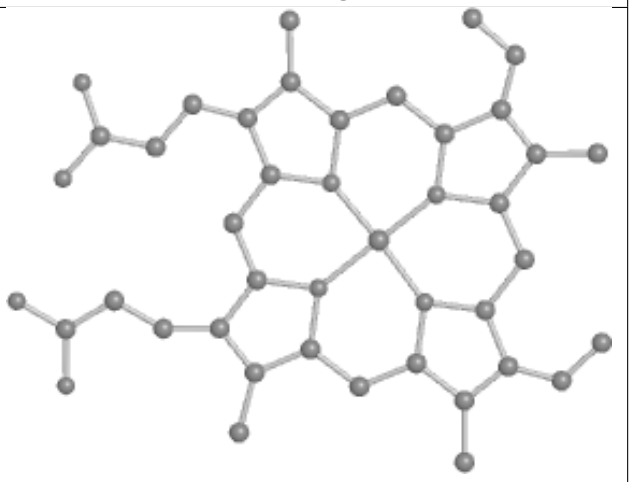
Bond lengths



Bond angles

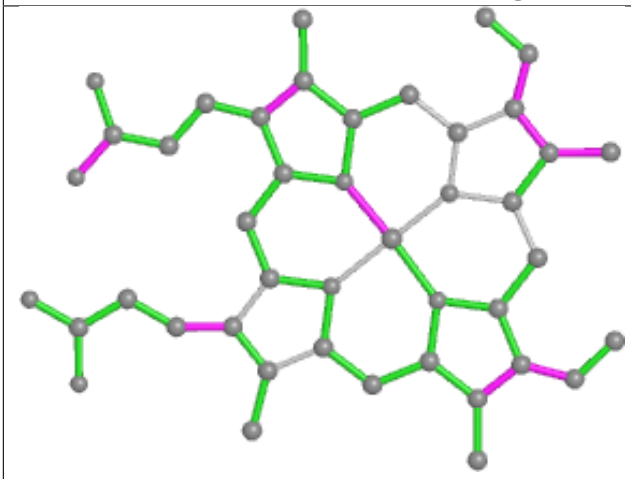


Torsions

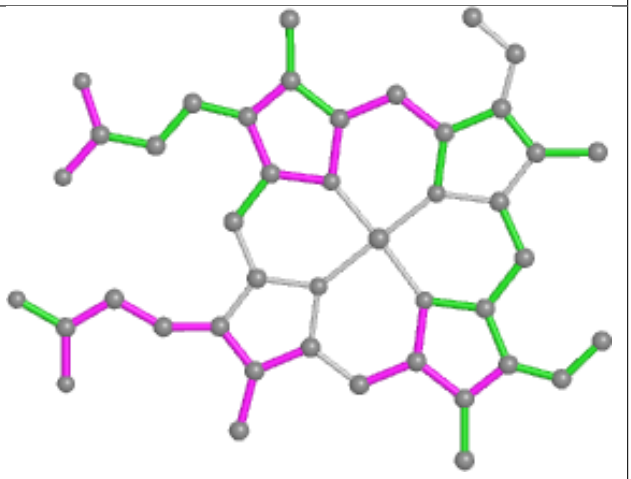


Rings

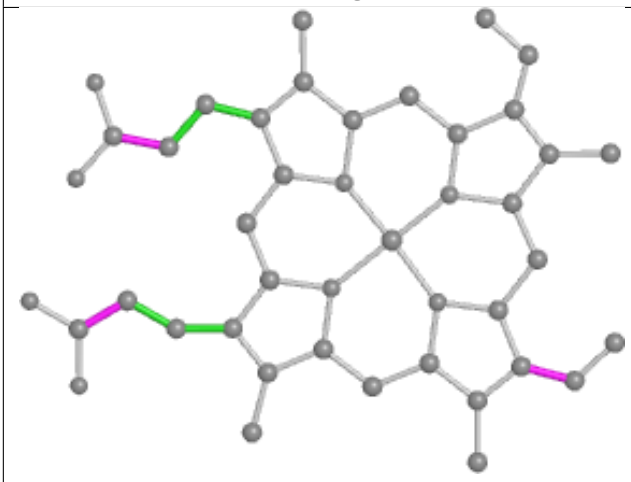
Ligand HEM O 1000



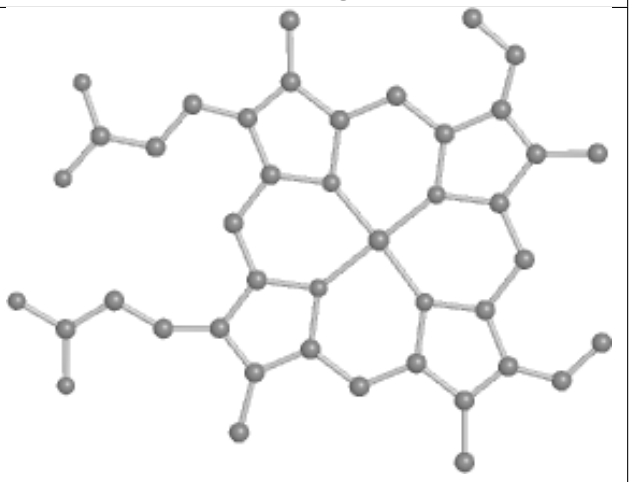
Bond lengths



Bond angles

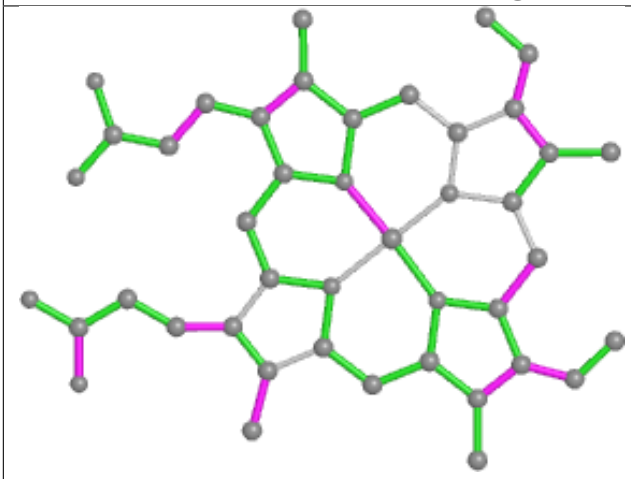


Torsions

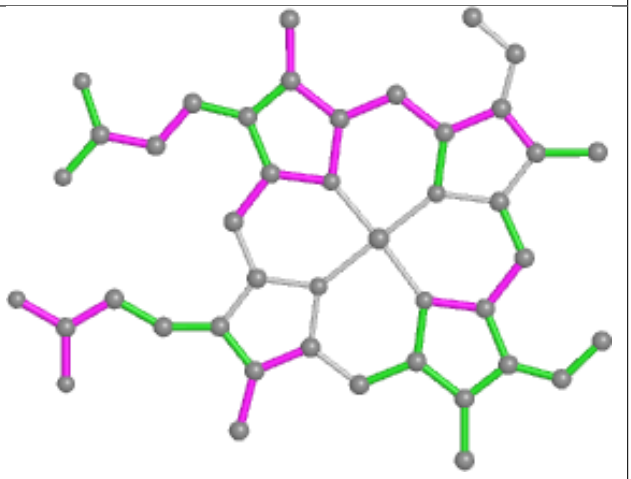


Rings

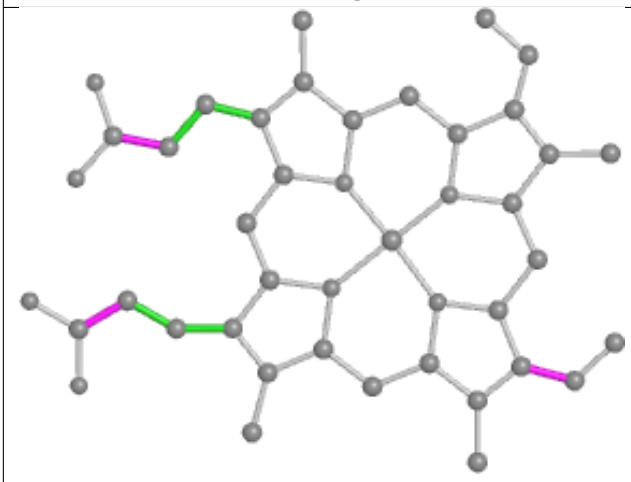
Ligand HEM D 1000



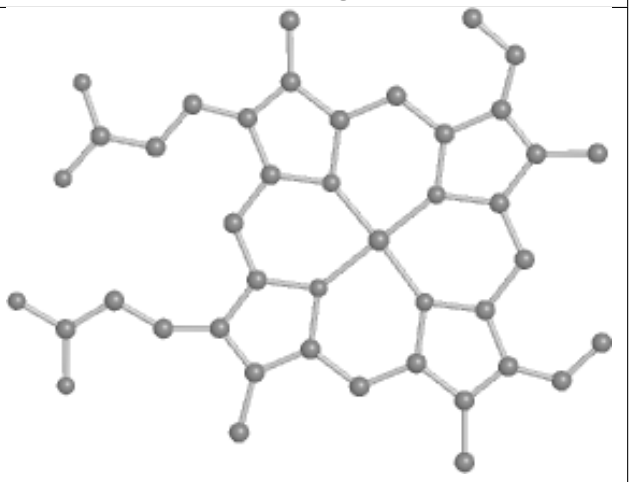
Bond lengths



Bond angles

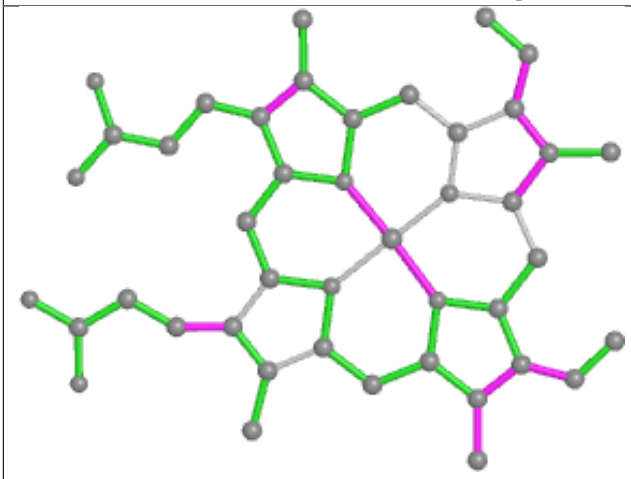


Torsions

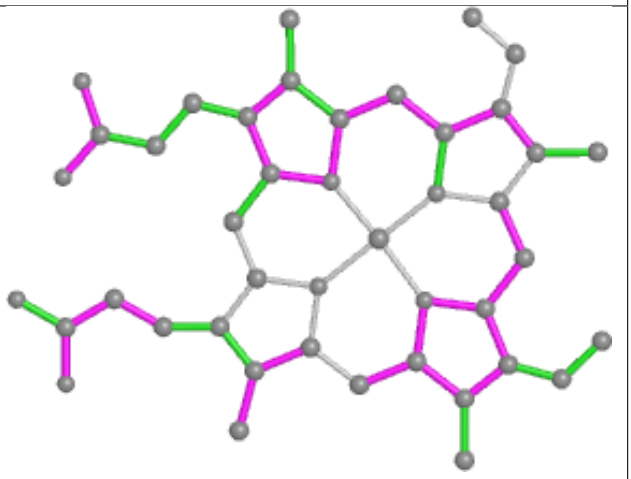


Rings

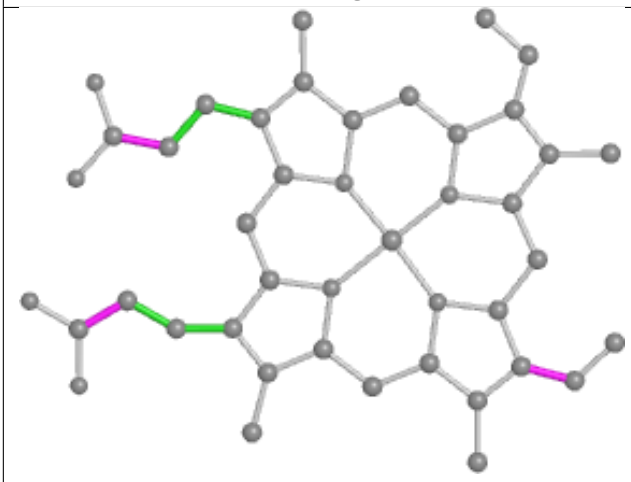
Ligand HEM T 1000



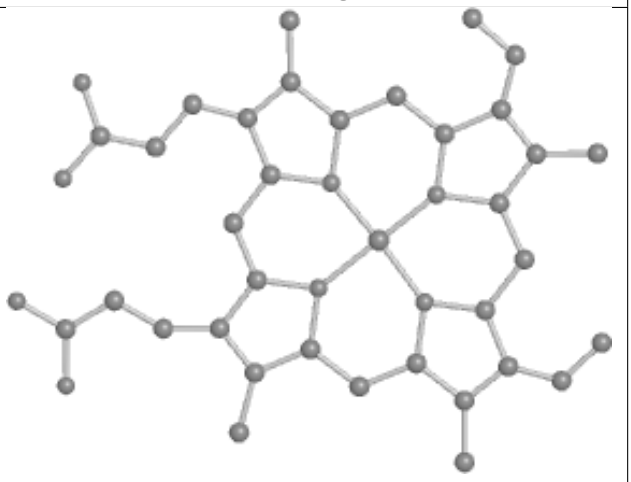
Bond lengths



Bond angles

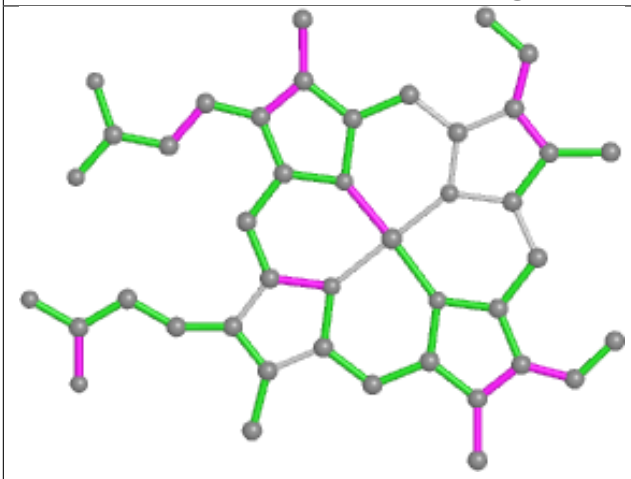


Torsions

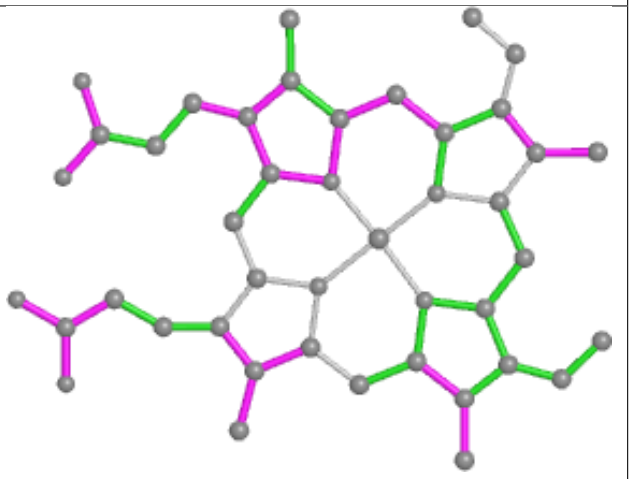


Rings

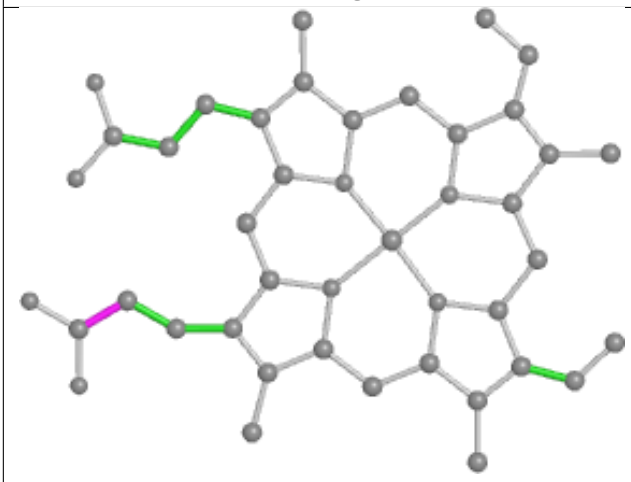
Ligand HEM K 1000



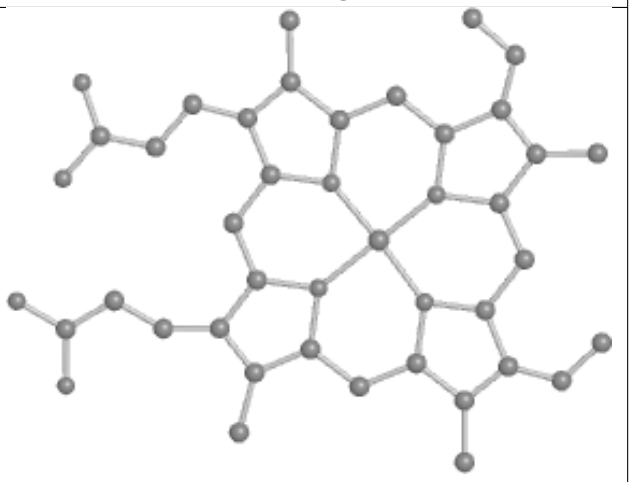
Bond lengths



Bond angles

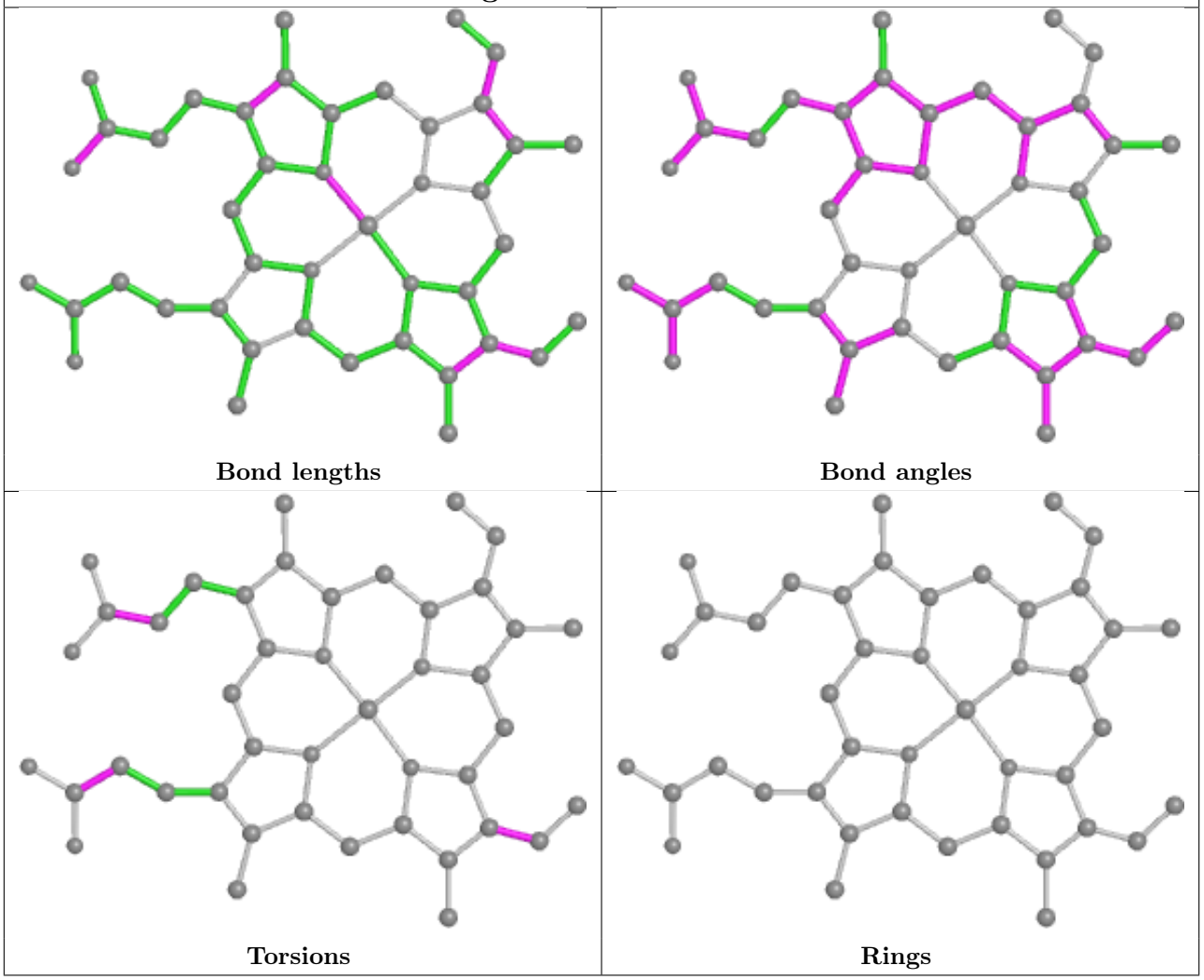


Torsions



Rings

Ligand HEM J 1000



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	241/248 (97%)	-0.78	0 100 100	11, 24, 52, 62	0
1	B	241/248 (97%)	-0.74	1 (0%) 92 79	13, 24, 48, 70	0
1	C	241/248 (97%)	-0.69	2 (0%) 86 65	11, 23, 50, 68	0
1	D	241/248 (97%)	-0.78	0 100 100	14, 27, 54, 77	0
1	E	241/248 (97%)	-0.83	0 100 100	9, 21, 47, 64	0
1	F	241/248 (97%)	-0.52	0 100 100	17, 40, 75, 96	0
1	G	241/248 (97%)	-0.69	0 100 100	18, 34, 61, 90	0
1	H	241/248 (97%)	-0.78	0 100 100	14, 27, 55, 74	0
1	I	241/248 (97%)	-0.70	0 100 100	13, 28, 62, 80	0
1	J	241/248 (97%)	-0.68	0 100 100	15, 32, 69, 88	0
1	K	241/248 (97%)	-0.66	0 100 100	19, 34, 64, 87	0
1	L	241/248 (97%)	-0.63	0 100 100	17, 31, 60, 81	0
1	M	241/248 (97%)	-0.68	0 100 100	16, 29, 56, 79	0
1	N	241/248 (97%)	-0.60	0 100 100	19, 36, 71, 82	0
1	O	241/248 (97%)	-0.54	0 100 100	22, 41, 71, 96	0
1	P	241/248 (97%)	-0.32	0 100 100	38, 62, 108, 134	0
1	Q	241/248 (97%)	-0.50	1 (0%) 92 79	23, 52, 99, 120	0
1	R	241/248 (97%)	-0.31	0 100 100	27, 56, 101, 124	0
1	S	241/248 (97%)	-0.14	3 (1%) 79 54	39, 68, 110, 129	0
1	T	241/248 (97%)	-0.25	0 100 100	32, 63, 111, 135	0
All	All	4820/4960 (97%)	-0.59	7 (0%) 95 89	9, 36, 86, 135	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	SER	3.6
1	S	132	SER	2.5
1	Q	132	SER	2.3
1	S	57	ASP	2.2
1	C	38	VAL	2.1
1	S	59	VAL	2.1
1	C	248	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	S	1001	1/1	0.84	0.14	60,60,60,60	0
4	CA	G	1001	1/1	0.92	0.14	24,24,24,24	0
4	CA	I	1001	1/1	0.94	0.11	23,23,23,23	0
4	CA	K	1001	1/1	0.94	0.18	26,26,26,26	0
4	CA	R	1001	1/1	0.94	0.14	50,50,50,50	0
2	HEM	S	1000	43/43	0.94	0.20	45,55,64,71	0
4	CA	T	1001	1/1	0.94	0.16	52,52,52,52	0
4	CA	L	1001	1/1	0.95	0.15	25,25,25,25	0
3	NO2	B	2000	3/3	0.95	0.23	32,32,36,43	0
4	CA	C	1001	1/1	0.96	0.14	20,20,20,20	0
2	HEM	G	1000	43/43	0.96	0.20	21,26,36,39	0
2	HEM	Q	1000	43/43	0.96	0.18	29,31,39,45	0
2	HEM	R	1000	43/43	0.96	0.19	30,36,43,53	0
2	HEM	B	1000	43/43	0.96	0.19	15,18,27,33	0
4	CA	N	1001	1/1	0.96	0.14	32,32,32,32	0
4	CA	O	1001	1/1	0.96	0.16	29,29,29,29	0
4	CA	Q	1001	1/1	0.96	0.12	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	T	1000	43/43	0.96	0.20	39,46,52,59	0
2	HEM	F	1000	43/43	0.96	0.20	24,33,42,47	0
3	NO2	M	2000	3/3	0.96	0.18	31,31,34,41	0
2	HEM	J	1000	43/43	0.97	0.17	15,20,28,35	0
3	NO2	N	2000	3/3	0.97	0.20	41,41,45,47	0
3	NO2	P	2000	3/3	0.97	0.16	55,55,55,55	0
3	NO2	R	2000	3/3	0.97	0.33	48,48,50,52	0
3	NO2	S	2000	3/3	0.97	0.18	63,63,64,65	0
4	CA	A	1001	1/1	0.97	0.12	21,21,21,21	0
2	HEM	K	1000	43/43	0.97	0.17	21,25,34,37	0
4	CA	D	1001	1/1	0.97	0.12	24,24,24,24	0
2	HEM	L	1000	43/43	0.97	0.17	18,22,30,35	0
4	CA	H	1001	1/1	0.97	0.13	22,22,22,22	0
2	HEM	M	1000	43/43	0.97	0.18	17,22,29,34	0
2	HEM	N	1000	43/43	0.97	0.17	22,31,40,48	0
2	HEM	O	1000	43/43	0.97	0.17	27,34,42,46	0
4	CA	M	1001	1/1	0.97	0.16	26,26,26,26	0
2	HEM	P	1000	43/43	0.97	0.17	41,45,52,55	0
2	HEM	E	1000	43/43	0.97	0.16	11,16,23,30	0
4	CA	P	1001	1/1	0.97	0.12	54,54,54,54	0
2	HEM	C	1000	43/43	0.97	0.16	13,17,24,31	0
2	HEM	D	1000	43/43	0.97	0.17	15,22,31,35	0
2	HEM	H	1000	43/43	0.97	0.17	12,19,29,33	0
2	HEM	I	1000	43/43	0.97	0.18	13,19,27,32	0
4	CA	B	1001	1/1	0.98	0.12	17,17,17,17	0
3	NO2	C	2000	3/3	0.98	0.18	25,25,28,31	0
3	NO2	F	2000	3/3	0.98	0.17	40,40,42,44	0
4	CA	E	1001	1/1	0.98	0.12	13,13,13,13	0
3	NO2	Q	2000	3/3	0.98	0.16	45,45,45,49	0
3	NO2	I	2000	3/3	0.98	0.20	27,27,29,32	0
3	NO2	K	2000	3/3	0.98	0.17	34,34,36,39	0
4	CA	J	1001	1/1	0.98	0.17	29,29,29,29	0
2	HEM	A	1000	43/43	0.98	0.17	13,19,28,36	0
3	NO2	O	2000	3/3	0.99	0.15	40,40,42,43	0
3	NO2	D	2000	3/3	0.99	0.16	30,30,32,34	0
3	NO2	J	2000	3/3	0.99	0.16	29,29,30,31	0
4	CA	F	1001	1/1	0.99	0.10	30,30,30,30	0
3	NO2	A	2000	3/3	0.99	0.22	29,29,31,34	0
3	NO2	L	2000	3/3	0.99	0.13	31,31,32,35	0
3	NO2	T	2000	3/3	0.99	0.17	57,57,57,58	0
3	NO2	G	2000	3/3	0.99	0.17	36,36,37,39	0
3	NO2	H	2000	3/3	0.99	0.17	28,28,30,33	0

Continued on next page...

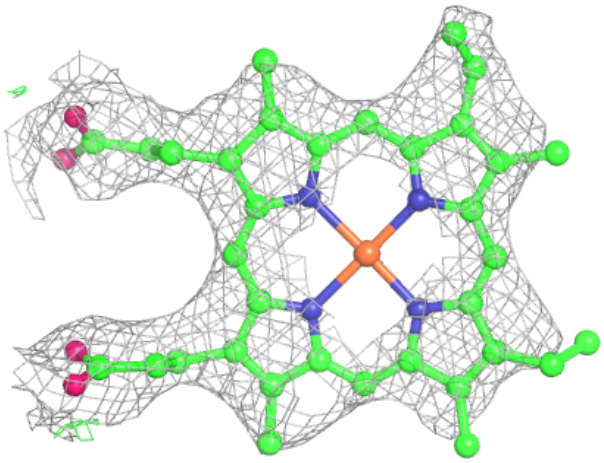
Continued from previous page...

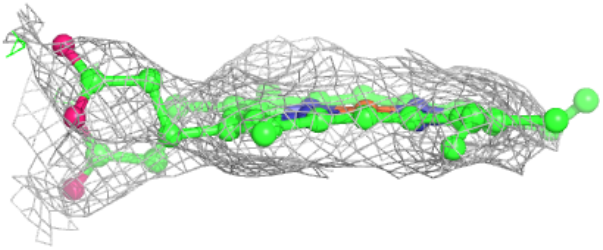
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NO2	E	2000	3/3	1.00	0.10	22,22,24,28	0

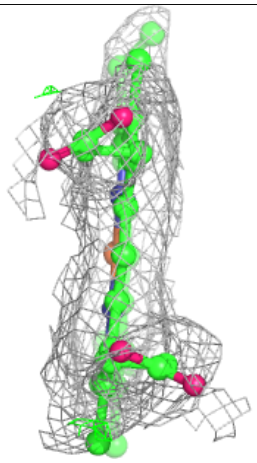
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM S 1000:

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

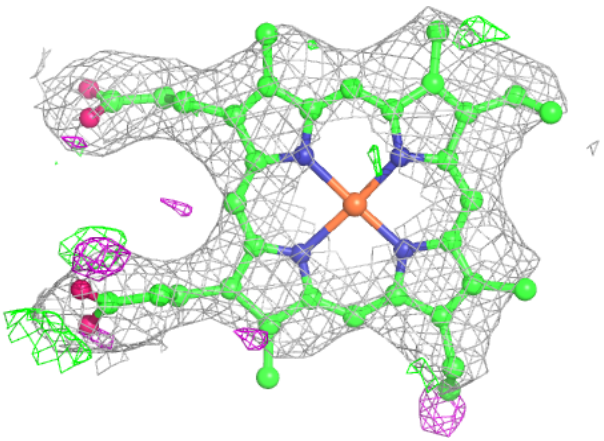


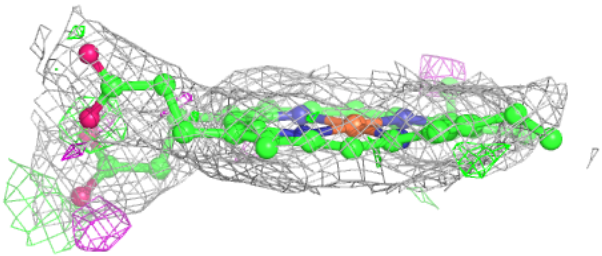


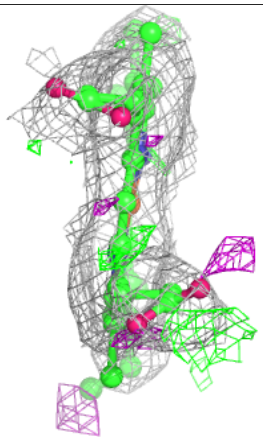


Electron density around HEM G 1000:

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

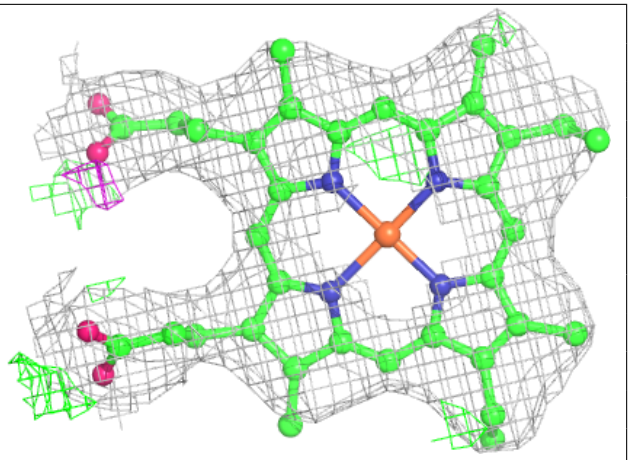


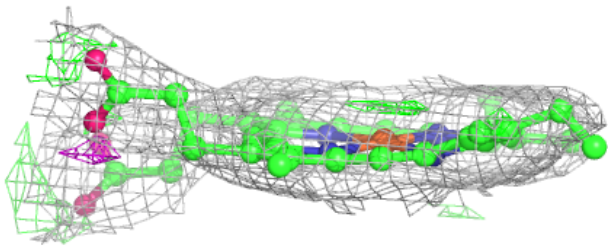


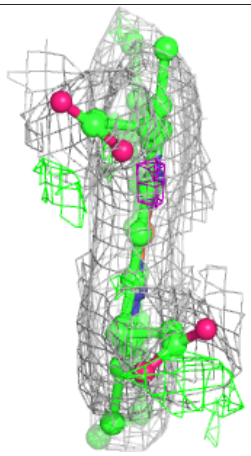


Electron density around HEM Q 1000:

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

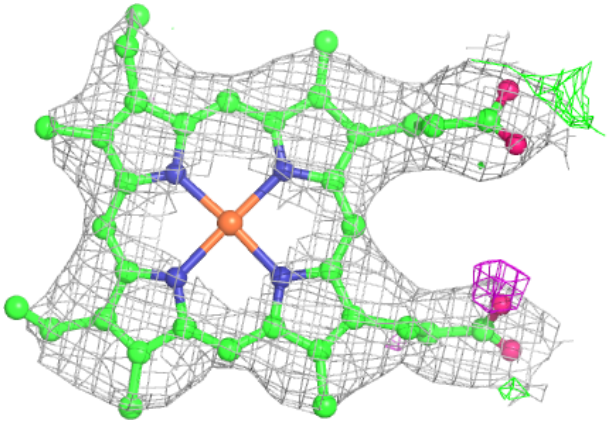


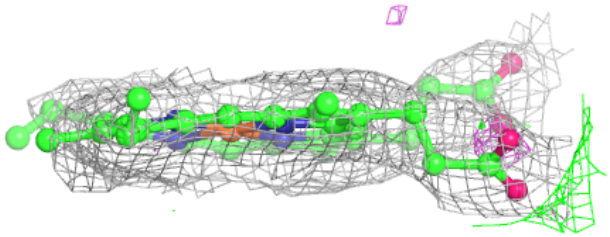


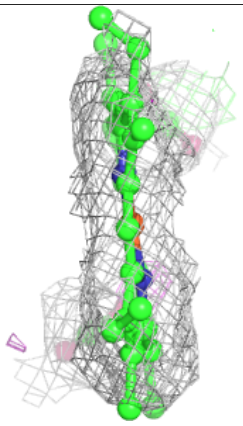


Electron density around HEM R 1000:

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

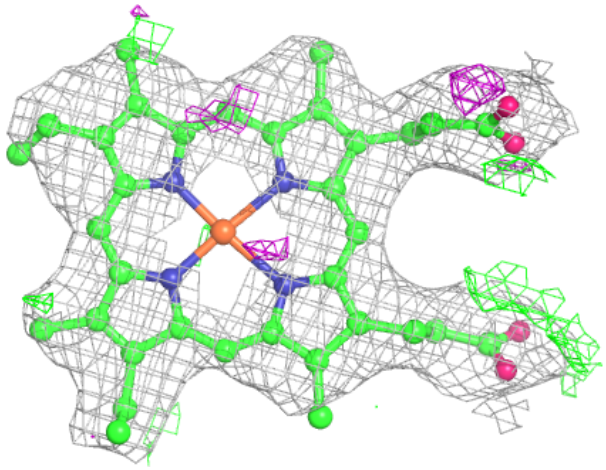


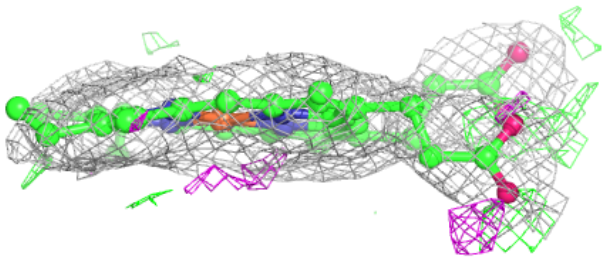


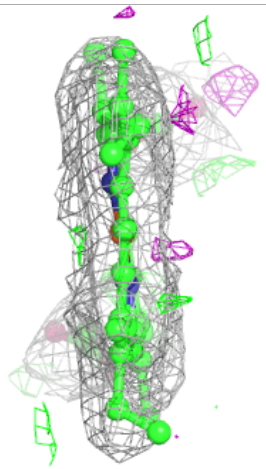


Electron density around HEM B 1000:

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

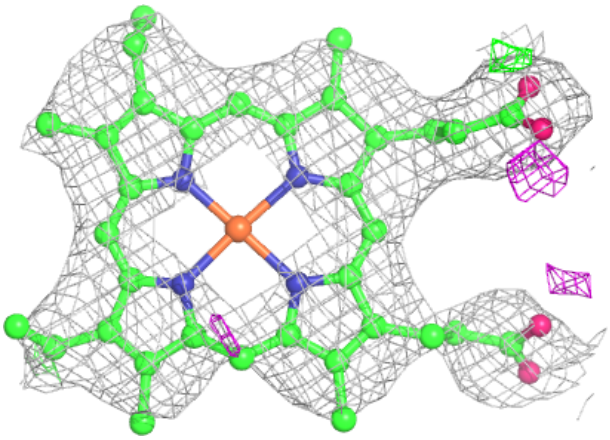


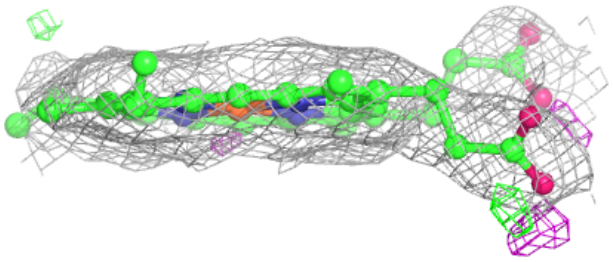


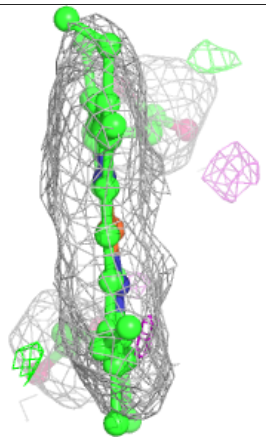


Electron density around HEM T 1000:

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

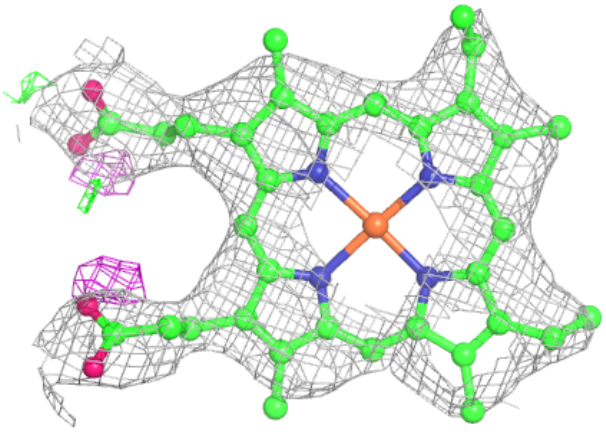


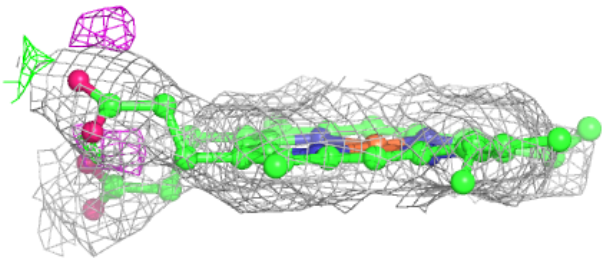


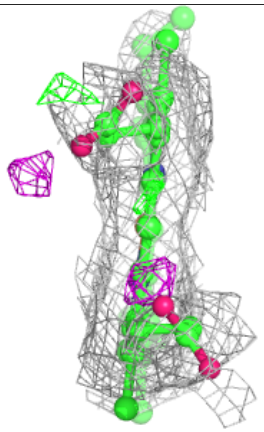


Electron density around HEM F 1000:

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

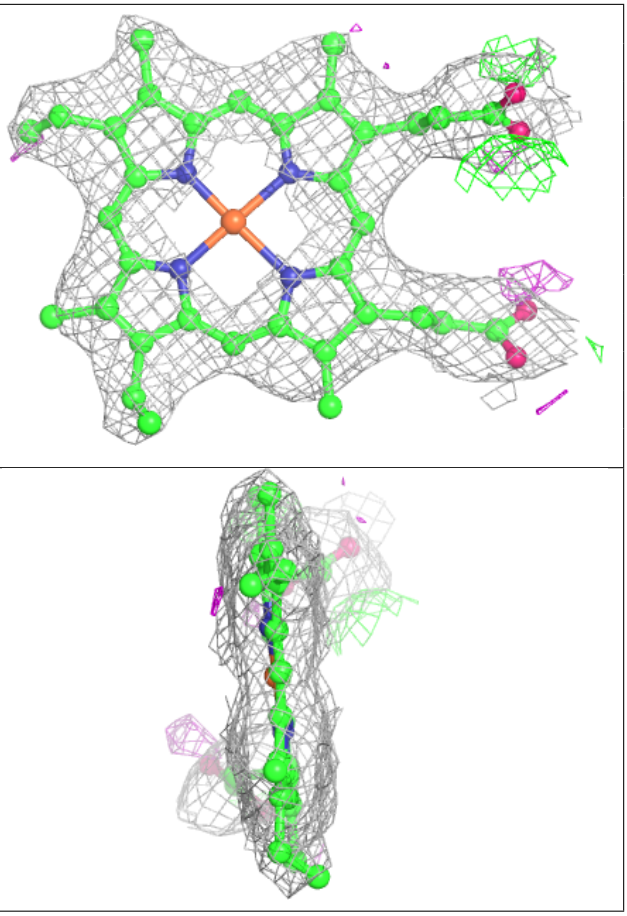


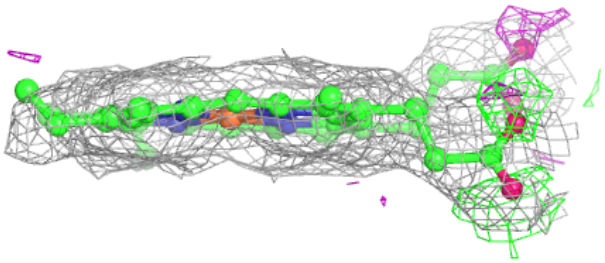




Electron density around HEM J 1000:

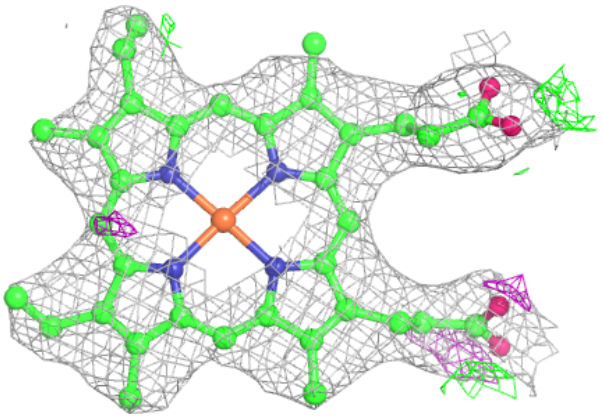
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

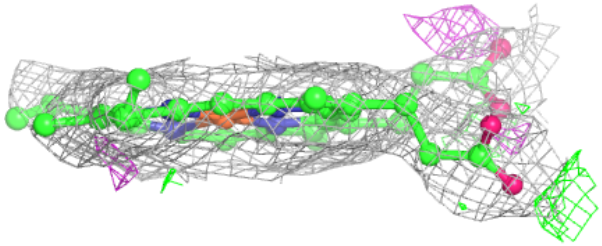


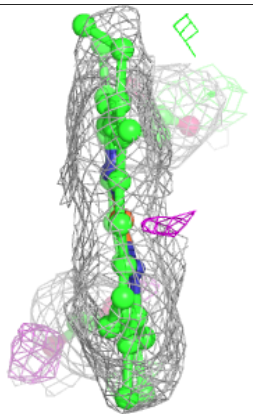


Electron density around HEM K 1000:

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

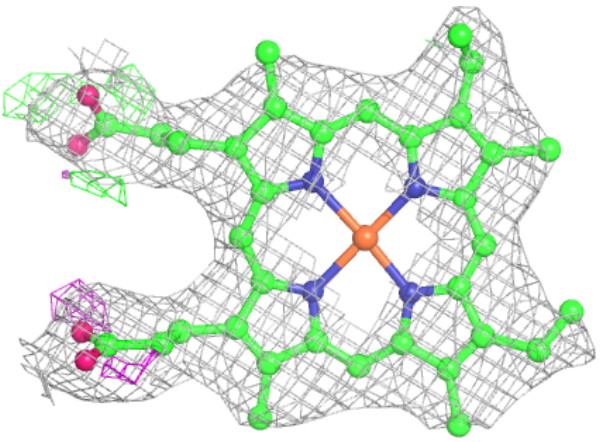


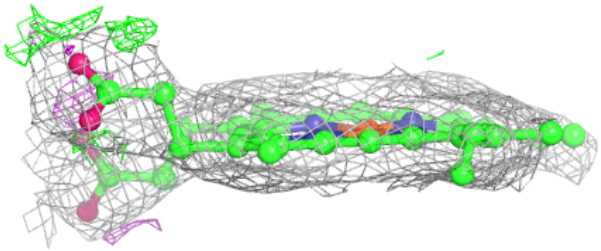


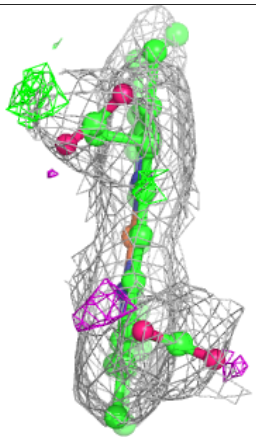


Electron density around HEM L 1000:

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

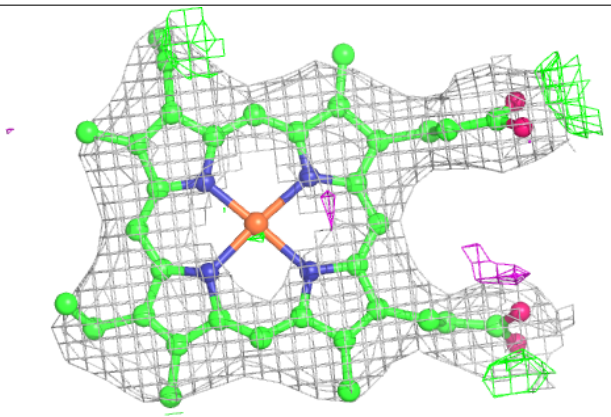


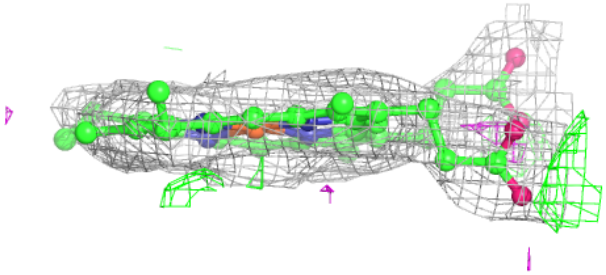


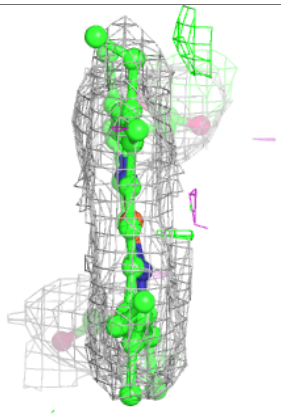


Electron density around HEM M 1000:

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

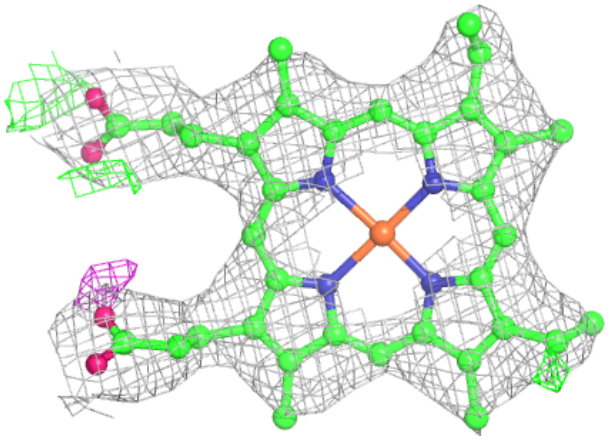


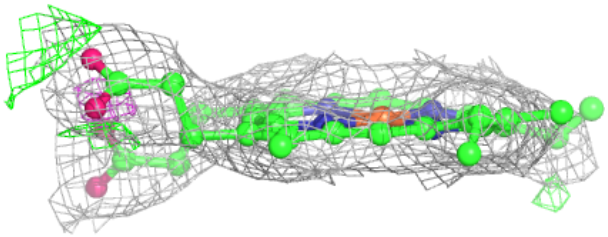


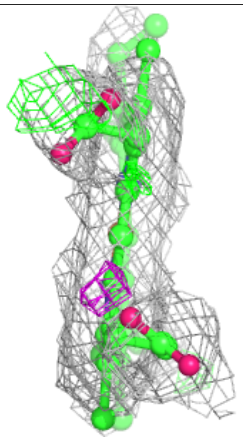


Electron density around HEM N 1000:

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

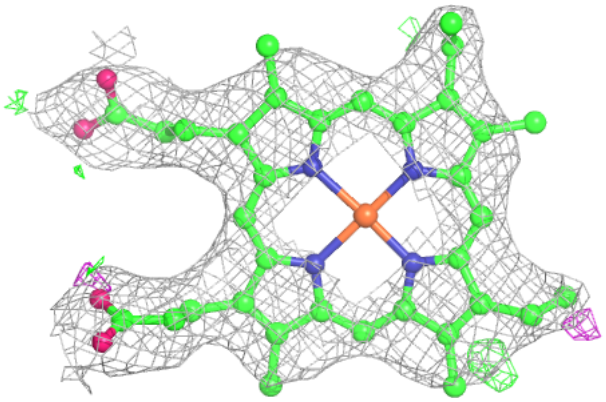


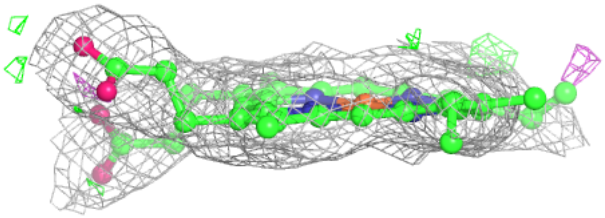


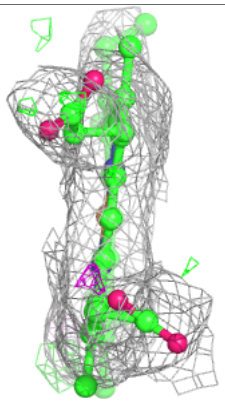


Electron density around HEM O 1000:

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

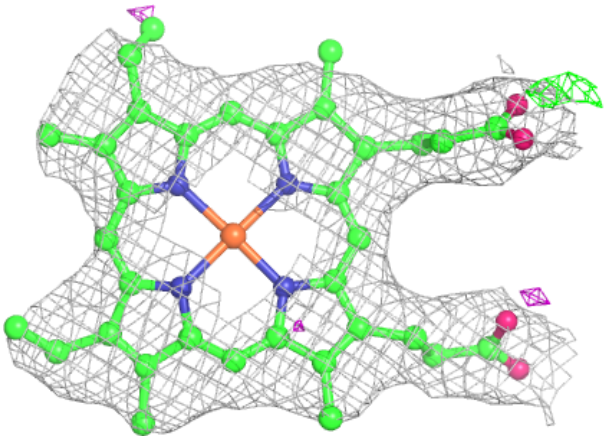


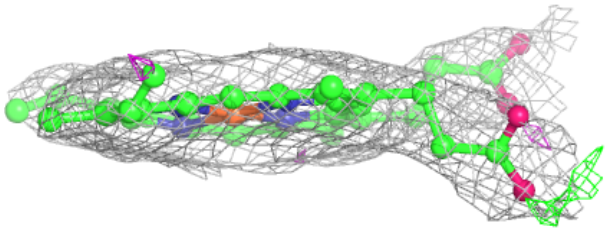


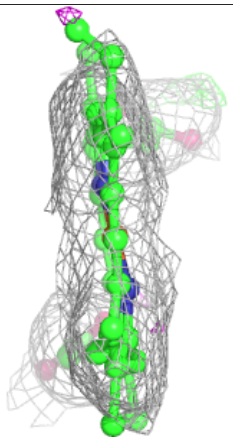


Electron density around HEM P 1000:

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

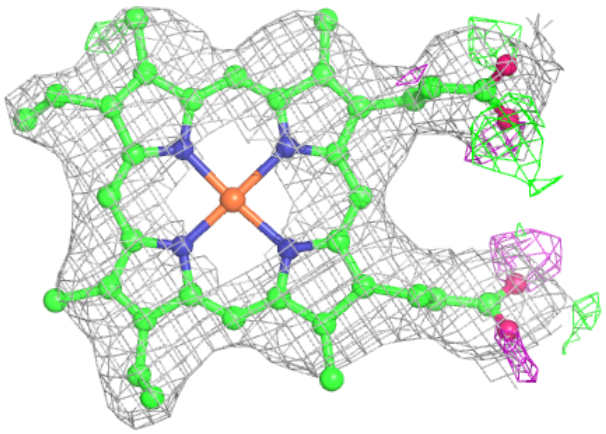


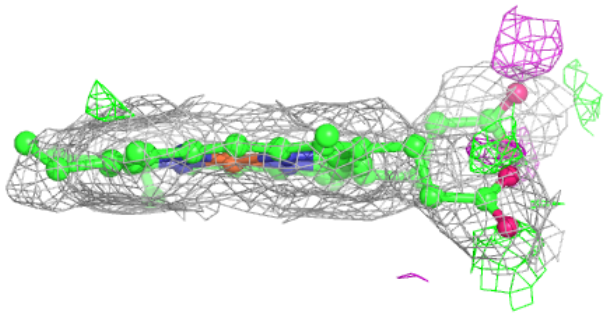


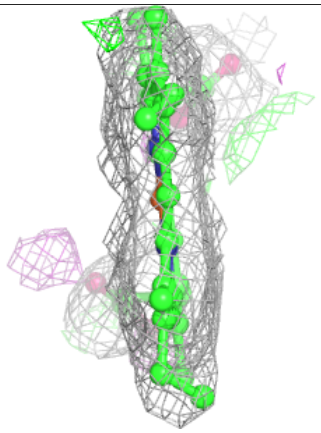


Electron density around HEM E 1000:

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

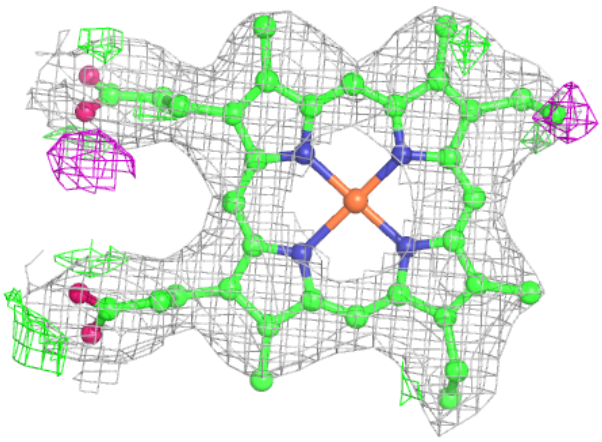


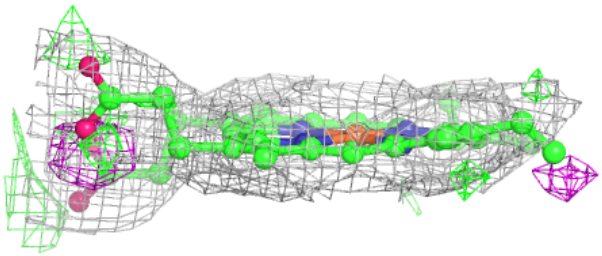


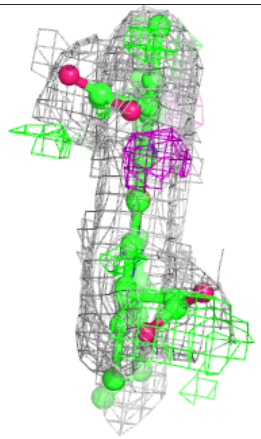


Electron density around HEM C 1000:

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

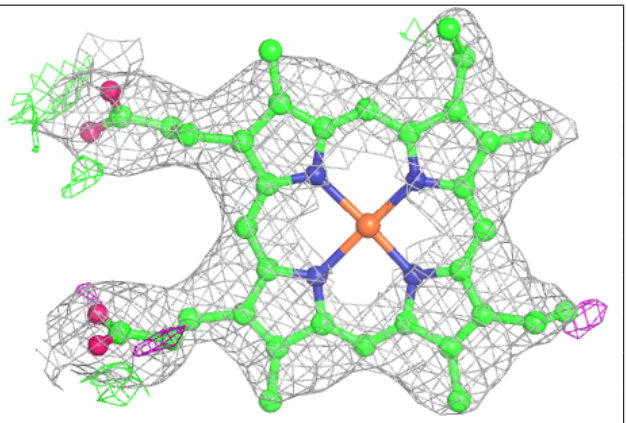


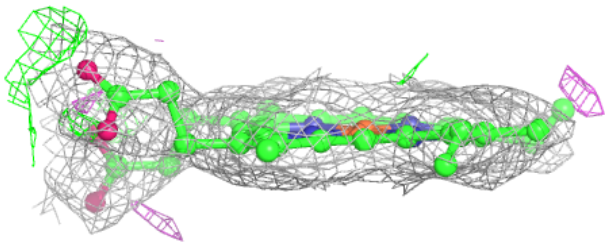


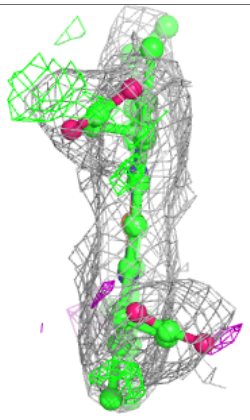


Electron density around HEM D 1000:

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

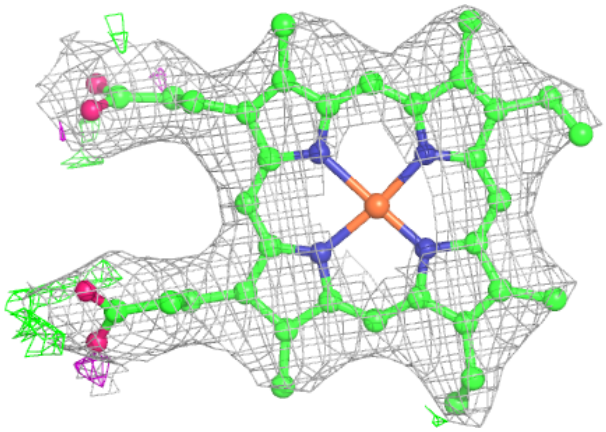


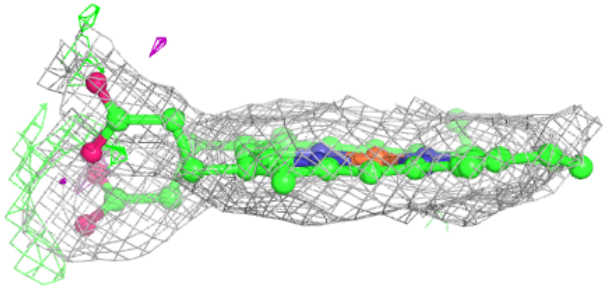


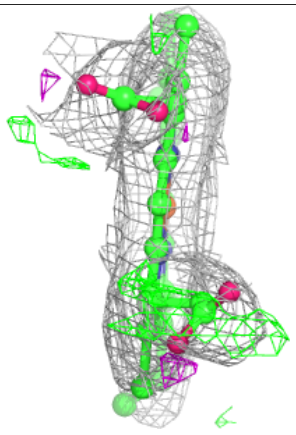


Electron density around HEM H 1000:

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

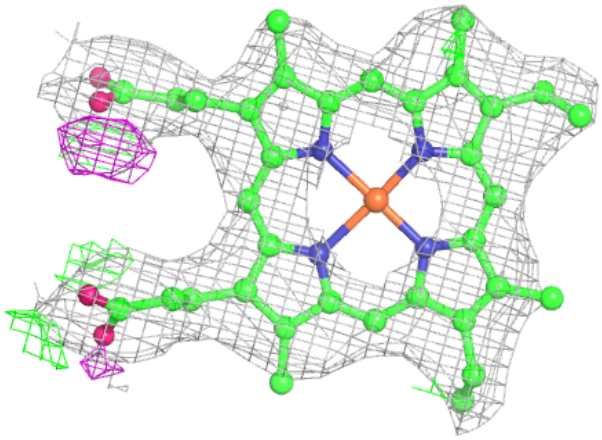


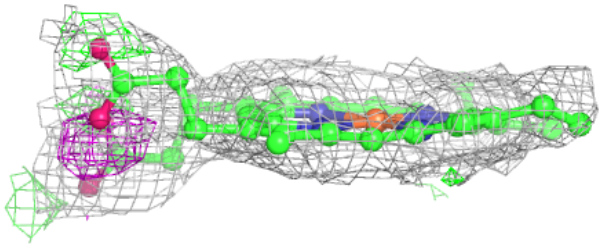


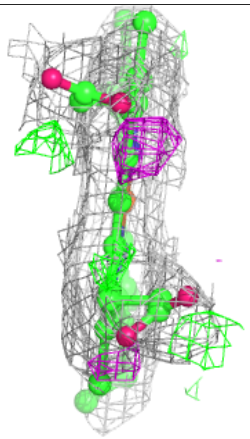


Electron density around HEM I 1000:

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

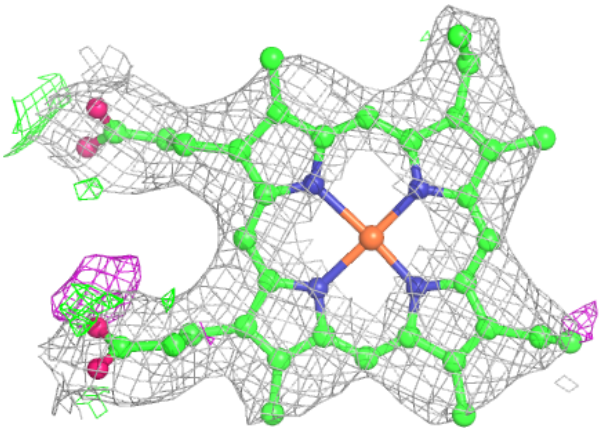


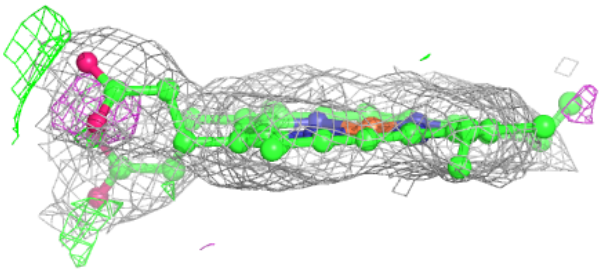


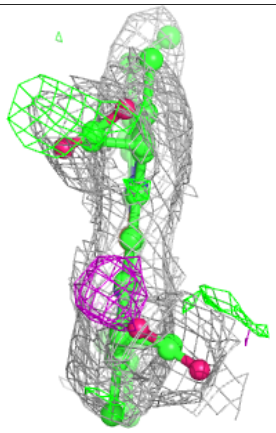


Electron density around HEM A 1000:

$2mF_o$-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.