Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 06:06 pm GMT

PDB ID	:	4BF4
Title	:	PikC D50N mutant in complex with the engineered cycloalkane substrate mimic bearing a termianl N,N-dimethylamino group
Authors	:	Podust, L.M.
Deposited on	:	2013-03-14
Resolution	:	2.70 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:

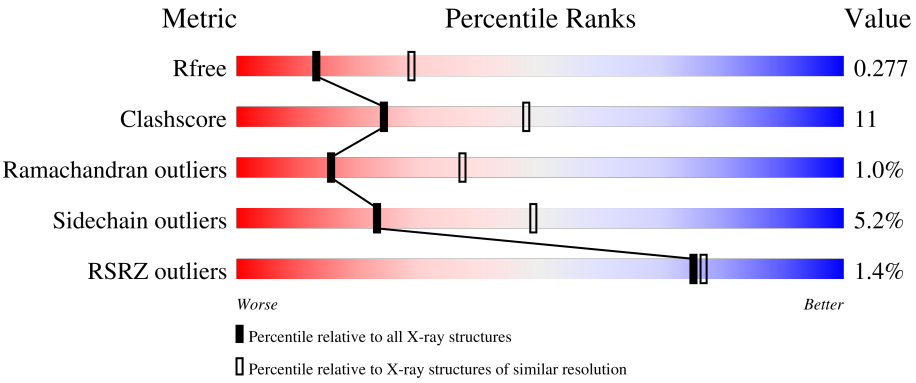
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	436	68% 22% • 9%
1	B	436	67% 22% • 9%
1	C	436	71% 18% • 9%
1	D	436	66% 23% • 9%
1	E	436	% 69% 19% • 9%

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Mol	Chain	Length	Quality of chain
1	F	436	71% 18% • 9%
1	G	436	70% 19% • 9%
1	H	436	% 70% 19% • 9%
1	I	436	71% 18% • 9%
1	J	436	72% 18% • 9%
1	K	436	68% 22% • 9%
1	L	436	69% 21% • 9%
1	M	436	% 66% 22% • 9%
1	N	436	4% 70% 19% • 9%
1	O	436	4% 66% 24% • 9%
1	P	436	7% 66% 24% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1408	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 50342 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 CYTOCHROME P450 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3031	1912	545	561	13			
1	B	397	Total	C	N	O	S	0	2	0
			3069	1939	553	564	13			
1	C	396	Total	C	N	O	S	0	1	0
			3063	1937	549	564	13			
1	D	397	Total	C	N	O	S	0	2	0
			3076	1942	552	569	13			
1	E	397	Total	C	N	O	S	0	1	0
			3068	1938	550	567	13			
1	F	396	Total	C	N	O	S	0	4	0
			3075	1944	552	566	13			
1	G	396	Total	C	N	O	S	0	4	0
			3093	1952	557	571	13			
1	H	396	Total	C	N	O	S	0	1	0
			3057	1935	549	560	13			
1	I	396	Total	C	N	O	S	0	2	0
			3066	1939	550	564	13			
1	J	397	Total	C	N	O	S	0	1	0
			3060	1934	551	562	13			
1	K	397	Total	C	N	O	S	0	2	0
			3076	1944	551	568	13			
1	L	397	Total	C	N	O	S	0	2	0
			3065	1938	551	563	13			
1	M	397	Total	C	N	O	S	0	1	0
			3065	1936	551	565	13			
1	N	397	Total	C	N	O	S	0	1	0
			3064	1938	550	563	13			
1	O	397	Total	C	N	O	S	0	0	0
			3052	1931	548	560	13			
1	P	396	Total	C	N	O	S	0	1	0
			3058	1932	548	565	13			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O87605
A	-18	GLY	-	expression tag	UNP O87605
A	-17	SER	-	expression tag	UNP O87605
A	-16	SER	-	expression tag	UNP O87605
A	-15	HIS	-	expression tag	UNP O87605
A	-14	HIS	-	expression tag	UNP O87605
A	-13	HIS	-	expression tag	UNP O87605
A	-12	HIS	-	expression tag	UNP O87605
A	-11	HIS	-	expression tag	UNP O87605
A	-10	HIS	-	expression tag	UNP O87605
A	-9	SER	-	expression tag	UNP O87605
A	-8	SER	-	expression tag	UNP O87605
A	-7	GLY	-	expression tag	UNP O87605
A	-6	LEU	-	expression tag	UNP O87605
A	-5	VAL	-	expression tag	UNP O87605
A	-4	PRO	-	expression tag	UNP O87605
A	-3	ARG	-	expression tag	UNP O87605
A	-2	GLY	-	expression tag	UNP O87605
A	-1	SER	-	expression tag	UNP O87605
A	0	HIS	-	expression tag	UNP O87605
A	50	ASN	ASP	engineered mutation	UNP O87605
B	-19	MET	-	expression tag	UNP O87605
B	-18	GLY	-	expression tag	UNP O87605
B	-17	SER	-	expression tag	UNP O87605
B	-16	SER	-	expression tag	UNP O87605
B	-15	HIS	-	expression tag	UNP O87605
B	-14	HIS	-	expression tag	UNP O87605
B	-13	HIS	-	expression tag	UNP O87605
B	-12	HIS	-	expression tag	UNP O87605
B	-11	HIS	-	expression tag	UNP O87605
B	-10	HIS	-	expression tag	UNP O87605
B	-9	SER	-	expression tag	UNP O87605
B	-8	SER	-	expression tag	UNP O87605
B	-7	GLY	-	expression tag	UNP O87605
B	-6	LEU	-	expression tag	UNP O87605
B	-5	VAL	-	expression tag	UNP O87605
B	-4	PRO	-	expression tag	UNP O87605
B	-3	ARG	-	expression tag	UNP O87605
B	-2	GLY	-	expression tag	UNP O87605
B	-1	SER	-	expression tag	UNP O87605
B	0	HIS	-	expression tag	UNP O87605
B	50	ASN	ASP	engineered mutation	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP O87605
C	-18	GLY	-	expression tag	UNP O87605
C	-17	SER	-	expression tag	UNP O87605
C	-16	SER	-	expression tag	UNP O87605
C	-15	HIS	-	expression tag	UNP O87605
C	-14	HIS	-	expression tag	UNP O87605
C	-13	HIS	-	expression tag	UNP O87605
C	-12	HIS	-	expression tag	UNP O87605
C	-11	HIS	-	expression tag	UNP O87605
C	-10	HIS	-	expression tag	UNP O87605
C	-9	SER	-	expression tag	UNP O87605
C	-8	SER	-	expression tag	UNP O87605
C	-7	GLY	-	expression tag	UNP O87605
C	-6	LEU	-	expression tag	UNP O87605
C	-5	VAL	-	expression tag	UNP O87605
C	-4	PRO	-	expression tag	UNP O87605
C	-3	ARG	-	expression tag	UNP O87605
C	-2	GLY	-	expression tag	UNP O87605
C	-1	SER	-	expression tag	UNP O87605
C	0	HIS	-	expression tag	UNP O87605
C	50	ASN	ASP	engineered mutation	UNP O87605
D	-19	MET	-	expression tag	UNP O87605
D	-18	GLY	-	expression tag	UNP O87605
D	-17	SER	-	expression tag	UNP O87605
D	-16	SER	-	expression tag	UNP O87605
D	-15	HIS	-	expression tag	UNP O87605
D	-14	HIS	-	expression tag	UNP O87605
D	-13	HIS	-	expression tag	UNP O87605
D	-12	HIS	-	expression tag	UNP O87605
D	-11	HIS	-	expression tag	UNP O87605
D	-10	HIS	-	expression tag	UNP O87605
D	-9	SER	-	expression tag	UNP O87605
D	-8	SER	-	expression tag	UNP O87605
D	-7	GLY	-	expression tag	UNP O87605
D	-6	LEU	-	expression tag	UNP O87605
D	-5	VAL	-	expression tag	UNP O87605
D	-4	PRO	-	expression tag	UNP O87605
D	-3	ARG	-	expression tag	UNP O87605
D	-2	GLY	-	expression tag	UNP O87605
D	-1	SER	-	expression tag	UNP O87605
D	0	HIS	-	expression tag	UNP O87605
D	50	ASN	ASP	engineered mutation	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	expression tag	UNP O87605
E	-18	GLY	-	expression tag	UNP O87605
E	-17	SER	-	expression tag	UNP O87605
E	-16	SER	-	expression tag	UNP O87605
E	-15	HIS	-	expression tag	UNP O87605
E	-14	HIS	-	expression tag	UNP O87605
E	-13	HIS	-	expression tag	UNP O87605
E	-12	HIS	-	expression tag	UNP O87605
E	-11	HIS	-	expression tag	UNP O87605
E	-10	HIS	-	expression tag	UNP O87605
E	-9	SER	-	expression tag	UNP O87605
E	-8	SER	-	expression tag	UNP O87605
E	-7	GLY	-	expression tag	UNP O87605
E	-6	LEU	-	expression tag	UNP O87605
E	-5	VAL	-	expression tag	UNP O87605
E	-4	PRO	-	expression tag	UNP O87605
E	-3	ARG	-	expression tag	UNP O87605
E	-2	GLY	-	expression tag	UNP O87605
E	-1	SER	-	expression tag	UNP O87605
E	0	HIS	-	expression tag	UNP O87605
E	50	ASN	ASP	engineered mutation	UNP O87605
F	-19	MET	-	expression tag	UNP O87605
F	-18	GLY	-	expression tag	UNP O87605
F	-17	SER	-	expression tag	UNP O87605
F	-16	SER	-	expression tag	UNP O87605
F	-15	HIS	-	expression tag	UNP O87605
F	-14	HIS	-	expression tag	UNP O87605
F	-13	HIS	-	expression tag	UNP O87605
F	-12	HIS	-	expression tag	UNP O87605
F	-11	HIS	-	expression tag	UNP O87605
F	-10	HIS	-	expression tag	UNP O87605
F	-9	SER	-	expression tag	UNP O87605
F	-8	SER	-	expression tag	UNP O87605
F	-7	GLY	-	expression tag	UNP O87605
F	-6	LEU	-	expression tag	UNP O87605
F	-5	VAL	-	expression tag	UNP O87605
F	-4	PRO	-	expression tag	UNP O87605
F	-3	ARG	-	expression tag	UNP O87605
F	-2	GLY	-	expression tag	UNP O87605
F	-1	SER	-	expression tag	UNP O87605
F	0	HIS	-	expression tag	UNP O87605
F	50	ASN	ASP	engineered mutation	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	expression tag	UNP O87605
G	-18	GLY	-	expression tag	UNP O87605
G	-17	SER	-	expression tag	UNP O87605
G	-16	SER	-	expression tag	UNP O87605
G	-15	HIS	-	expression tag	UNP O87605
G	-14	HIS	-	expression tag	UNP O87605
G	-13	HIS	-	expression tag	UNP O87605
G	-12	HIS	-	expression tag	UNP O87605
G	-11	HIS	-	expression tag	UNP O87605
G	-10	HIS	-	expression tag	UNP O87605
G	-9	SER	-	expression tag	UNP O87605
G	-8	SER	-	expression tag	UNP O87605
G	-7	GLY	-	expression tag	UNP O87605
G	-6	LEU	-	expression tag	UNP O87605
G	-5	VAL	-	expression tag	UNP O87605
G	-4	PRO	-	expression tag	UNP O87605
G	-3	ARG	-	expression tag	UNP O87605
G	-2	GLY	-	expression tag	UNP O87605
G	-1	SER	-	expression tag	UNP O87605
G	0	HIS	-	expression tag	UNP O87605
G	50	ASN	ASP	engineered mutation	UNP O87605
H	-19	MET	-	expression tag	UNP O87605
H	-18	GLY	-	expression tag	UNP O87605
H	-17	SER	-	expression tag	UNP O87605
H	-16	SER	-	expression tag	UNP O87605
H	-15	HIS	-	expression tag	UNP O87605
H	-14	HIS	-	expression tag	UNP O87605
H	-13	HIS	-	expression tag	UNP O87605
H	-12	HIS	-	expression tag	UNP O87605
H	-11	HIS	-	expression tag	UNP O87605
H	-10	HIS	-	expression tag	UNP O87605
H	-9	SER	-	expression tag	UNP O87605
H	-8	SER	-	expression tag	UNP O87605
H	-7	GLY	-	expression tag	UNP O87605
H	-6	LEU	-	expression tag	UNP O87605
H	-5	VAL	-	expression tag	UNP O87605
H	-4	PRO	-	expression tag	UNP O87605
H	-3	ARG	-	expression tag	UNP O87605
H	-2	GLY	-	expression tag	UNP O87605
H	-1	SER	-	expression tag	UNP O87605
H	0	HIS	-	expression tag	UNP O87605
H	50	ASN	ASP	engineered mutation	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-19	MET	-	expression tag	UNP O87605
I	-18	GLY	-	expression tag	UNP O87605
I	-17	SER	-	expression tag	UNP O87605
I	-16	SER	-	expression tag	UNP O87605
I	-15	HIS	-	expression tag	UNP O87605
I	-14	HIS	-	expression tag	UNP O87605
I	-13	HIS	-	expression tag	UNP O87605
I	-12	HIS	-	expression tag	UNP O87605
I	-11	HIS	-	expression tag	UNP O87605
I	-10	HIS	-	expression tag	UNP O87605
I	-9	SER	-	expression tag	UNP O87605
I	-8	SER	-	expression tag	UNP O87605
I	-7	GLY	-	expression tag	UNP O87605
I	-6	LEU	-	expression tag	UNP O87605
I	-5	VAL	-	expression tag	UNP O87605
I	-4	PRO	-	expression tag	UNP O87605
I	-3	ARG	-	expression tag	UNP O87605
I	-2	GLY	-	expression tag	UNP O87605
I	-1	SER	-	expression tag	UNP O87605
I	0	HIS	-	expression tag	UNP O87605
I	50	ASN	ASP	engineered mutation	UNP O87605
J	-19	MET	-	expression tag	UNP O87605
J	-18	GLY	-	expression tag	UNP O87605
J	-17	SER	-	expression tag	UNP O87605
J	-16	SER	-	expression tag	UNP O87605
J	-15	HIS	-	expression tag	UNP O87605
J	-14	HIS	-	expression tag	UNP O87605
J	-13	HIS	-	expression tag	UNP O87605
J	-12	HIS	-	expression tag	UNP O87605
J	-11	HIS	-	expression tag	UNP O87605
J	-10	HIS	-	expression tag	UNP O87605
J	-9	SER	-	expression tag	UNP O87605
J	-8	SER	-	expression tag	UNP O87605
J	-7	GLY	-	expression tag	UNP O87605
J	-6	LEU	-	expression tag	UNP O87605
J	-5	VAL	-	expression tag	UNP O87605
J	-4	PRO	-	expression tag	UNP O87605
J	-3	ARG	-	expression tag	UNP O87605
J	-2	GLY	-	expression tag	UNP O87605
J	-1	SER	-	expression tag	UNP O87605
J	0	HIS	-	expression tag	UNP O87605
J	50	ASN	ASP	engineered mutation	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-19	MET	-	expression tag	UNP O87605
K	-18	GLY	-	expression tag	UNP O87605
K	-17	SER	-	expression tag	UNP O87605
K	-16	SER	-	expression tag	UNP O87605
K	-15	HIS	-	expression tag	UNP O87605
K	-14	HIS	-	expression tag	UNP O87605
K	-13	HIS	-	expression tag	UNP O87605
K	-12	HIS	-	expression tag	UNP O87605
K	-11	HIS	-	expression tag	UNP O87605
K	-10	HIS	-	expression tag	UNP O87605
K	-9	SER	-	expression tag	UNP O87605
K	-8	SER	-	expression tag	UNP O87605
K	-7	GLY	-	expression tag	UNP O87605
K	-6	LEU	-	expression tag	UNP O87605
K	-5	VAL	-	expression tag	UNP O87605
K	-4	PRO	-	expression tag	UNP O87605
K	-3	ARG	-	expression tag	UNP O87605
K	-2	GLY	-	expression tag	UNP O87605
K	-1	SER	-	expression tag	UNP O87605
K	0	HIS	-	expression tag	UNP O87605
K	50	ASN	ASP	engineered mutation	UNP O87605
L	-19	MET	-	expression tag	UNP O87605
L	-18	GLY	-	expression tag	UNP O87605
L	-17	SER	-	expression tag	UNP O87605
L	-16	SER	-	expression tag	UNP O87605
L	-15	HIS	-	expression tag	UNP O87605
L	-14	HIS	-	expression tag	UNP O87605
L	-13	HIS	-	expression tag	UNP O87605
L	-12	HIS	-	expression tag	UNP O87605
L	-11	HIS	-	expression tag	UNP O87605
L	-10	HIS	-	expression tag	UNP O87605
L	-9	SER	-	expression tag	UNP O87605
L	-8	SER	-	expression tag	UNP O87605
L	-7	GLY	-	expression tag	UNP O87605
L	-6	LEU	-	expression tag	UNP O87605
L	-5	VAL	-	expression tag	UNP O87605
L	-4	PRO	-	expression tag	UNP O87605
L	-3	ARG	-	expression tag	UNP O87605
L	-2	GLY	-	expression tag	UNP O87605
L	-1	SER	-	expression tag	UNP O87605
L	0	HIS	-	expression tag	UNP O87605
L	50	ASN	ASP	engineered mutation	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	expression tag	UNP O87605
M	-18	GLY	-	expression tag	UNP O87605
M	-17	SER	-	expression tag	UNP O87605
M	-16	SER	-	expression tag	UNP O87605
M	-15	HIS	-	expression tag	UNP O87605
M	-14	HIS	-	expression tag	UNP O87605
M	-13	HIS	-	expression tag	UNP O87605
M	-12	HIS	-	expression tag	UNP O87605
M	-11	HIS	-	expression tag	UNP O87605
M	-10	HIS	-	expression tag	UNP O87605
M	-9	SER	-	expression tag	UNP O87605
M	-8	SER	-	expression tag	UNP O87605
M	-7	GLY	-	expression tag	UNP O87605
M	-6	LEU	-	expression tag	UNP O87605
M	-5	VAL	-	expression tag	UNP O87605
M	-4	PRO	-	expression tag	UNP O87605
M	-3	ARG	-	expression tag	UNP O87605
M	-2	GLY	-	expression tag	UNP O87605
M	-1	SER	-	expression tag	UNP O87605
M	0	HIS	-	expression tag	UNP O87605
M	50	ASN	ASP	engineered mutation	UNP O87605
N	-19	MET	-	expression tag	UNP O87605
N	-18	GLY	-	expression tag	UNP O87605
N	-17	SER	-	expression tag	UNP O87605
N	-16	SER	-	expression tag	UNP O87605
N	-15	HIS	-	expression tag	UNP O87605
N	-14	HIS	-	expression tag	UNP O87605
N	-13	HIS	-	expression tag	UNP O87605
N	-12	HIS	-	expression tag	UNP O87605
N	-11	HIS	-	expression tag	UNP O87605
N	-10	HIS	-	expression tag	UNP O87605
N	-9	SER	-	expression tag	UNP O87605
N	-8	SER	-	expression tag	UNP O87605
N	-7	GLY	-	expression tag	UNP O87605
N	-6	LEU	-	expression tag	UNP O87605
N	-5	VAL	-	expression tag	UNP O87605
N	-4	PRO	-	expression tag	UNP O87605
N	-3	ARG	-	expression tag	UNP O87605
N	-2	GLY	-	expression tag	UNP O87605
N	-1	SER	-	expression tag	UNP O87605
N	0	HIS	-	expression tag	UNP O87605
N	50	ASN	ASP	engineered mutation	UNP O87605

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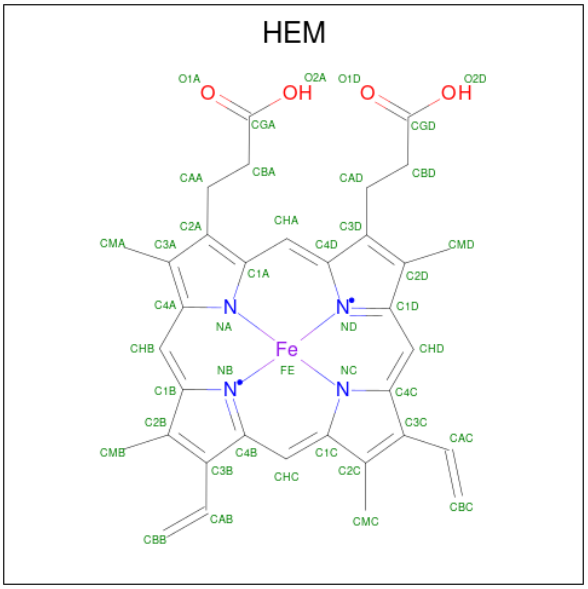
Chain	Residue	Modelled	Actual	Comment	Reference
O	-19	MET	-	expression tag	UNP O87605
O	-18	GLY	-	expression tag	UNP O87605
O	-17	SER	-	expression tag	UNP O87605
O	-16	SER	-	expression tag	UNP O87605
O	-15	HIS	-	expression tag	UNP O87605
O	-14	HIS	-	expression tag	UNP O87605
O	-13	HIS	-	expression tag	UNP O87605
O	-12	HIS	-	expression tag	UNP O87605
O	-11	HIS	-	expression tag	UNP O87605
O	-10	HIS	-	expression tag	UNP O87605
O	-9	SER	-	expression tag	UNP O87605
O	-8	SER	-	expression tag	UNP O87605
O	-7	GLY	-	expression tag	UNP O87605
O	-6	LEU	-	expression tag	UNP O87605
O	-5	VAL	-	expression tag	UNP O87605
O	-4	PRO	-	expression tag	UNP O87605
O	-3	ARG	-	expression tag	UNP O87605
O	-2	GLY	-	expression tag	UNP O87605
O	-1	SER	-	expression tag	UNP O87605
O	0	HIS	-	expression tag	UNP O87605
O	50	ASN	ASP	engineered mutation	UNP O87605
P	-19	MET	-	expression tag	UNP O87605
P	-18	GLY	-	expression tag	UNP O87605
P	-17	SER	-	expression tag	UNP O87605
P	-16	SER	-	expression tag	UNP O87605
P	-15	HIS	-	expression tag	UNP O87605
P	-14	HIS	-	expression tag	UNP O87605
P	-13	HIS	-	expression tag	UNP O87605
P	-12	HIS	-	expression tag	UNP O87605
P	-11	HIS	-	expression tag	UNP O87605
P	-10	HIS	-	expression tag	UNP O87605
P	-9	SER	-	expression tag	UNP O87605
P	-8	SER	-	expression tag	UNP O87605
P	-7	GLY	-	expression tag	UNP O87605
P	-6	LEU	-	expression tag	UNP O87605
P	-5	VAL	-	expression tag	UNP O87605
P	-4	PRO	-	expression tag	UNP O87605
P	-3	ARG	-	expression tag	UNP O87605
P	-2	GLY	-	expression tag	UNP O87605
P	-1	SER	-	expression tag	UNP O87605
P	0	HIS	-	expression tag	UNP O87605
P	50	ASN	ASP	engineered mutation	UNP O87605

- 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		
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		

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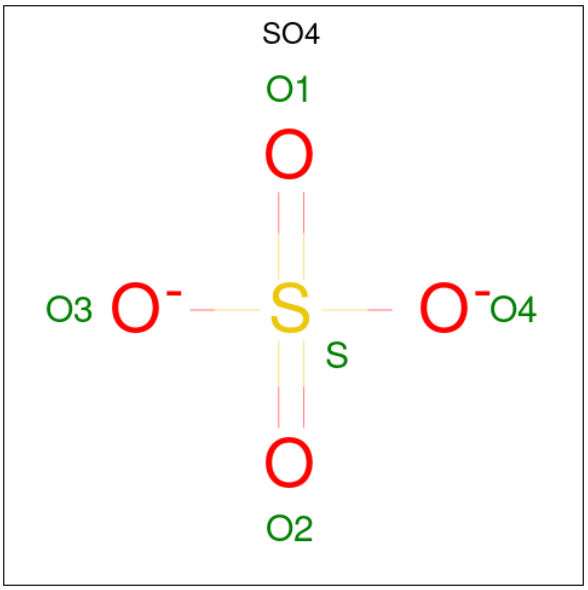
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

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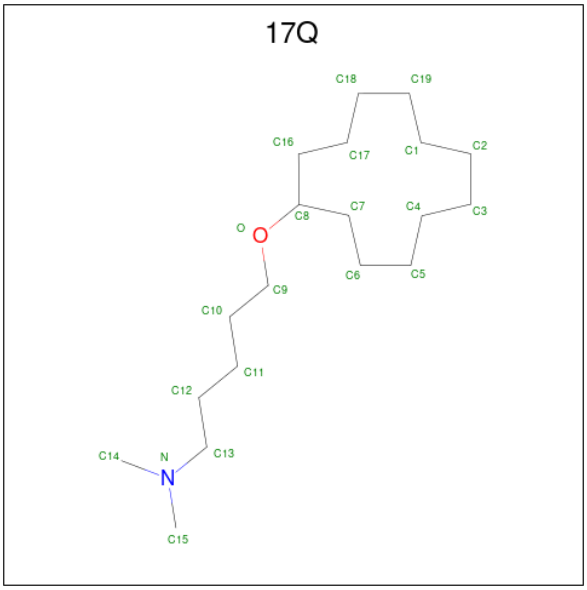
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0

- Molecule 4 is 1.7.6 5-cyclododecyloxy-N,N-dimethyl-pentan-1-amine (three-letter code: 17Q) (formula: $C_{19}H_{39}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 21 19 1 1	0	0
4	G	1	Total C N O 21 19 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	35	Total O 35 35	0	0
5	B	32	Total O 32 32	0	0

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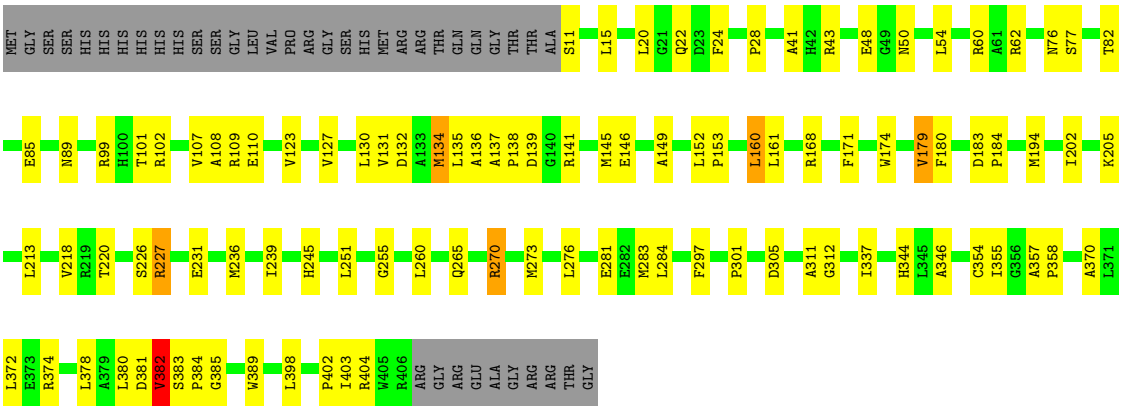
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	43	Total O 43 43	0	0
5	D	46	Total O 46 46	0	0
5	E	37	Total O 37 37	0	0
5	F	39	Total O 39 39	0	0
5	G	57	Total O 57 57	0	0
5	H	35	Total O 35 35	0	0
5	I	39	Total O 39 39	0	0
5	J	34	Total O 34 34	0	0
5	K	28	Total O 28 28	0	0
5	L	21	Total O 21 21	0	0
5	M	16	Total O 16 16	0	0
5	N	15	Total O 15 15	0	0
5	O	20	Total O 20 20	0	0
5	P	17	Total O 17 17	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.

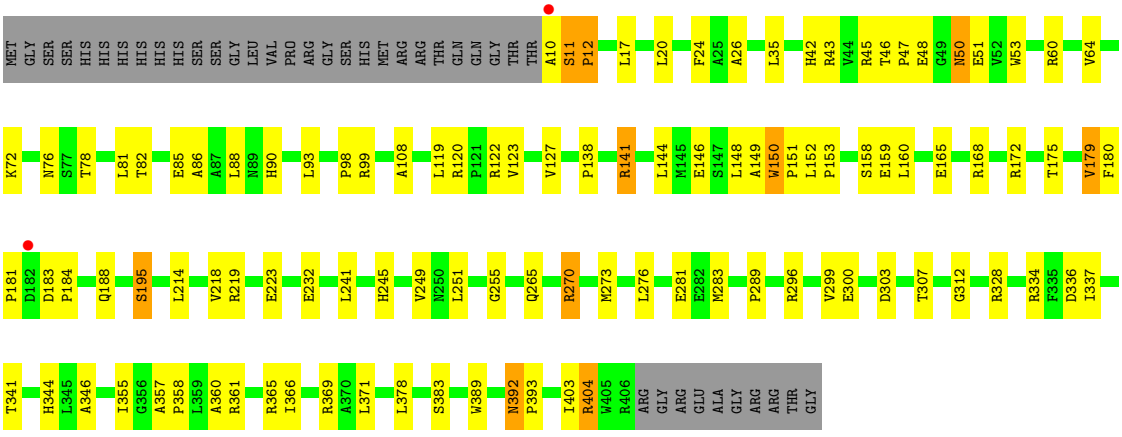
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain A:



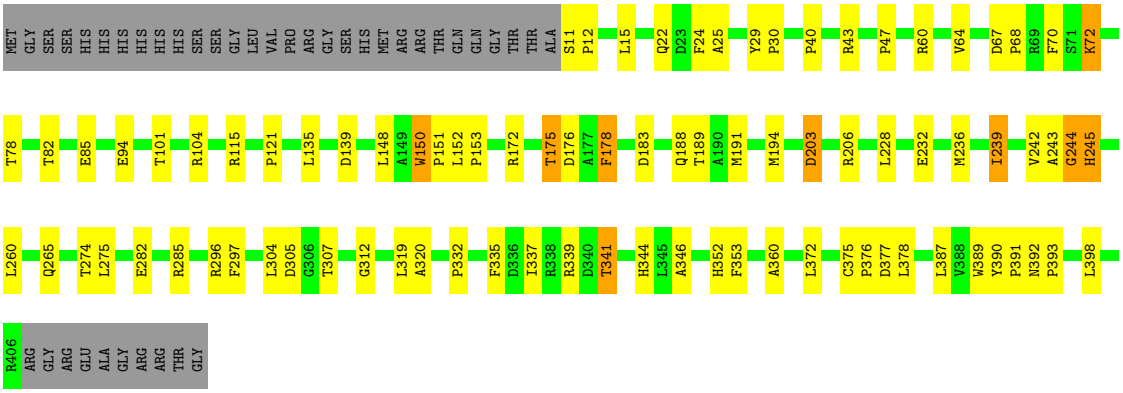
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain B:



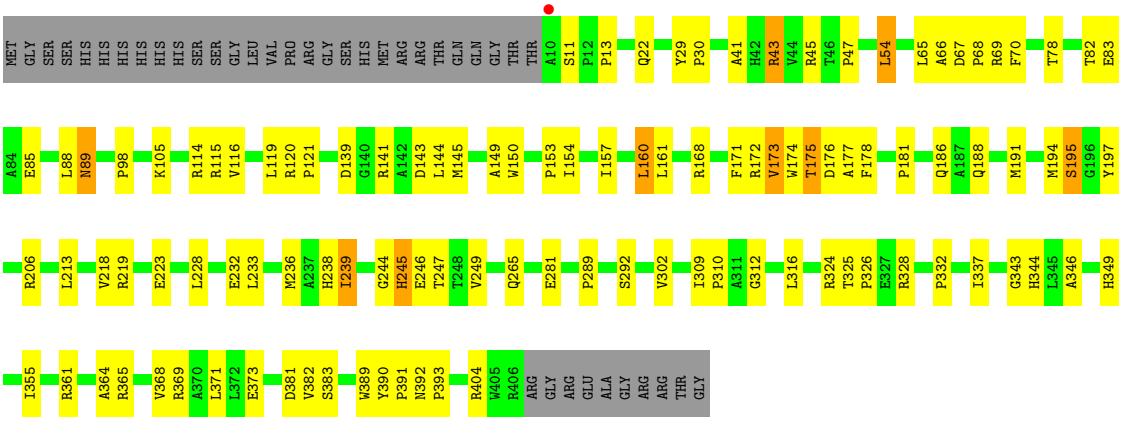
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain C:



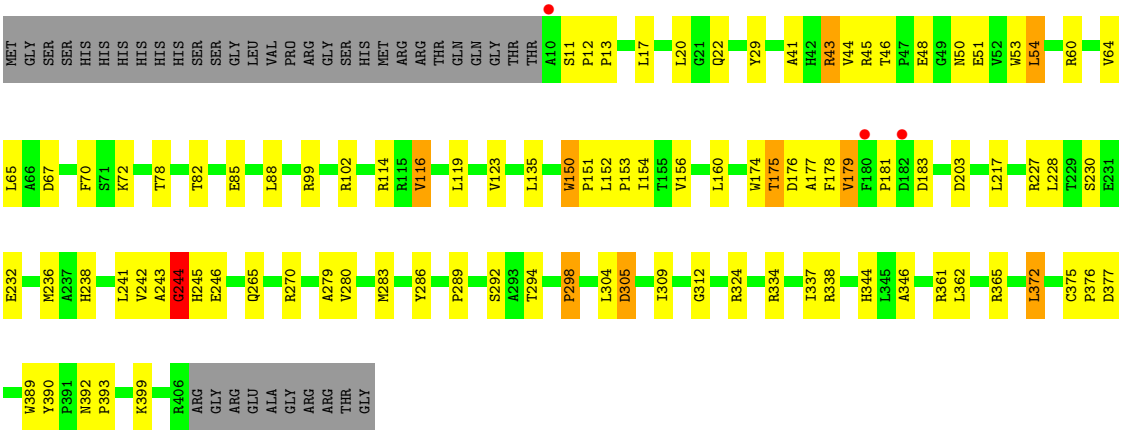
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain D:



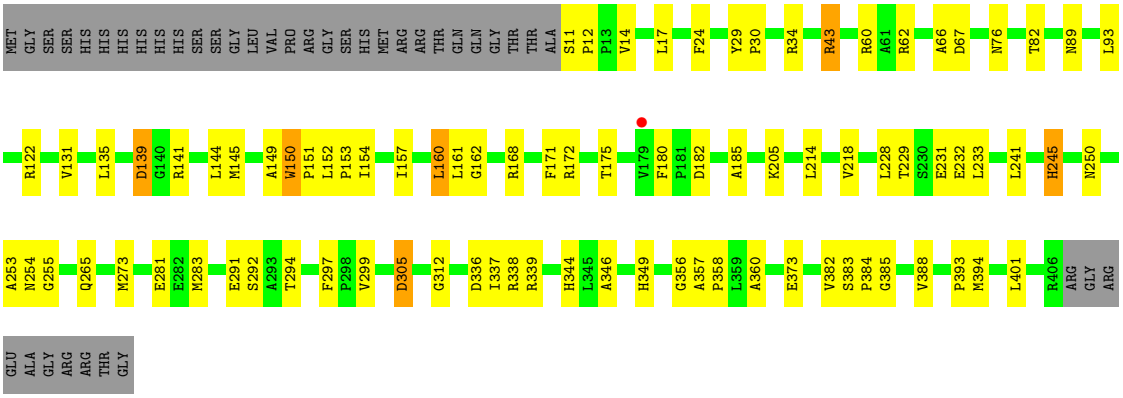
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain E:



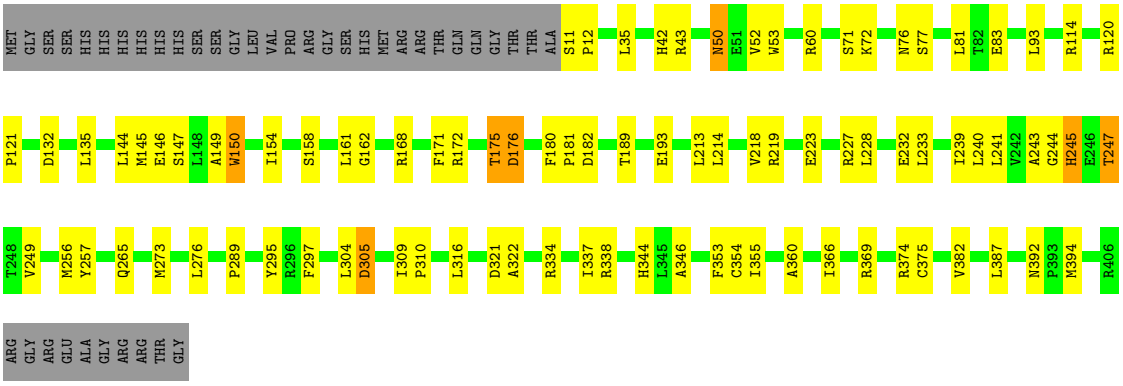
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain F:



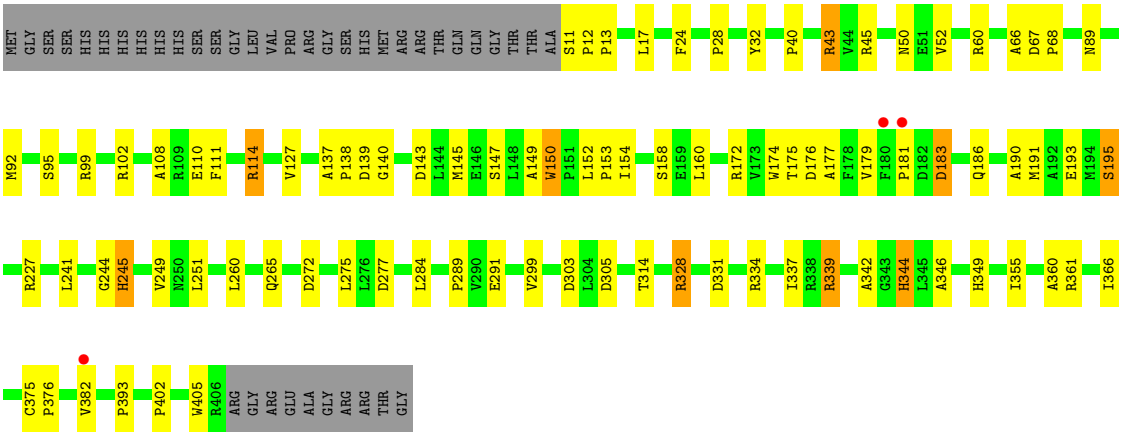
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain G:



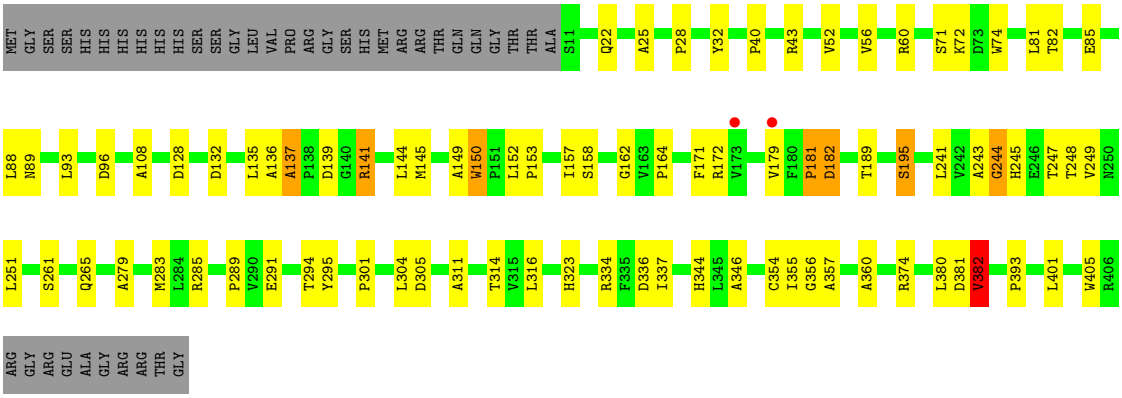
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain H:



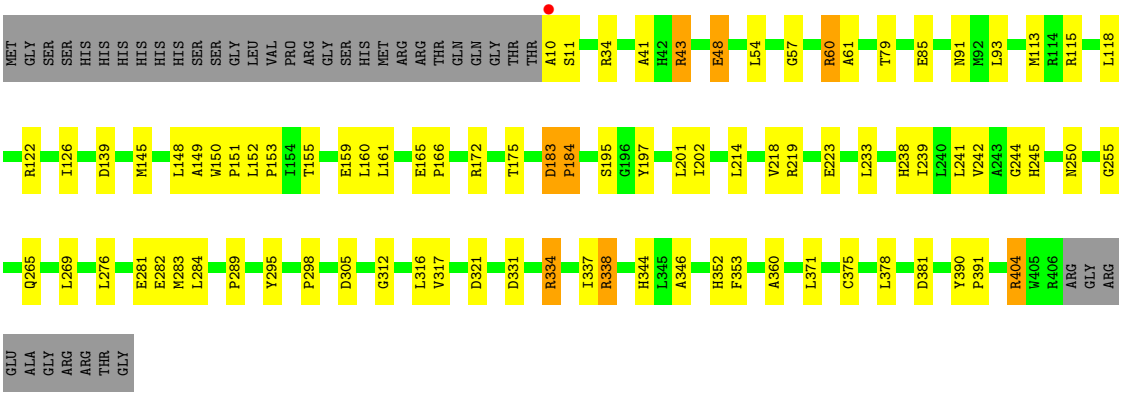
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain I:



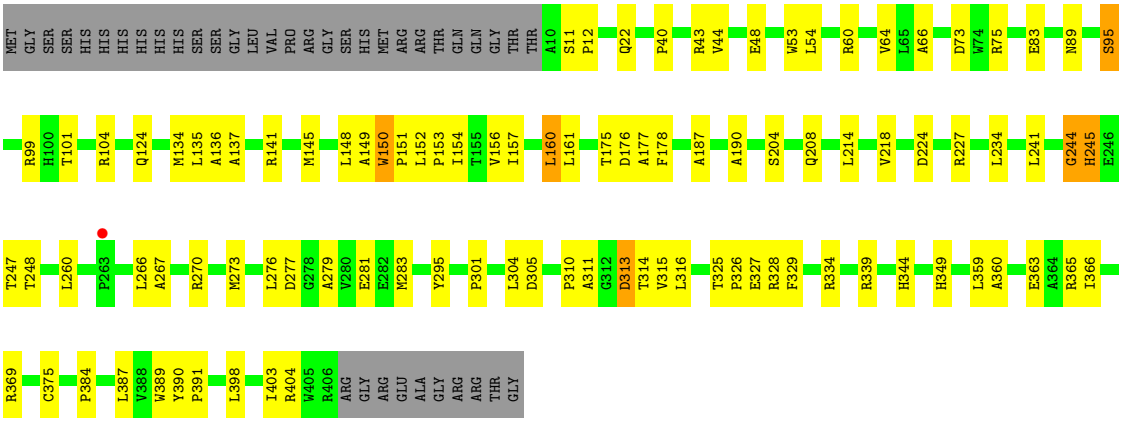
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain J:



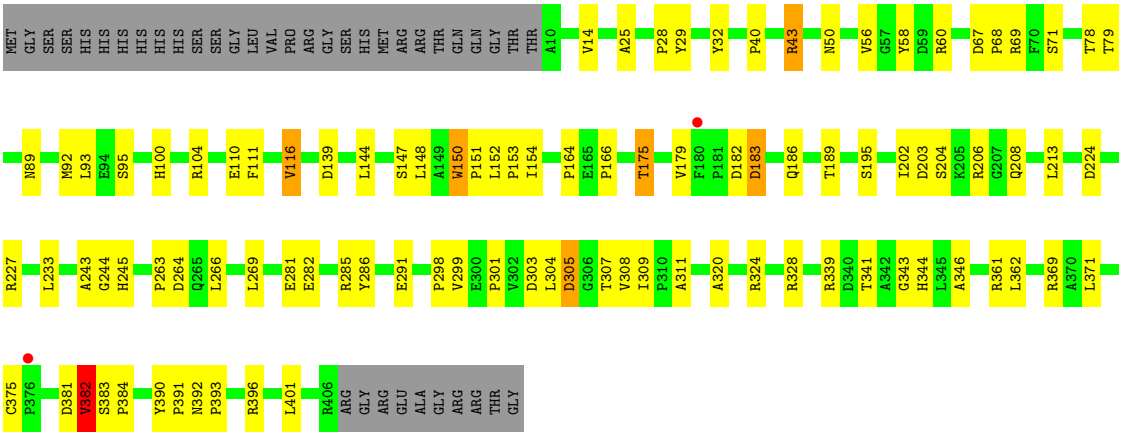
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain K:



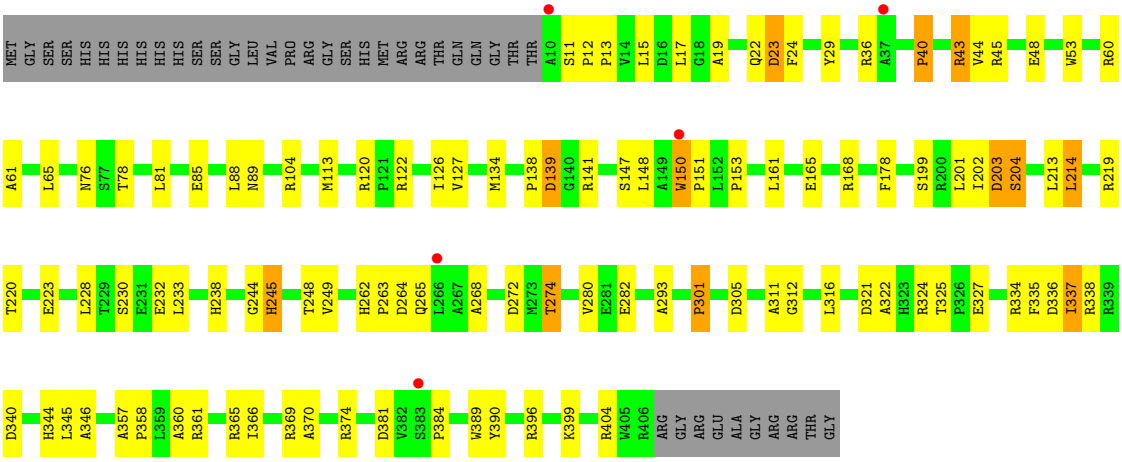
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain L:



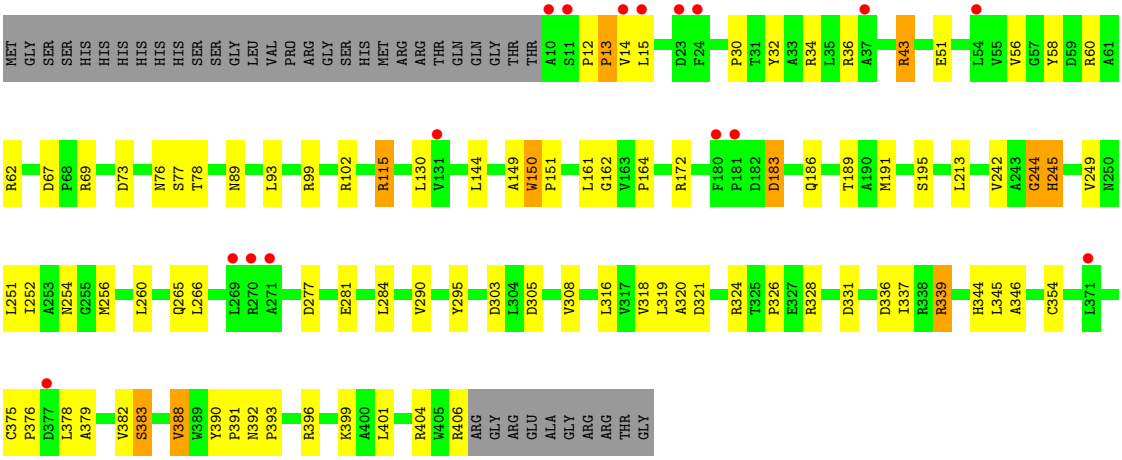
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain M:



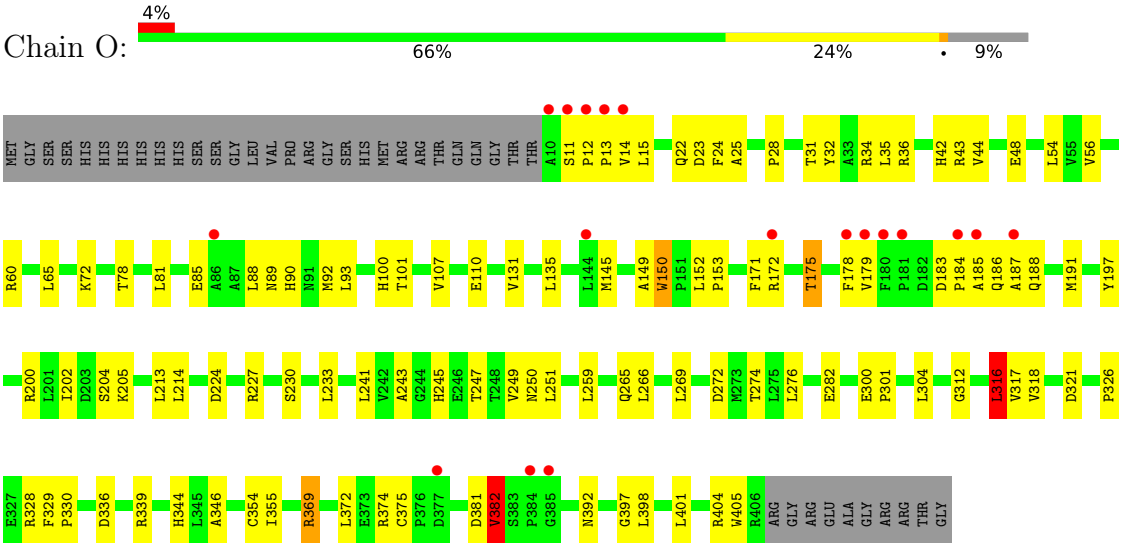
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain N:



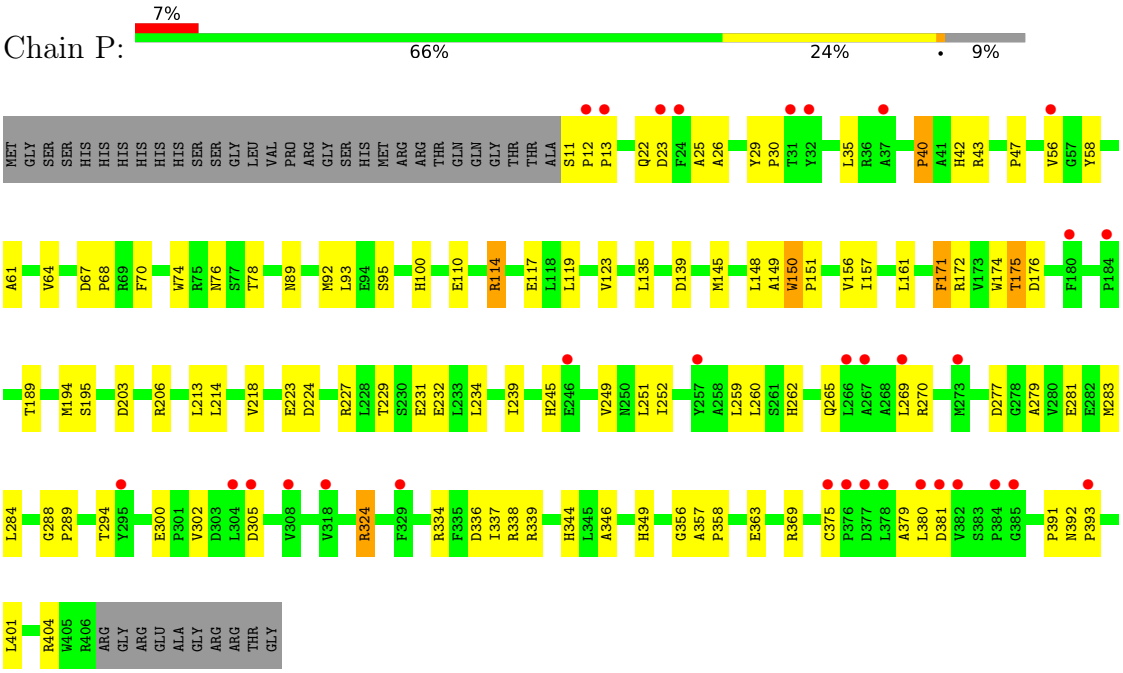
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain O:



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	110.27Å 130.11Å 134.90Å 66.48° 70.25° 72.23°	Depositor
Resolution (Å)	119.84 – 2.70 91.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (119.84-2.70) 97.3 (91.88-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.196 , 0.279 0.199 , 0.277	Depositor DCC
R_{free} test set	8479 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.030 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	50342	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8815e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4, 17Q

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	0.61	0/3100	0.75	0/4234
1	B	0.60	0/3142	0.72	0/4292
1	C	0.62	0/3136	0.75	1/4283 (0.0%)
1	D	0.63	0/3149	0.75	1/4301 (0.0%)
1	E	0.66	0/3141	0.77	1/4290 (0.0%)
1	F	0.59	0/3149	0.71	0/4303
1	G	0.61	0/3166	0.71	0/4324
1	H	0.62	0/3130	0.74	0/4275
1	I	0.57	0/3139	0.72	0/4288
1	J	0.58	0/3133	0.69	0/4280
1	K	0.55	0/3149	0.70	0/4301
1	L	0.54	0/3138	0.70	0/4287
1	M	0.54	0/3138	0.68	0/4286
1	N	0.48	0/3137	0.63	0/4285
1	O	0.51	0/3125	0.67	1/4269 (0.0%)
1	P	0.47	0/3131	0.64	0/4276
All	All	0.58	0/50203	0.71	4/68574 (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	E	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	E	54	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	65	LEU	CA-CB-CG	5.05	126.92	115.30
1	O	316	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	244	GLY	Peptide
1	I	179	VAL	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	3031	0	2990	67	0
1	B	3069	0	3026	93	0
1	C	3063	0	3024	71	0
1	D	3076	0	3027	78	0
1	E	3068	0	3022	63	0
1	F	3075	0	3019	70	0
1	G	3093	0	3049	78	0
1	H	3057	0	3020	57	0
1	I	3066	0	3020	65	0
1	J	3060	0	3016	61	0
1	K	3076	0	3032	60	0
1	L	3065	0	3014	61	0
1	M	3065	0	3014	68	0
1	N	3064	0	3025	63	0
1	O	3052	0	3008	70	0
1	P	3058	0	3006	60	0
2	A	43	0	30	1	0
2	B	43	0	30	6	0
2	C	43	0	30	6	0
2	D	43	0	30	8	0
2	E	43	0	30	5	0
2	F	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	43	0	30	6	0
2	H	43	0	30	7	0
2	I	43	0	30	5	0
2	J	43	0	30	4	0
2	K	43	0	30	3	0
2	L	43	0	30	4	0
2	M	43	0	30	5	0
2	N	43	0	30	7	0
2	O	43	0	30	4	0
2	P	43	0	30	5	0
3	A	5	0	0	2	0
3	B	10	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	1	0
3	H	10	0	0	1	0
3	I	10	0	0	0	0
3	J	5	0	0	0	0
3	O	10	0	0	1	0
4	C	21	0	39	6	0
4	G	21	0	39	5	0
5	A	35	0	0	0	0
5	B	32	0	0	0	0
5	C	43	0	0	3	0
5	D	46	0	0	3	0
5	E	37	0	0	1	0
5	F	39	0	0	2	0
5	G	57	0	0	2	0
5	H	35	0	0	4	0
5	I	39	0	0	0	0
5	J	34	0	0	1	0
5	K	28	0	0	1	0
5	L	21	0	0	0	0
5	M	16	0	0	0	0
5	N	15	0	0	0	0
5	O	20	0	0	0	0
5	P	17	0	0	1	0
All	All	50342	0	48870	1084	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 11.

All (1084) 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:227:ARG:NH1	1:O:227:ARG:HB3	1.69	1.07
1:I:128:ASP:HA	1:I:374:ARG:HH12	1.21	1.06
1:G:171:PHE:O	1:G:175:THR:HG22	1.56	1.05
1:N:390:TYR:HE1	1:N:399:LYS:HG3	1.20	1.04
1:F:171:PHE:O	1:F:175:THR:HG22	1.59	1.02
1:K:11:SER:HB2	1:K:12:PRO:HD3	1.43	1.00
3:A:1408:SO4:O1	1:E:227:ARG:NH1	1.94	0.98
1:C:11:SER:CB	1:C:12:PRO:HD3	1.99	0.93
1:C:150:TRP:HZ3	1:C:245:HIS:CE1	1.88	0.92
1:L:150:TRP:HZ3	1:L:245:HIS:HE2	1.11	0.91
1:B:165:GLU:HA	1:B:168:ARG:HD2	1.52	0.89
1:F:265:GLN:NE2	1:F:337:ILE:H	1.70	0.89
1:P:224:ASP:OD2	1:P:227:ARG:HG3	1.73	0.89
1:O:227:ARG:HB3	1:O:227:ARG:HH11	1.26	0.89
1:D:361:ARG:O	1:D:365:ARG:HG3	1.73	0.88
1:N:390:TYR:CE1	1:N:399:LYS:HG3	2.07	0.87
1:C:344:HIS:HD2	1:C:346:ALA:H	1.21	0.87
1:L:144:LEU:HD23	1:L:401:LEU:HD23	1.57	0.86
1:A:381:ASP:O	1:A:382:VAL:HB	1.75	0.85
1:A:132:ASP:OD1	1:A:374:ARG:NH2	2.08	0.85
1:I:334:ARG:HE	1:I:336:ASP:HB2	1.42	0.84
1:B:245[B]:HIS:CD2	1:B:249:VAL:HG21	2.11	0.84
1:E:344:HIS:HD2	1:E:346:ALA:H	1.25	0.84
1:J:265:GLN:NE2	1:J:337:ILE:H	1.75	0.84
1:A:174:TRP:HE3	1:A:194:MET:CE	1.90	0.83
1:G:60:ARG:NH2	1:G:305:ASP:OD2	2.12	0.82
1:H:60:ARG:NH2	1:H:305:ASP:HB2	1.94	0.82
1:G:189:THR:O	1:G:193:GLU:HG3	1.79	0.82
1:L:150:TRP:CZ3	1:L:245:HIS:NE2	2.46	0.82
1:E:116:VAL:HG13	1:E:362:LEU:HD22	1.62	0.82
1:C:60:ARG:HH22	1:C:305:ASP:HB2	1.45	0.81
1:F:11:SER:HB2	1:F:12:PRO:HD3	1.60	0.81
1:J:183:ASP:HB2	1:J:184:PRO:HD2	1.60	0.81
1:P:114:ARG:HG2	1:P:114:ARG:HH11	1.45	0.81
1:E:242:VAL:O	1:E:245:HIS:HB3	1.81	0.80
1:N:36:ARG:HH12	1:N:326:PRO:HD3	1.46	0.80
1:E:22:GLN:HE22	1:E:389:TRP:H	1.28	0.80
1:J:172:ARG:HA	1:J:175:THR:HG22	1.63	0.79
1:A:174:TRP:HE3	1:A:194:MET:HE3	1.45	0.79
1:K:359:LEU:O	1:K:363:GLU:HG3	1.82	0.79
1:C:11:SER:HB3	1:C:12:PRO:HD3	1.62	0.79
1:L:392:ASN:OD1	1:L:393:PRO:HD2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG12	1:A:180:PHE:H	1.47	0.78
1:C:85:GLU:HG3	1:C:191:MET:CE	2.13	0.78
1:B:179:VAL:HG12	1:B:180:PHE:H	1.48	0.78
1:L:93:LEU:HD13	2:L:1407:HEM:HAD2	1.66	0.78
1:M:344:HIS:HD2	1:M:346:ALA:H	1.33	0.77
1:K:60:ARG:NH2	1:K:305:ASP:HB2	2.01	0.76
1:K:325:THR:HG22	1:K:327:GLU:OE1	1.85	0.76
1:D:145:MET:HA	1:D:149:ALA:HB3	1.68	0.76
1:B:392:ASN:OD1	1:B:393:PRO:HD2	1.86	0.75
1:B:51:GLU:OE2	1:L:369:ARG:NH1	2.19	0.75
1:B:82:THR:HG23	1:B:85:GLU:OE1	1.86	0.75
1:B:150:TRP:CH2	1:B:172:ARG:HB2	2.21	0.75
1:G:171:PHE:O	1:G:175:THR:CG2	2.35	0.74
1:H:227:ARG:NH1	3:H:1409:SO4:O2	2.21	0.73
1:K:40:PRO:HG3	1:K:305:ASP:HB3	1.70	0.73
1:M:161:LEU:HD23	1:M:213:LEU:HB3	1.70	0.73
1:P:11:SER:HB2	1:P:12:PRO:HD3	1.71	0.73
1:I:141:ARG:HD3	1:I:381:ASP:OD2	1.89	0.73
1:K:150:TRP:HE3	1:K:245:HIS:HE1	1.35	0.73
1:A:265:GLN:NE2	1:A:337:ILE:HG12	2.03	0.73
1:D:67:ASP:HB3	1:D:70:PHE:HD1	1.53	0.72
1:D:150:TRP:CZ2	1:D:172:ARG:HB2	2.23	0.72
1:G:219:ARG:O	1:G:223:GLU:HG3	1.88	0.72
1:C:11:SER:HB2	1:C:12:PRO:HD3	1.70	0.72
1:A:60:ARG:HH22	1:A:305:ASP:HB2	1.54	0.72
1:A:174:TRP:CE3	1:A:194:MET:HE3	2.24	0.72
1:F:60:ARG:HD3	5:F:2007:HOH:O	1.90	0.72
1:G:161:LEU:CD2	1:G:213:LEU:HD23	2.20	0.72
1:O:245:HIS:O	1:O:249:VAL:HG23	1.89	0.72
1:C:150:TRP:CZ3	1:C:245:HIS:CE1	2.76	0.71
1:E:265:GLN:NE2	1:E:337:ILE:HG12	2.05	0.71
1:I:344:HIS:HD2	1:I:346:ALA:H	1.37	0.71
1:L:154:ILE:HB	1:L:245:HIS:HE1	1.54	0.71
1:O:35:LEU:HB3	1:O:42:HIS:CD2	2.25	0.71
1:K:150:TRP:CE3	1:K:245:HIS:HE1	2.09	0.71
1:B:179:VAL:HG12	1:B:180:PHE:N	2.05	0.71
1:B:141:ARG:HH11	1:B:141:ARG:HB2	1.56	0.71
1:C:60:ARG:NH2	1:C:305:ASP:HB2	2.05	0.71
1:G:243:ALA:O	1:G:247:THR:OG1	2.09	0.71
1:G:273:MET:HE2	1:G:369:ARG:HG3	1.73	0.70
1:K:316[B]:LEU:N	1:K:316[B]:LEU:HD12	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:O	1:B:181:PRO:HD3	1.91	0.70
1:M:13:PRO:HD2	1:P:369:ARG:HH12	1.56	0.70
1:B:344:HIS:HD2	1:B:346:ALA:H	1.36	0.70
1:F:344:HIS:HD2	1:F:346:ALA:H	1.36	0.70
1:G:214:LEU:O	1:G:218:VAL:HG23	1.91	0.70
1:F:150:TRP:CD1	1:F:151:PRO:HD3	2.27	0.70
1:A:174:TRP:CE3	1:A:194:MET:CE	2.75	0.69
1:E:181:PRO:HB2	1:E:183:ASP:O	1.91	0.69
1:P:357:ALA:HB3	1:P:358:PRO:HD3	1.74	0.69
1:H:11:SER:HB3	1:H:12:PRO:HD3	1.74	0.69
1:J:93:LEU:HD13	2:J:1407:HEM:HAD2	1.73	0.69
1:B:265:GLN:NE2	1:B:337:ILE:H	1.89	0.69
2:N:1407:HEM:HMC1	2:N:1407:HEM:HBC2	1.74	0.69
1:O:227:ARG:HH11	1:O:227:ARG:CB	2.03	0.69
1:A:179:VAL:HG12	1:A:180:PHE:N	2.07	0.69
1:F:265:GLN:HE22	1:F:337:ILE:H	1.37	0.69
1:I:150:TRP:CZ2	1:I:172:ARG:HB2	2.27	0.69
1:C:228:LEU:HD12	1:C:232:GLU:HB3	1.75	0.69
1:E:265:GLN:NE2	1:E:337:ILE:H	1.90	0.69
1:B:11:SER:N	1:B:12:PRO:HD3	2.08	0.69
1:B:138:PRO:HB2	1:F:185:ALA:HB3	1.75	0.69
1:F:241:LEU:O	1:F:245[B]:HIS:CE1	2.47	0.68
1:G:360:ALA:HB1	2:G:1407:HEM:HAB	1.75	0.68
1:I:128:ASP:HA	1:I:374:ARG:NH1	2.03	0.68
1:D:143:ASP:HB2	1:G:83:GLU:HG3	1.75	0.68
1:I:22:GLN:HA	1:I:25:ALA:HB3	1.75	0.68
1:B:127:VAL:HG21	1:B:366:ILE:HG22	1.74	0.68
1:C:344:HIS:CD2	1:C:346:ALA:H	2.10	0.68
1:O:282:GLU:HG2	1:O:336:ASP:O	1.94	0.68
1:F:139:ASP:HB3	1:F:141:ARG:HB2	1.76	0.68
1:D:265:GLN:HE21	1:D:337:ILE:H	1.40	0.67
1:F:360:ALA:CB	2:F:1407:HEM:HAB	2.25	0.67
1:L:263:PRO:HA	1:L:266:LEU:HB3	1.75	0.67
1:D:392:ASN:OD1	1:D:393:PRO:HD2	1.95	0.67
1:O:344:HIS:HD2	1:O:346:ALA:H	1.42	0.67
1:C:265:GLN:NE2	1:C:337:ILE:H	1.92	0.67
1:D:236:MET:O	1:D:239:ILE:HG22	1.93	0.67
1:D:265:GLN:NE2	1:D:337:ILE:H	1.93	0.67
1:G:132:ASP:OD1	1:G:374:ARG:NH2	2.28	0.67
1:I:82:THR:HG23	1:I:85:GLU:OE1	1.94	0.67
1:A:60:ARG:NH2	1:A:305:ASP:HB2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HG3	1:B:404:ARG:HB3	1.76	0.67
1:G:265:GLN:NE2	1:G:337:ILE:HG12	2.08	0.67
1:M:360:ALA:HB1	2:M:1407:HEM:HAB	1.76	0.67
1:L:344:HIS:HD2	1:L:346:ALA:H	1.40	0.67
1:B:150:TRP:CE3	1:B:245[B]:HIS:NE2	2.63	0.67
1:B:150:TRP:HE3	1:B:245[B]:HIS:NE2	1.93	0.67
1:C:11:SER:CB	1:C:12:PRO:CD	2.73	0.66
1:G:72:LYS:NZ	1:G:72:LYS:HB3	2.10	0.66
1:L:154:ILE:HB	1:L:245:HIS:CE1	2.31	0.66
1:F:150:TRP:CZ3	1:F:172:ARG:HB2	2.31	0.66
1:N:150:TRP:CE3	1:N:245:HIS:HE1	2.14	0.66
1:C:265:GLN:HE21	1:C:337:ILE:HG23	1.60	0.66
1:E:289:PRO:HG2	2:E:1407:HEM:HMB2	1.77	0.66
1:G:227:ARG:HH21	1:O:328:ARG:HH21	1.43	0.66
1:D:244:GLY:CA	2:D:1407:HEM:HBC2	2.26	0.66
1:J:250:ASN:HB2	1:J:289:PRO:HB3	1.77	0.66
1:L:144:LEU:CD2	1:L:401:LEU:HD23	2.26	0.65
1:P:260:LEU:HD22	1:P:379:ALA:HA	1.77	0.65
1:C:40:PRO:HG3	1:C:305:ASP:HB3	1.79	0.65
1:I:40:PRO:HG3	1:I:305:ASP:CB	2.26	0.65
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.79	0.65
1:P:114:ARG:HG2	1:P:114:ARG:NH1	2.11	0.65
1:M:219:ARG:O	1:M:223:GLU:HG3	1.96	0.65
1:P:277:ASP:O	1:P:281:GLU:HG2	1.96	0.65
1:O:381:ASP:O	1:O:382:VAL:HB	1.96	0.65
1:I:381:ASP:O	1:I:382:VAL:HB	1.97	0.65
1:G:360:ALA:CB	2:G:1407:HEM:HAB	2.27	0.65
2:H:1407:HEM:HBB2	2:H:1407:HEM:HMB2	1.77	0.64
1:K:60:ARG:HD3	5:K:2004:HOH:O	1.95	0.64
1:O:282:GLU:OE1	1:O:282:GLU:HA	1.97	0.64
1:C:152:LEU:HB3	1:C:153:PRO:HD3	1.77	0.64
1:G:50[A]:ASN:HD22	1:G:50[A]:ASN:N	1.94	0.64
1:C:85:GLU:HG3	1:C:191:MET:HE1	1.78	0.64
1:C:344:HIS:HD2	1:C:346:ALA:N	1.93	0.64
1:G:161:LEU:HD21	1:G:213:LEU:HD23	1.80	0.64
1:O:110:GLU:HG3	1:O:213:LEU:HD13	1.80	0.64
1:K:214:LEU:O	1:K:218:VAL:HG23	1.97	0.64
1:F:162:GLY:O	1:F:205:LYS:NZ	2.27	0.64
1:O:150:TRP:CH2	1:O:172:ARG:HB2	2.33	0.64
1:C:85:GLU:HG3	1:C:191:MET:HE3	1.79	0.63
1:G:172:ARG:O	1:G:176:ASP:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLN:HE21	1:A:337:ILE:HG12	1.62	0.63
1:D:120:ARG:HB3	1:D:121:PRO:HD3	1.78	0.63
1:H:339:ARG:HD3	5:H:2031:HOH:O	1.97	0.63
1:N:295:TYR:CD1	1:N:316[A]:LEU:HD21	2.33	0.63
1:D:22:GLN:HE22	1:D:389:TRP:H	1.45	0.63
1:F:11:SER:CB	1:F:12:PRO:HD3	2.27	0.63
1:M:301:PRO:HD3	1:M:311:ALA:HB2	1.81	0.63
1:I:301:PRO:HD3	1:I:311:ALA:HB2	1.80	0.63
1:C:150:TRP:CH2	1:C:172:ARG:HB2	2.34	0.63
1:A:255:GLY:HA2	1:A:283:MET:HG2	1.80	0.63
1:O:60:ARG:HD2	1:O:304:LEU:HD22	1.80	0.63
1:H:150:TRP:HZ3	1:H:245:HIS:CE1	2.17	0.63
1:D:344:HIS:HD2	1:D:346:ALA:H	1.45	0.63
2:N:1407:HEM:HBC2	2:N:1407:HEM:CMC	2.29	0.63
1:H:11:SER:HB3	1:H:12:PRO:CD	2.29	0.62
1:M:40:PRO:HG3	1:M:305:ASP:HB3	1.80	0.62
1:N:344:HIS:HD2	1:N:346:ALA:H	1.45	0.62
1:C:265:GLN:NE2	1:C:337:ILE:HG12	2.14	0.62
1:B:51:GLU:CD	1:L:369:ARG:HH22	2.03	0.62
4:G:1410:17Q:H61C	4:G:1410:17Q:H172	1.82	0.62
1:L:243:ALA:C	1:L:245:HIS:H	2.02	0.62
1:N:191:MET:O	1:N:195:SER:HB2	1.98	0.62
1:J:183:ASP:HB2	1:J:184:PRO:CD	2.27	0.62
1:J:344:HIS:HD2	1:J:346:ALA:H	1.47	0.62
1:I:71:SER:OG	1:I:96:ASP:OD2	2.18	0.62
1:A:381:ASP:O	1:A:402:PRO:HB2	1.99	0.62
1:H:174:TRP:NE1	1:H:193:GLU:OE1	2.28	0.62
1:P:381:ASP:HA	1:P:404:ARG:HH11	1.64	0.62
1:B:148:LEU:HD23	1:B:371:LEU:HD11	1.82	0.62
1:G:114:ARG:NH1	5:G:2026:HOH:O	2.29	0.62
1:J:244:GLY:HA2	2:J:1407:HEM:C3C	2.35	0.62
1:J:265:GLN:HE21	1:J:337:ILE:H	1.48	0.62
1:D:328:ARG:NH2	1:D:343:GLY:HA3	2.15	0.62
1:G:273:MET:CE	1:G:369:ARG:HG3	2.30	0.62
1:M:344:HIS:CD2	1:M:346:ALA:H	2.16	0.62
1:B:93:LEU:HD13	2:B:1407:HEM:HAD2	1.82	0.61
1:E:72:LYS:HE3	1:E:294:THR:OG1	1.99	0.61
1:I:141:ARG:HG3	1:I:141:ARG:NH1	2.14	0.61
1:K:360:ALA:CB	2:K:1407:HEM:HAB	2.30	0.61
1:C:11:SER:HB3	1:C:12:PRO:CD	2.31	0.61
1:C:242:VAL:O	1:C:245:HIS:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:GLN:HE21	1:I:337:ILE:H	1.48	0.61
1:J:202:ILE:HG23	1:J:218:VAL:HG22	1.82	0.61
1:O:93:LEU:HD13	2:O:1407:HEM:HAD2	1.81	0.61
1:K:360:ALA:HB1	2:K:1407:HEM:HAB	1.83	0.61
1:B:82:THR:OG1	1:B:188:GLN:NE2	2.33	0.61
1:I:40:PRO:HG3	1:I:305:ASP:HB2	1.83	0.61
1:B:357:ALA:HB3	1:B:358:PRO:HD3	1.81	0.61
1:G:353:PHE:CD1	1:P:223:GLU:HG2	2.36	0.61
1:D:244:GLY:HA3	2:D:1407:HEM:HBC2	1.82	0.61
1:N:36:ARG:NH1	1:N:326:PRO:HD3	2.14	0.61
1:H:145:MET:HA	1:H:149:ALA:HB3	1.82	0.61
1:H:152:LEU:HB3	1:H:153:PRO:HD3	1.82	0.61
2:C:1407:HEM:NA	4:C:1410:17Q:H32C	2.16	0.61
1:F:228:LEU:HD12	1:F:232:GLU:CB	2.31	0.61
1:B:245[B]:HIS:CD2	1:B:249:VAL:CG2	2.83	0.60
1:M:22:GLN:HE22	1:M:389:TRP:H	1.49	0.60
1:N:376:PRO:HG2	1:N:406:ARG:CB	2.30	0.60
1:B:150:TRP:CZ2	1:B:172:ARG:HB2	2.37	0.60
1:B:245[B]:HIS:HD2	1:B:249:VAL:CG2	2.15	0.60
1:C:150:TRP:CZ2	1:C:172:ARG:HB2	2.37	0.60
1:B:214:LEU:O	1:B:218:VAL:HG23	2.01	0.60
1:D:114:ARG:NH1	5:D:2021:HOH:O	2.30	0.60
1:E:265:GLN:HE21	1:E:337:ILE:H	1.50	0.59
1:D:191:MET:O	1:D:195:SER:HB2	2.02	0.59
1:I:149:ALA:O	1:I:249:VAL:HG22	2.02	0.59
1:F:62:ARG:NH2	3:F:1408:SO4:O3	2.33	0.59
1:L:381:ASP:O	1:L:382:VAL:HB	2.02	0.59
2:O:1407:HEM:HBB2	2:O:1407:HEM:HMB2	1.84	0.59
1:E:154:ILE:HD13	1:E:245:HIS:NE2	2.17	0.59
1:I:150:TRP:CH2	1:I:172:ARG:HB2	2.38	0.59
1:N:260:LEU:HD22	1:N:379:ALA:HA	1.84	0.59
1:I:141:ARG:HG3	1:I:141:ARG:HH11	1.68	0.58
1:I:141:ARG:CG	1:I:141:ARG:HH11	2.16	0.58
1:B:26:ALA:HA	1:B:389:TRP:CD1	2.37	0.58
1:N:318:VAL:HG12	1:N:321:ASP:H	1.67	0.58
1:A:220:THR:HG23	1:A:227:ARG:HH11	1.67	0.58
1:D:381:ASP:HB2	1:D:404:ARG:HB3	1.86	0.58
1:E:217:LEU:HD11	1:E:236:MET:HG2	1.85	0.58
1:O:54:LEU:HD23	1:O:316:LEU:HB2	1.86	0.58
1:I:144:LEU:HD23	1:I:401:LEU:HD23	1.85	0.58
1:N:336:ASP:HB3	1:N:339:ARG:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:GLN:HE22	1:C:389:TRP:H	1.52	0.58
1:E:135:LEU:HD21	1:E:375:CYS:SG	2.43	0.58
1:F:150:TRP:CZ3	1:F:245[A]:HIS:HE1	2.21	0.58
1:B:82:THR:CG2	1:B:85:GLU:OE1	2.51	0.58
1:J:295:TYR:CD1	1:J:316:LEU:HD21	2.39	0.58
1:G:344:HIS:HD2	1:G:346:ALA:H	1.50	0.57
1:I:150:TRP:CZ3	1:I:245:HIS:CE1	2.92	0.57
1:M:13:PRO:HD2	1:P:369:ARG:NH1	2.18	0.57
1:E:178:PHE:O	1:E:179:VAL:HG23	2.04	0.57
2:H:1407:HEM:HBB2	2:H:1407:HEM:CMB	2.34	0.57
1:A:251:LEU:HD13	1:A:284:LEU:HD23	1.85	0.57
1:B:11:SER:N	1:B:12:PRO:CD	2.68	0.57
1:K:152:LEU:HB3	1:K:153:PRO:HD3	1.86	0.57
1:C:150:TRP:HZ3	1:C:245:HIS:HE1	1.51	0.57
1:E:286:TYR:O	1:E:324:ARG:NH2	2.37	0.57
1:I:291:GLU:HB3	1:I:393:PRO:O	2.03	0.57
1:J:202:ILE:HG12	1:J:214:LEU:HD11	1.87	0.57
1:N:43:ARG:NH1	1:N:51:GLU:HB3	2.20	0.57
1:P:22:GLN:HE21	1:P:26:ALA:HB2	1.70	0.57
1:P:119:LEU:O	1:P:123:VAL:HG23	2.05	0.57
1:B:289:PRO:HG3	2:B:1407:HEM:HBB2	1.87	0.57
1:C:244:GLY:HA2	2:C:1407:HEM:CMC	2.34	0.57
1:N:93:LEU:HD13	2:N:1407:HEM:HAD2	1.87	0.57
1:I:72:LYS:HE2	1:I:295:TYR:O	2.05	0.57
1:A:301:PRO:HD3	1:A:311:ALA:HB2	1.87	0.56
1:E:53:TRP:CD2	1:E:309:ILE:HG12	2.40	0.56
1:D:67:ASP:HB3	1:D:70:PHE:CD1	2.38	0.56
1:D:244:GLY:HA2	2:D:1407:HEM:HMC2	1.87	0.56
1:K:11:SER:HB2	1:K:12:PRO:CD	2.26	0.56
1:P:380:LEU:O	1:P:404:ARG:NH1	2.38	0.56
1:A:174:TRP:HE3	1:A:194:MET:HE2	1.70	0.56
1:B:148:LEU:O	1:B:151:PRO:HD2	2.05	0.56
1:C:203:ASP:OD1	1:C:206:ARG:NH1	2.39	0.56
1:E:361:ARG:O	1:E:365:ARG:HG3	2.05	0.56
1:G:135:LEU:HD21	1:G:375:CYS:SG	2.45	0.56
1:F:228:LEU:HD12	1:F:232:GLU:HB2	1.87	0.56
1:E:304:LEU:HD12	1:E:309:ILE:HD12	1.87	0.56
1:G:289:PRO:HG2	2:G:1407:HEM:HMB3	1.87	0.56
1:H:244:GLY:HA2	2:H:1407:HEM:C3C	2.41	0.56
1:G:171:PHE:CE2	1:G:241:LEU:HD13	2.41	0.56
1:I:360:ALA:HB1	2:I:1407:HEM:HAB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:LEU:O	1:J:245:HIS:HD2	1.89	0.56
1:P:336:ASP:O	1:P:339:ARG:HG2	2.06	0.56
1:I:244:GLY:HA2	2:I:1407:HEM:C2C	2.40	0.56
1:K:150:TRP:HE3	1:K:245:HIS:CE1	2.22	0.56
1:A:273:MET:HE3	1:A:276:LEU:HB2	1.87	0.56
1:B:150:TRP:CZ3	1:B:245[B]:HIS:CE1	2.94	0.56
1:H:60:ARG:HH22	1:H:305:ASP:HB2	1.70	0.56
1:O:227:ARG:HB3	1:O:227:ARG:CZ	2.35	0.56
1:B:255:GLY:HA2	1:B:283:MET:HG2	1.88	0.55
1:C:243:ALA:HB2	4:C:1410:17Q:H52C	1.87	0.55
1:H:328:ARG:NH1	1:H:342:ALA:O	2.39	0.55
1:D:150:TRP:HZ3	1:D:245:HIS:CE1	2.24	0.55
1:M:282:GLU:HG3	1:M:335:PHE:CE1	2.41	0.55
1:M:360:ALA:CB	2:M:1407:HEM:HAB	2.36	0.55
1:D:172:ARG:O	1:D:173:VAL:C	2.45	0.55
1:N:244:GLY:O	1:N:245:HIS:C	2.45	0.55
1:N:183:ASP:OD1	1:N:186:GLN:HB2	2.05	0.55
1:O:88:LEU:C	1:O:90:HIS:H	2.09	0.55
1:B:120:ARG:HG3	1:B:366:ILE:HD11	1.89	0.55
1:F:154:ILE:HD12	1:F:245[B]:HIS:CE1	2.42	0.55
1:F:265:GLN:NE2	1:F:337:ILE:HG12	2.21	0.55
1:P:93:LEU:HD13	2:P:1407:HEM:HAD2	1.87	0.55
1:C:243:ALA:CB	4:C:1410:17Q:H52C	2.37	0.55
1:G:52:VAL:HG21	1:G:316[B]:LEU:HD22	1.89	0.55
1:B:17:LEU:HB2	1:B:47:PRO:HD3	1.88	0.55
1:N:396:ARG:HG3	1:N:396:ARG:HH11	1.72	0.55
1:C:244:GLY:HA2	2:C:1407:HEM:HMC2	1.89	0.54
1:L:150:TRP:HZ3	1:L:245:HIS:NE2	1.89	0.54
1:N:375:CYS:HB3	1:N:378:LEU:HB2	1.89	0.54
1:O:22:GLN:HA	1:O:25:ALA:HB3	1.88	0.54
1:A:24:PHE:CE1	1:A:28:PRO:HB3	2.42	0.54
1:I:265:GLN:NE2	1:I:337:ILE:H	2.04	0.54
1:J:250:ASN:CB	1:J:289:PRO:HB3	2.36	0.54
1:O:35:LEU:O	1:O:42:HIS:NE2	2.40	0.54
1:P:259:LEU:HD21	1:P:269:LEU:HD23	1.89	0.54
1:B:11:SER:H	1:B:12:PRO:HD3	1.72	0.54
1:B:35:LEU:HD22	1:B:42:HIS:CG	2.43	0.54
1:B:88:LEU:HD21	1:B:195:SER:HB2	1.89	0.54
1:L:224:ASP:OD2	1:L:227:ARG:HG3	2.07	0.54
1:O:110:GLU:HG3	1:O:213:LEU:CD1	2.36	0.54
1:E:338:ARG:HG2	1:E:338:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:ASP:HB3	1:H:275:LEU:HD12	1.88	0.54
1:K:60:ARG:HD2	1:K:304:LEU:HD22	1.88	0.54
1:M:161:LEU:HD22	1:M:214:LEU:HD13	1.89	0.54
1:M:244:GLY:HA2	2:M:1407:HEM:C2C	2.42	0.54
1:B:10:ALA:HB1	1:B:53:TRP:HH2	1.71	0.54
1:B:265:GLN:NE2	1:B:337:ILE:HG12	2.23	0.54
1:G:228:LEU:HD12	1:G:232:GLU:HB3	1.90	0.54
1:E:265:GLN:HE21	1:E:337:ILE:HG12	1.72	0.54
1:B:149:ALA:O	1:B:249:VAL:HG13	2.08	0.54
1:J:375:CYS:HB2	1:J:378:LEU:HB2	1.90	0.54
1:M:23:ASP:OD1	1:M:23:ASP:N	2.33	0.54
1:O:31:THR:HG23	1:O:34:ARG:HH22	1.73	0.54
1:O:145:MET:HA	1:O:149:ALA:HB3	1.88	0.54
1:A:354:CYS:HB2	2:A:1407:HEM:NA	2.22	0.54
1:C:150:TRP:HZ3	1:C:245:HIS:NE2	2.06	0.54
1:C:150:TRP:CE2	1:C:172:ARG:HD2	2.43	0.54
1:H:382:VAL:HG11	1:H:402:PRO:HD2	1.90	0.54
1:L:93:LEU:HD11	2:L:1407:HEM:HBA1	1.90	0.54
1:O:15:LEU:HB3	1:O:44:VAL:HG12	1.90	0.54
1:E:60:ARG:HH22	1:E:305:ASP:HB2	1.73	0.54
1:H:265:GLN:NE2	1:H:337:ILE:H	2.05	0.54
1:J:48:GLU:CD	1:J:48:GLU:H	2.10	0.54
1:J:269:LEU:HD11	1:J:276:LEU:HA	1.90	0.54
1:M:148:LEU:C	1:M:151:PRO:HD2	2.28	0.54
1:A:174:TRP:CE3	1:A:194:MET:HE2	2.43	0.53
1:C:60:ARG:HD2	1:C:304:LEU:HD22	1.89	0.53
1:D:150:TRP:CH2	1:D:172:ARG:HB2	2.43	0.53
1:P:150:TRP:CE3	1:P:245:HIS:CE1	2.96	0.53
1:A:108:ALA:O	1:A:109:ARG:C	2.47	0.53
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.89	0.53
1:B:150:TRP:HE3	1:B:245[B]:HIS:HE2	1.56	0.53
1:L:71:SER:HB2	1:L:299:VAL:CG1	2.38	0.53
1:H:154:ILE:O	1:H:158:SER:HB2	2.07	0.53
1:J:238:HIS:CE1	1:J:242:VAL:HG21	2.44	0.53
2:O:1407:HEM:HBB2	2:O:1407:HEM:CMB	2.38	0.53
1:I:88:LEU:HD21	1:I:195:SER:HB2	1.90	0.53
1:B:148:LEU:C	1:B:151:PRO:HD2	2.29	0.53
1:J:61:ALA:HB1	1:J:317:VAL:HG13	1.91	0.53
1:K:73:ASP:OD2	1:K:75:ARG:NH2	2.42	0.53
1:M:29:TYR:CD1	1:M:324:ARG:HG3	2.44	0.53
1:M:265:GLN:HE21	1:M:337:ILE:HG12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:294:THR:OG1	2:P:1407:HEM:O1A	2.25	0.53
1:D:41:ALA:HA	1:D:54:LEU:O	2.09	0.53
1:E:11:SER:N	1:E:12:PRO:HD2	2.24	0.53
1:A:183:ASP:HB2	1:A:184:PRO:CD	2.39	0.52
1:B:122:ARG:NH2	1:B:159:GLU:OE2	2.42	0.52
1:B:273:MET:HE3	1:B:276:LEU:HB2	1.90	0.52
1:C:387:LEU:HD22	1:C:398:LEU:HD22	1.91	0.52
1:M:245:HIS:O	1:M:249:VAL:HG23	2.09	0.52
1:F:14:VAL:HG22	1:F:43:ARG:O	2.09	0.52
1:J:34:ARG:HD3	5:J:2006:HOH:O	2.09	0.52
1:D:144:LEU:HD11	1:D:371:LEU:HD11	1.90	0.52
1:G:180:PHE:O	1:G:182:ASP:N	2.42	0.52
1:G:338:ARG:HG2	1:G:338:ARG:HH11	1.75	0.52
1:I:145:MET:HA	1:I:149:ALA:HB3	1.90	0.52
1:M:78:THR:HG23	1:M:312:GLY:HA3	1.91	0.52
1:D:174:TRP:CE3	1:D:194:MET:HG3	2.45	0.52
1:I:241:LEU:O	1:I:245:HIS:HB3	2.10	0.52
1:I:244:GLY:HA2	2:I:1407:HEM:C3C	2.45	0.52
1:L:204:SER:O	1:L:208:GLN:HG3	2.10	0.52
1:P:174:TRP:HB3	1:P:194:MET:HE3	1.92	0.52
1:D:244:GLY:HA2	2:D:1407:HEM:CMC	2.39	0.52
1:O:78:THR:HG23	1:O:312:GLY:HA3	1.91	0.52
1:D:139:ASP:HB3	1:D:141:ARG:HB2	1.92	0.52
1:E:150:TRP:CD1	1:E:151:PRO:HD3	2.45	0.52
1:H:277:ASP:HB3	5:H:2027:HOH:O	2.08	0.52
1:I:251:LEU:HB2	1:I:289:PRO:HG3	1.91	0.52
1:B:165:GLU:HA	1:B:168:ARG:CD	2.34	0.52
1:C:148:LEU:C	1:C:151:PRO:HD2	2.30	0.52
1:G:273:MET:CE	1:G:276:LEU:HD22	2.39	0.52
1:A:273:MET:HE1	1:A:276:LEU:HD13	1.92	0.52
1:G:295:TYR:CE1	1:G:316[B]:LEU:HD11	2.45	0.52
1:H:17:LEU:HD22	1:H:24:PHE:CZ	2.45	0.52
1:O:152:LEU:HB3	1:O:153:PRO:HD3	1.93	0.52
1:J:126:ILE:HD13	1:J:155:THR:HG22	1.92	0.51
1:O:171:PHE:O	1:O:175:THR:HB	2.09	0.51
1:A:179:VAL:CG1	1:A:180:PHE:H	2.14	0.51
1:G:11:SER:HB2	1:G:12:PRO:HD3	1.91	0.51
1:G:60:ARG:HD2	1:G:304:LEU:HD22	1.92	0.51
1:K:260:LEU:HD23	1:K:266:LEU:HD22	1.91	0.51
1:N:149:ALA:O	1:N:249:VAL:HG22	2.10	0.51
1:P:150:TRP:CH2	1:P:172:ARG:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:THR:HG23	1:D:312:GLY:HA3	1.92	0.51
1:H:28:PRO:HB2	1:H:32:TYR:CE2	2.45	0.51
1:N:320:ALA:O	1:N:324:ARG:HG2	2.10	0.51
1:P:150:TRP:HE3	1:P:245:HIS:CE1	2.28	0.51
1:F:360:ALA:HB1	2:F:1407:HEM:HAB	1.92	0.51
1:N:58:TYR:CD2	1:N:328:ARG:HG2	2.46	0.51
1:N:295:TYR:HD1	1:N:316[A]:LEU:HD21	1.75	0.51
1:B:10:ALA:HB1	1:B:53:TRP:CH2	2.45	0.51
1:D:150:TRP:O	1:D:153:PRO:HD2	2.11	0.51
1:D:161:LEU:CD2	1:D:213:LEU:HD23	2.40	0.51
1:E:17:LEU:HA	1:E:20:LEU:HD12	1.92	0.51
1:D:47:PRO:HG2	1:D:393:PRO:HD3	1.92	0.51
1:D:289:PRO:HG2	2:D:1407:HEM:HMB3	1.92	0.51
1:F:171:PHE:O	1:F:175:THR:CG2	2.46	0.51
1:N:62:ARG:HH11	1:N:345:LEU:HD21	1.76	0.51
1:D:228:LEU:HD12	1:D:232:GLU:HB3	1.93	0.51
1:F:383:SER:C	1:F:385:GLY:H	2.13	0.51
1:L:152:LEU:HB3	1:L:153:PRO:HD3	1.92	0.51
1:I:150:TRP:CE3	1:I:245:HIS:HE1	2.28	0.51
1:K:295:TYR:CE2	1:K:314:THR:HG21	2.46	0.51
1:L:150:TRP:CZ3	1:L:245:HIS:CE1	2.98	0.51
1:O:150:TRP:CZ2	1:O:172:ARG:HB2	2.45	0.51
1:O:243:ALA:O	1:O:247:THR:OG1	2.25	0.51
1:A:378:LEU:HD12	1:A:404:ARG:O	2.11	0.51
1:E:228:LEU:CD1	1:E:232:GLU:HB3	2.41	0.51
1:E:244:GLY:HA2	2:E:1407:HEM:C3C	2.46	0.51
1:J:381:ASP:OD1	1:J:404:ARG:NH1	2.44	0.51
1:A:270:ARG:NH1	1:A:372:LEU:O	2.43	0.51
1:D:161:LEU:HD21	1:D:213:LEU:HD23	1.93	0.51
1:I:40:PRO:HG3	1:I:305:ASP:HB3	1.92	0.50
1:L:282:GLU:OE1	1:L:285:ARG:HB3	2.11	0.50
1:N:99:ARG:HG3	1:N:102:ARG:NH2	2.26	0.50
1:H:244:GLY:HA2	2:H:1407:HEM:C2C	2.46	0.50
1:P:40:PRO:HG3	1:P:305:ASP:HB3	1.92	0.50
1:M:325:THR:HG23	1:M:327:GLU:OE1	2.11	0.50
1:N:130:LEU:HD11	1:N:151:PRO:HB2	1.93	0.50
1:C:104:ARG:NH1	2:C:1407:HEM:O2D	2.44	0.50
1:N:77:SER:OG	1:N:78:THR:N	2.44	0.50
1:A:15:LEU:HD11	1:A:20:LEU:HD11	1.93	0.50
1:B:90:HIS:HB3	1:B:232:GLU:HG3	1.94	0.50
1:D:281:GLU:OE1	1:D:344:HIS:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:GLU:HB3	1:F:393:PRO:O	2.11	0.50
1:G:35:LEU:HB3	1:G:42:HIS:CD2	2.46	0.50
1:L:281:GLU:OE1	1:L:361:ARG:NH2	2.45	0.50
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.94	0.50
1:L:392:ASN:OD1	1:L:393:PRO:CD	2.58	0.50
1:D:244:GLY:HA2	2:D:1407:HEM:HBC2	1.93	0.50
1:K:135:LEU:HD21	1:K:375:CYS:SG	2.52	0.50
1:C:67:ASP:HB3	1:C:70:PHE:HD2	1.77	0.50
1:F:265:GLN:HE21	1:F:337:ILE:HG23	1.77	0.50
1:J:281:GLU:OE1	1:J:344:HIS:HE1	1.95	0.50
1:J:338:ARG:HG2	1:J:338:ARG:HH11	1.77	0.50
1:L:14:VAL:HG22	1:L:43:ARG:O	2.12	0.50
1:L:320:ALA:O	1:L:324:ARG:HG2	2.12	0.50
1:E:279:ALA:O	1:E:283:MET:HG3	2.12	0.50
1:F:154:ILE:CD1	1:F:245[B]:HIS:CE1	2.95	0.50
1:H:92:MET:O	1:H:95:SER:HB2	2.12	0.50
1:H:191:MET:O	1:H:195:SER:HB2	2.12	0.50
1:N:162:GLY:O	1:N:164:PRO:HD3	2.12	0.50
1:N:213:LEU:O	1:N:213:LEU:HG	2.12	0.50
1:D:344:HIS:CD2	1:D:346:ALA:H	2.29	0.49
1:M:120:ARG:HG3	1:M:366:ILE:HD11	1.94	0.49
1:C:121:PRO:HD2	5:C:2017:HOH:O	2.12	0.49
1:F:255:GLY:HA3	1:F:283:MET:SD	2.52	0.49
1:N:60:ARG:NH1	1:N:305:ASP:HB2	2.26	0.49
1:O:65:LEU:HG	1:O:317:VAL:HG11	1.93	0.49
1:C:47:PRO:HD2	1:C:393:PRO:HD3	1.92	0.49
1:J:60:ARG:NH2	1:J:305:ASP:HB2	2.27	0.49
1:J:250:ASN:HB2	1:J:289:PRO:CB	2.41	0.49
1:M:336:ASP:C	1:M:338:ARG:H	2.14	0.49
1:B:344:HIS:HD2	1:B:346:ALA:N	2.06	0.49
1:O:81:LEU:HD22	1:O:85:GLU:HB3	1.94	0.49
1:G:72:LYS:HB3	1:G:72:LYS:HZ2	1.77	0.49
1:G:161:LEU:HD12	1:G:241:LEU:HG	1.93	0.49
1:K:11:SER:CB	1:K:12:PRO:HD3	2.28	0.49
1:D:369:ARG:O	1:D:373:GLU:HG3	2.13	0.49
1:O:24:PHE:CD1	1:O:28:PRO:HA	2.47	0.49
1:F:34:ARG:NH1	5:F:2004:HOH:O	2.44	0.49
1:F:93:LEU:HD13	2:F:1407:HEM:HAD2	1.95	0.49
1:F:228:LEU:HD12	1:F:232:GLU:HB3	1.92	0.49
1:I:150:TRP:CD2	1:I:172:ARG:HD2	2.47	0.49
1:K:387:LEU:HD22	1:K:398:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:262:HIS:O	1:M:264:ASP:N	2.45	0.49
1:E:376:PRO:O	1:E:377:ASP:HB2	2.13	0.49
1:E:390:TYR:CE1	1:E:399:LYS:HG2	2.47	0.49
1:H:181:PRO:C	1:H:183:ASP:N	2.66	0.49
1:I:279:ALA:O	1:I:283:MET:HG3	2.13	0.49
1:J:298:PRO:HD2	1:J:312:GLY:H	1.78	0.49
1:D:157:ILE:HD12	1:D:160:LEU:HD23	1.94	0.49
1:N:144:LEU:HD23	1:N:401:LEU:HD23	1.95	0.49
1:B:175:THR:HG21	1:B:245[B]:HIS:CE1	2.48	0.49
1:E:244:GLY:HA2	2:E:1407:HEM:CAC	2.43	0.49
1:H:289:PRO:HG2	2:H:1407:HEM:HMB2	1.95	0.49
1:B:51:GLU:OE2	1:L:369:ARG:NH2	2.45	0.48
1:C:72:LYS:HE2	1:C:296:ARG:NH1	2.28	0.48
1:C:236:MET:O	1:C:239:ILE:HG22	2.12	0.48
1:C:260:LEU:HD21	1:C:378:LEU:HD23	1.94	0.48
1:E:67:ASP:HB3	1:E:70:PHE:HD2	1.76	0.48
1:E:152:LEU:HB3	1:E:153:PRO:HD3	1.95	0.48
1:E:243:ALA:O	2:E:1407:HEM:C4C	2.67	0.48
1:J:115:ARG:HD3	1:J:118:LEU:HD12	1.94	0.48
1:J:360:ALA:HB1	2:J:1407:HEM:CBB	2.43	0.48
1:K:279:ALA:O	1:K:283:MET:HG3	2.13	0.48
1:P:135:LEU:HD21	1:P:375:CYS:SG	2.53	0.48
1:B:245[B]:HIS:O	1:B:249:VAL:HG23	2.13	0.48
1:D:153:PRO:HG2	1:D:249:VAL:HG22	1.96	0.48
1:F:281:GLU:OE1	1:F:344:HIS:HE1	1.96	0.48
1:H:13:PRO:HG2	1:H:45:ARG:HH21	1.78	0.48
1:I:60:ARG:HD2	1:I:304:LEU:HD22	1.95	0.48
1:L:32:TYR:OH	1:L:291:GLU:OE2	2.29	0.48
1:O:265:GLN:HE21	1:O:336:ASP:HA	1.77	0.48
1:B:175:THR:HG21	1:B:245[B]:HIS:ND1	2.29	0.48
1:K:66:ALA:HB2	1:K:349:HIS:CD2	2.48	0.48
1:C:360:ALA:HB1	2:C:1407:HEM:HAB	1.95	0.48
1:D:66:ALA:HB2	1:D:349:HIS:CD2	2.48	0.48
1:E:183:ASP:OD1	1:E:183:ASP:N	2.32	0.48
1:M:201:LEU:O	1:M:204:SER:HB3	2.13	0.48
1:O:272:ASP:OD1	1:O:274:THR:HG23	2.13	0.48
1:B:270:ARG:HH22	1:B:378:LEU:HB3	1.77	0.48
1:E:29:TYR:CD1	1:E:324:ARG:HG3	2.48	0.48
1:F:150:TRP:CE3	1:F:245[A]:HIS:CE1	3.01	0.48
1:G:158:SER:O	1:G:162:GLY:N	2.47	0.48
1:N:244:GLY:HA2	2:N:1407:HEM:HMC3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:290:VAL:HB	1:N:319:LEU:HD12	1.94	0.48
1:J:145:MET:HA	1:J:149:ALA:HB3	1.95	0.48
1:J:295:TYR:CE1	1:J:316:LEU:HD21	2.49	0.48
1:G:180:PHE:HA	1:G:392[B]:ASN:HD21	1.79	0.48
1:G:257:TYR:CE1	1:G:387:LEU:HD11	2.49	0.48
1:I:295:TYR:CD1	1:I:316[B]:LEU:HD11	2.49	0.48
1:J:338:ARG:HG2	1:J:338:ARG:NH1	2.29	0.48
1:N:260:LEU:HD23	1:N:266:LEU:HD22	1.95	0.48
1:B:299:VAL:HG23	1:B:300:GLU:N	2.28	0.48
1:C:275:LEU:HD13	1:C:337:ILE:HD11	1.95	0.48
1:D:265:GLN:NE2	1:D:337:ILE:HG12	2.28	0.48
1:E:88:LEU:HD22	1:E:238:HIS:CG	2.49	0.48
1:L:243:ALA:C	1:L:245:HIS:N	2.66	0.48
1:M:43:ARG:HG2	1:M:53:TRP:CE2	2.49	0.48
1:O:88:LEU:O	1:O:90:HIS:N	2.46	0.48
1:H:251:LEU:HD22	1:H:284:LEU:HD21	1.95	0.47
1:O:282:GLU:HG2	1:O:336:ASP:C	2.34	0.47
1:P:13:PRO:HB3	1:P:43:ARG:HH11	1.79	0.47
1:A:370:ALA:O	1:A:374:ARG:HG3	2.13	0.47
1:B:281:GLU:HB3	1:B:341:THR:OG1	2.14	0.47
1:C:285:ARG:NH1	1:C:332:PRO:O	2.39	0.47
1:F:17:LEU:HD22	1:F:24:PHE:CZ	2.49	0.47
1:G:265:GLN:HE21	1:G:337:ILE:HG23	1.79	0.47
1:K:234:LEU:HD12	1:K:234:LEU:O	2.13	0.47
1:N:150:TRP:HE3	1:N:245:HIS:HE1	1.57	0.47
1:O:269:LEU:HD11	1:O:276:LEU:HA	1.95	0.47
1:P:214:LEU:O	1:P:218:VAL:HG23	2.14	0.47
1:D:89:ASN:CG	1:D:89:ASN:O	2.52	0.47
1:E:154:ILE:HD13	1:E:245:HIS:CD2	2.49	0.47
1:G:265:GLN:NE2	1:G:337:ILE:H	2.11	0.47
1:K:281:GLU:OE1	1:K:344:HIS:HE1	1.97	0.47
1:M:357:ALA:HB3	1:M:358:PRO:HD3	1.96	0.47
1:B:265:GLN:HE21	1:B:337:ILE:H	1.61	0.47
4:G:1410:17Q:H91C	4:G:1410:17Q:H72C	1.65	0.47
1:N:396:ARG:HH11	1:N:396:ARG:CG	2.27	0.47
1:A:107:VAL:O	1:A:110:GLU:HB2	2.13	0.47
1:A:127:VAL:O	1:A:131:VAL:HG23	2.14	0.47
1:B:98:PRO:O	1:B:99:ARG:C	2.53	0.47
1:C:339:ARG:HG3	1:C:341:THR:HG23	1.95	0.47
1:D:69:ARG:NH1	1:D:302:VAL:HG13	2.29	0.47
1:F:131:VAL:O	1:F:135:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:162:GLY:O	1:I:164:PRO:HD3	2.14	0.47
1:K:22:GLN:HE22	1:K:389:TRP:H	1.63	0.47
1:L:183:ASP:N	1:L:183:ASP:OD1	2.48	0.47
1:M:88:LEU:HD22	1:M:238:HIS:ND1	2.29	0.47
1:M:122:ARG:O	1:M:126:ILE:HG13	2.14	0.47
1:O:36:ARG:HH12	1:O:326:PRO:HD3	1.80	0.47
1:O:250:ASN:OD1	1:O:397:GLY:HA2	2.15	0.47
1:P:29:TYR:N	1:P:30:PRO:HD2	2.29	0.47
1:A:273:MET:CE	1:A:276:LEU:HD22	2.45	0.47
1:G:145:MET:HA	1:G:149:ALA:HB3	1.97	0.47
1:I:150:TRP:CE2	1:I:172:ARG:HD2	2.50	0.47
1:N:115:ARG:HA	1:N:115:ARG:HD3	1.77	0.47
1:A:62:ARG:NH2	3:A:1408:SO4:O4	2.40	0.47
1:A:381:ASP:O	1:A:382:VAL:CB	2.53	0.47
1:C:29:TYR:N	1:C:30:PRO:HD2	2.29	0.47
1:H:114:ARG:NH1	5:H:2017:HOH:O	2.47	0.47
1:H:127:VAL:HG21	1:H:366:ILE:HG22	1.97	0.47
1:I:381:ASP:O	1:I:382:VAL:CB	2.62	0.47
1:H:291:GLU:HB3	1:H:393:PRO:O	2.15	0.47
1:M:19:ALA:HB3	1:P:117:GLU:HG2	1.97	0.47
1:B:60:ARG:O	1:B:64:VAL:HG23	2.15	0.46
1:B:158:SER:HB3	1:B:168:ARG:NE	2.30	0.46
1:E:152:LEU:O	1:E:156:VAL:HG23	2.15	0.46
1:F:336:ASP:C	1:F:338:ARG:H	2.18	0.46
1:L:301:PRO:HD3	1:L:311:ALA:HB2	1.97	0.46
1:B:183:ASP:HB2	1:B:184:PRO:CD	2.45	0.46
1:B:241:LEU:O	1:B:245[A]:HIS:CE1	2.68	0.46
1:F:150:TRP:O	1:F:153:PRO:HD2	2.14	0.46
1:G:149:ALA:O	1:G:249:VAL:HG22	2.16	0.46
1:I:128:ASP:CA	1:I:374:ARG:HH12	2.09	0.46
1:K:187:ALA:O	1:K:190:ALA:HB3	2.15	0.46
1:M:282:GLU:HG2	1:M:336:ASP:C	2.36	0.46
1:N:13:PRO:O	1:N:15:LEU:N	2.48	0.46
1:N:281:GLU:HA	1:N:284:LEU:HD12	1.97	0.46
1:N:390:TYR:HA	1:N:391:PRO:HD3	1.77	0.46
1:O:36:ARG:NH1	1:O:326:PRO:HD3	2.30	0.46
1:A:344:HIS:CD2	1:A:346:ALA:HB3	2.51	0.46
1:G:150:TRP:CZ3	1:G:154:ILE:HG21	2.50	0.46
1:J:150:TRP:HZ3	1:J:245:HIS:CE1	2.33	0.46
1:K:267:ALA:HA	1:K:270:ARG:HB2	1.97	0.46
1:C:282:GLU:HG3	1:C:335:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:ASN:OD1	1:E:393:PRO:HD2	2.15	0.46
1:B:81:LEU:HD13	1:B:86:ALA:HA	1.96	0.46
1:P:171:PHE:O	1:P:175:THR:HB	2.15	0.46
1:J:183:ASP:OD1	1:J:183:ASP:N	2.49	0.46
1:L:298:PRO:HG2	1:L:309:ILE:HG22	1.98	0.46
1:N:150:TRP:CD1	1:N:151:PRO:HD3	2.51	0.46
1:A:123:VAL:O	1:A:127:VAL:HG23	2.16	0.46
1:B:179:VAL:CG1	1:B:180:PHE:N	2.73	0.46
1:C:82:THR:OG1	1:C:188:GLN:NE2	2.48	0.46
1:E:228:LEU:HD12	1:E:232:GLU:HB3	1.97	0.46
1:H:227:ARG:NH2	5:H:2025:HOH:O	2.48	0.46
1:I:354:CYS:HB2	2:I:1407:HEM:NA	2.30	0.46
1:J:122:ARG:NH2	1:J:159:GLU:OE2	2.48	0.46
1:K:301:PRO:HD3	1:K:311:ALA:HB2	1.97	0.46
1:P:35:LEU:HD13	1:P:42:HIS:HB2	1.98	0.46
1:P:279:ALA:O	1:P:283:MET:HG3	2.16	0.46
1:F:76:ASN:O	1:F:312:GLY:HA2	2.15	0.46
1:F:265:GLN:HE22	1:F:337:ILE:HG12	1.81	0.46
1:O:179:VAL:O	1:O:392:ASN:HB2	2.16	0.46
1:A:161:LEU:CD2	1:A:213:LEU:HB3	2.46	0.46
1:C:178:PHE:HZ	1:C:194:MET:CE	2.28	0.46
1:E:114:ARG:NH2	5:E:2018:HOH:O	2.48	0.46
1:K:161:LEU:CD1	1:K:241:LEU:HG	2.45	0.46
1:K:390:TYR:HA	1:K:391:PRO:HD3	1.81	0.46
1:M:248:THR:HA	2:M:1407:HEM:HBB1	1.98	0.46
1:P:203[A]:ASP:OD1	1:P:206:ARG:NH1	2.45	0.46
1:H:331:ASP:OD2	1:H:334:ARG:HD3	2.16	0.46
1:I:150:TRP:CE3	1:I:245:HIS:CE1	3.04	0.46
1:J:150:TRP:HB3	1:J:151:PRO:HD3	1.97	0.46
1:F:265:GLN:HE22	1:F:337:ILE:N	2.11	0.45
1:F:357:ALA:HB3	1:F:358:PRO:HD3	1.97	0.45
1:J:331:ASP:OD2	1:J:334:ARG:HD3	2.16	0.45
1:K:136:ALA:O	1:K:137:ALA:C	2.54	0.45
1:K:145:MET:HA	1:K:149:ALA:HB3	1.97	0.45
1:M:81:LEU:HD22	1:M:85:GLU:HB3	1.99	0.45
1:N:354:CYS:HB2	2:N:1407:HEM:NA	2.31	0.45
1:O:318:VAL:HG12	1:O:321:ASP:H	1.81	0.45
1:O:344:HIS:HD2	1:O:346:ALA:N	2.13	0.45
1:P:148:LEU:C	1:P:151:PRO:HD2	2.36	0.45
1:C:64:VAL:HG13	1:C:70:PHE:CD2	2.50	0.45
1:G:353:PHE:CE1	1:P:223:GLU:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:375:CYS:HA	1:H:376:PRO:HD2	1.74	0.45
1:K:148:LEU:C	1:K:151:PRO:HD2	2.36	0.45
1:P:231:GLU:O	1:P:234:LEU:HB3	2.16	0.45
1:F:150:TRP:CE3	1:F:245[A]:HIS:HE1	2.34	0.45
1:I:248:THR:O	1:I:249:VAL:C	2.53	0.45
1:J:148:LEU:HD23	1:J:371:LEU:HD21	1.99	0.45
1:J:152:LEU:HB3	1:J:153:PRO:HD3	1.99	0.45
1:A:131:VAL:O	1:A:135:LEU:HG	2.15	0.45
1:B:344:HIS:CD2	1:B:346:ALA:HB3	2.51	0.45
1:C:94:GLU:OE1	4:C:1410:17Q:H112	2.17	0.45
1:H:137:ALA:HA	1:H:138:PRO:HD3	1.85	0.45
1:D:11:SER:HB3	1:O:369:ARG:NH2	2.32	0.45
1:D:29:TYR:O	1:D:30:PRO:C	2.54	0.45
1:D:181:PRO:HA	1:D:186:GLN:OE1	2.17	0.45
1:H:40:PRO:HG3	1:H:305:ASP:HB3	1.99	0.45
1:K:141:ARG:HG3	1:K:404:ARG:HB3	1.99	0.45
1:L:110:GLU:HG3	1:L:213:LEU:HD13	1.98	0.45
1:N:303:ASP:HA	1:N:308:VAL:HA	1.99	0.45
1:A:48:GLU:CD	1:A:48:GLU:H	2.19	0.45
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.99	0.45
1:C:244:GLY:HA2	2:C:1407:HEM:C2C	2.51	0.45
1:C:352:HIS:O	1:C:353:PHE:C	2.55	0.45
1:H:344:HIS:CD2	1:H:346:ALA:H	2.35	0.45
1:L:29:TYR:HE1	1:L:320:ALA:HB1	1.82	0.45
1:N:252:ILE:O	1:N:256:MET:HB2	2.16	0.45
1:N:254:ASN:ND2	1:N:396:ARG:O	2.44	0.45
1:D:219:ARG:O	1:D:223:GLU:HG3	2.17	0.45
1:G:93:LEU:HD13	2:G:1407:HEM:HAD2	1.98	0.45
1:H:140:GLY:HA2	1:H:405:TRP:CE2	2.51	0.45
1:M:148:LEU:O	1:M:151:PRO:HD2	2.16	0.45
1:P:229:THR:OG1	1:P:232:GLU:HG3	2.17	0.45
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.98	0.45
1:D:153:PRO:HG2	1:D:249:VAL:CG2	2.47	0.45
1:D:324:ARG:HA	1:D:332:PRO:HB2	1.99	0.45
1:E:13:PRO:HA	1:E:43:ARG:O	2.17	0.45
1:F:29:TYR:N	1:F:30:PRO:CD	2.80	0.45
1:G:168:ARG:O	1:G:171:PHE:HB2	2.17	0.45
1:K:326:PRO:HA	1:K:329:PHE:O	2.17	0.45
1:N:150:TRP:CZ3	1:N:245:HIS:CE1	3.04	0.45
1:P:284:LEU:O	1:P:346:ALA:HB2	2.15	0.45
1:J:202:ILE:HD13	1:J:233:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:390:TYR:HA	1:J:391:PRO:HD3	1.84	0.45
1:O:107:VAL:HG23	1:O:355:ILE:CD1	2.46	0.45
1:O:197:TYR:HA	1:O:200:ARG:NH2	2.32	0.45
1:H:52:VAL:HG12	1:H:314:THR:HB	2.00	0.45
1:J:150:TRP:CZ3	1:J:245:HIS:CE1	3.05	0.45
1:M:228:LEU:HD12	1:M:232:GLU:HB2	1.99	0.45
1:N:73:ASP:HB3	1:N:76:ASN:ND2	2.32	0.45
1:N:388:VAL:HG23	1:N:399:LYS:HB2	1.99	0.45
1:P:245:HIS:O	1:P:249:VAL:HG23	2.17	0.45
1:P:324:ARG:HA	1:P:324:ARG:HD3	1.64	0.45
1:A:41:ALA:HA	1:A:54:LEU:O	2.17	0.44
1:K:53:TRP:HB2	1:K:315:VAL:HG22	1.99	0.44
1:M:11:SER:N	1:M:12:PRO:HD2	2.32	0.44
1:O:36:ARG:HA	1:O:56:VAL:HG21	1.99	0.44
1:P:92:MET:O	1:P:100:HIS:HD2	2.00	0.44
1:P:110:GLU:HG3	1:P:213:LEU:HD13	1.99	0.44
1:E:64:VAL:O	1:E:65:LEU:C	2.56	0.44
1:E:78:THR:HG23	1:E:312:GLY:HA3	1.98	0.44
1:E:150:TRP:HD1	1:E:151:PRO:HD3	1.81	0.44
1:E:344:HIS:CD2	1:E:346:ALA:H	2.17	0.44
1:F:66:ALA:HB2	1:F:349:HIS:CD2	2.52	0.44
1:J:281:GLU:HA	1:J:284:LEU:HD12	1.98	0.44
1:K:204:SER:O	1:K:208:GLN:HG3	2.17	0.44
1:K:273:MET:CE	1:K:276:LEU:HD22	2.48	0.44
1:M:40:PRO:HG3	1:M:305:ASP:CB	2.44	0.44
1:A:22:GLN:HE22	1:A:389:TRP:H	1.66	0.44
1:A:251:LEU:HD13	1:A:284:LEU:CD2	2.47	0.44
1:B:46:THR:OG1	1:B:50:ASN:N	2.50	0.44
1:G:344:HIS:CD2	1:G:346:ALA:HB3	2.52	0.44
1:I:243:ALA:C	1:I:245:HIS:H	2.20	0.44
1:J:48:GLU:CD	1:J:48:GLU:N	2.71	0.44
1:L:25:ALA:HB2	1:L:391:PRO:HA	1.99	0.44
1:M:272:ASP:OD1	1:M:274:THR:OG1	2.36	0.44
1:N:150:TRP:CE3	1:N:245:HIS:CE1	3.01	0.44
2:N:1407:HEM:HMC1	2:N:1407:HEM:CBC	2.45	0.44
1:P:145:MET:HA	1:P:149:ALA:HB3	1.99	0.44
1:F:180:PHE:O	1:F:180:PHE:CG	2.70	0.44
1:G:265:GLN:HE21	1:G:337:ILE:HG12	1.83	0.44
1:G:354:CYS:HA	2:G:1407:HEM:CHA	2.48	0.44
1:I:152:LEU:HB3	1:I:153:PRO:HD3	1.98	0.44
1:K:273:MET:HE2	1:K:369:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:VAL:HG11	1:L:390:TYR:CD2	2.52	0.44
1:M:17:LEU:HD22	1:M:24:PHE:CE1	2.53	0.44
1:M:202:ILE:HD13	1:M:233:LEU:HG	1.99	0.44
1:M:344:HIS:CD2	1:M:344:HIS:C	2.90	0.44
1:O:202:ILE:HD13	1:O:233:LEU:HG	1.98	0.44
1:O:381:ASP:O	1:O:382:VAL:CB	2.65	0.44
1:D:344:HIS:CD2	1:D:344:HIS:C	2.91	0.44
1:E:298:PRO:HG2	1:E:309:ILE:HG22	2.00	0.44
1:H:172:ARG:O	1:H:175:THR:HG22	2.18	0.44
1:H:244:GLY:HA2	2:H:1407:HEM:CAC	2.47	0.44
1:O:72:LYS:HD3	1:O:93:LEU:O	2.18	0.44
1:O:107:VAL:HG23	1:O:355:ILE:HD13	1.99	0.44
1:A:136:ALA:HB2	1:M:268:ALA:HA	2.00	0.44
1:G:72:LYS:HB3	1:G:72:LYS:HZ3	1.82	0.44
1:H:99:ARG:HG3	1:H:102:ARG:HH21	1.82	0.44
1:L:58:TYR:C	1:L:58:TYR:CD1	2.90	0.44
1:L:175:THR:O	1:L:179:VAL:HG23	2.17	0.44
1:F:60:ARG:HH12	1:F:305:ASP:HB2	1.81	0.44
1:F:145:MET:HA	1:F:149:ALA:HB3	1.99	0.44
1:G:146:GLU:OE2	1:G:172:ARG:NH1	2.50	0.44
1:G:265:GLN:HE22	1:G:337:ILE:HG12	1.81	0.44
1:I:28:PRO:HB2	1:I:32:TYR:CE2	2.52	0.44
1:J:295:TYR:HD1	1:J:316:LEU:CD2	2.29	0.44
1:M:134:MET:HG3	1:M:147:SER:HB3	2.00	0.44
1:O:92:MET:O	1:O:100:HIS:HD2	2.01	0.44
1:O:250:ASN:O	1:O:251:LEU:C	2.56	0.44
1:P:356:GLY:HA3	2:P:1407:HEM:C3C	2.53	0.44
1:P:392:ASN:HA	1:P:393:PRO:HD3	1.70	0.44
1:B:76:ASN:O	1:B:312:GLY:HA2	2.18	0.44
1:B:336:ASP:C	1:B:336:ASP:OD1	2.55	0.44
1:G:120:ARG:HB3	1:G:121:PRO:HD3	1.99	0.44
1:G:144:LEU:HD21	1:G:256:MET:HG3	2.00	0.44
1:M:203:ASP:O	1:M:204:SER:C	2.56	0.44
1:O:28:PRO:HB2	1:O:32:TYR:CE2	2.53	0.44
1:B:150:TRP:HZ3	1:B:245[B]:HIS:CE1	2.35	0.44
1:B:344:HIS:CD2	1:B:346:ALA:H	2.25	0.44
1:I:144:LEU:HB3	1:I:401:LEU:HB3	2.00	0.44
1:L:71:SER:HB2	1:L:299:VAL:HG13	1.98	0.44
1:N:382:VAL:HG22	1:N:383:SER:H	1.83	0.44
1:O:183:ASP:OD1	1:O:186:GLN:N	2.51	0.44
1:B:72:LYS:HE2	1:B:296:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:THR:HG21	1:D:246:GLU:HG2	2.00	0.43
1:G:239:ILE:HD11	4:G:1410:17Q:H51C	2.00	0.43
1:G:321:ASP:O	1:G:322:ALA:C	2.57	0.43
1:K:156:VAL:HG12	1:K:157:ILE:N	2.33	0.43
1:L:28:PRO:HB2	1:L:32:TYR:CE2	2.53	0.43
1:L:371:LEU:O	1:L:375:CYS:HB2	2.17	0.43
1:M:282:GLU:HG3	1:M:335:PHE:CD1	2.53	0.43
1:N:251:LEU:HD22	2:N:1407:HEM:HBB1	2.00	0.43
1:O:265:GLN:NE2	1:O:336:ASP:HA	2.32	0.43
1:C:29:TYR:CE1	1:C:320:ALA:HB1	2.53	0.43
1:P:252:ILE:H	1:P:252:ILE:HG13	1.65	0.43
1:B:219:ARG:O	1:B:223:GLU:HG3	2.18	0.43
1:C:152:LEU:CB	1:C:153:PRO:HD3	2.48	0.43
1:F:161:LEU:O	1:F:214:LEU:HB2	2.19	0.43
1:G:71:SER:CB	1:G:76:ASN:HD22	2.31	0.43
1:P:64:VAL:HG13	1:P:70:PHE:CD2	2.54	0.43
1:P:157:ILE:HG13	1:P:161:LEU:HD12	2.00	0.43
1:B:251:LEU:HB2	2:B:1407:HEM:HBB1	2.00	0.43
1:F:273:MET:HG3	1:F:373:GLU:OE2	2.19	0.43
1:N:186:GLN:O	1:N:189:THR:HB	2.18	0.43
1:A:134:MET:CE	1:A:403:ILE:HD11	2.49	0.43
1:B:360:ALA:CB	2:B:1407:HEM:HAB	2.49	0.43
1:F:152:LEU:HB3	1:F:153:PRO:HD3	2.01	0.43
1:H:140:GLY:HA2	1:H:405:TRP:CZ2	2.53	0.43
1:I:108:ALA:HA	1:I:355:ILE:HD11	2.01	0.43
1:M:293:ALA:O	1:M:316:LEU:HD22	2.18	0.43
1:M:381:ASP:CG	1:M:381:ASP:O	2.56	0.43
1:M:390:TYR:CZ	1:M:399:LYS:HG2	2.54	0.43
1:O:88:LEU:C	1:O:90:HIS:N	2.72	0.43
1:O:205:LYS:HD2	1:O:214:LEU:HD23	1.99	0.43
1:B:328:ARG:O	1:B:328:ARG:NH1	2.46	0.43
1:L:244:GLY:HA2	2:L:1407:HEM:HMC3	2.01	0.43
1:B:51:GLU:OE2	1:L:369:ARG:CZ	2.66	0.43
1:G:50[A]:ASN:N	1:G:50[A]:ASN:ND2	2.66	0.43
1:H:145:MET:O	1:H:150:TRP:HB3	2.18	0.43
1:H:344:HIS:CD2	1:H:344:HIS:C	2.92	0.43
1:N:30:PRO:O	1:N:34:ARG:HB2	2.19	0.43
1:O:183:ASP:C	1:O:185:ALA:H	2.21	0.43
1:P:300:GLU:O	1:P:302:VAL:HG23	2.19	0.43
1:A:130:LEU:O	1:A:134:MET:HB2	2.18	0.43
4:C:1410:17Q:H11C	4:C:1410:17Q:H42C	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:LEU:O	1:E:123:VAL:HG23	2.19	0.43
1:F:218:VAL:HG22	1:F:233:LEU:HD21	2.01	0.43
1:G:228:LEU:HD12	1:G:232:GLU:CB	2.49	0.43
1:I:136:ALA:O	1:I:137:ALA:C	2.57	0.43
1:K:44:VAL:HG11	1:K:54:LEU:HD12	2.00	0.43
1:O:178:PHE:HB3	1:O:187:ALA:CB	2.48	0.43
1:E:270:ARG:NH1	1:E:372:LEU:O	2.45	0.43
1:J:91:ASN:OD1	1:J:239:ILE:HD13	2.18	0.43
1:J:165:GLU:N	1:J:166:PRO:CD	2.81	0.43
1:N:396:ARG:CG	1:N:396:ARG:NH1	2.81	0.43
1:A:82:THR:HG23	1:A:85:GLU:OE1	2.19	0.43
1:E:41:ALA:HA	1:E:54:LEU:O	2.19	0.43
1:E:176:ASP:O	1:E:177:ALA:C	2.57	0.43
1:F:160:LEU:HD12	1:F:160:LEU:HA	1.86	0.43
1:G:53:TRP:CD1	1:G:309:ILE:HG23	2.54	0.43
1:I:60:ARG:HH11	1:I:304:LEU:HD22	1.84	0.43
1:P:337:ILE:O	5:P:2016:HOH:O	2.22	0.43
1:A:76:ASN:O	1:A:312:GLY:HA2	2.19	0.42
1:A:77:SER:HB2	1:A:297:PHE:CE2	2.54	0.42
1:A:145:MET:HA	1:A:149:ALA:HB3	2.01	0.42
1:B:273:MET:HE2	1:B:369:ARG:HD2	1.99	0.42
1:I:285:ARG:O	1:I:323:HIS:HB3	2.19	0.42
1:K:244:GLY:O	1:K:245:HIS:C	2.58	0.42
1:M:139:ASP:O	1:M:141:ARG:HG3	2.19	0.42
1:N:67:ASP:OD1	1:N:69:ARG:N	2.52	0.42
1:O:178:PHE:HB3	1:O:187:ALA:HB1	2.00	0.42
1:B:20:LEU:HB3	1:B:24:PHE:HB2	2.00	0.42
1:C:150:TRP:CZ3	1:C:245:HIS:HE1	2.29	0.42
1:D:114:ARG:NH1	1:D:114:ARG:HG2	2.34	0.42
1:D:114:ARG:HG2	1:D:114:ARG:HH11	1.84	0.42
1:E:48:GLU:CD	1:E:48:GLU:H	2.22	0.42
1:G:245:HIS:CE1	5:G:2042:HOH:O	2.72	0.42
1:I:132:ASP:OD1	1:I:374:ARG:NH2	2.51	0.42
1:K:95:SER:HB3	1:K:99:ARG:HB3	2.00	0.42
1:K:316[B]:LEU:N	1:K:316[B]:LEU:CD1	2.80	0.42
1:L:148:LEU:C	1:L:151:PRO:HD2	2.39	0.42
1:P:251:LEU:HD22	2:P:1407:HEM:HBB1	2.01	0.42
1:A:161:LEU:HD21	1:A:213:LEU:HD23	2.01	0.42
1:D:82:THR:OG1	1:D:188:GLN:NE2	2.51	0.42
1:D:218:VAL:HG22	1:D:233:LEU:HD21	2.02	0.42
1:F:67:ASP:C	1:F:67:ASP:OD1	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:282:GLU:OE1	1:J:282:GLU:HA	2.20	0.42
1:L:148:LEU:O	1:L:151:PRO:HD2	2.18	0.42
1:N:60:ARG:HH12	1:N:305:ASP:HB2	1.84	0.42
1:P:288:GLY:HA2	1:P:289:PRO:HD3	1.88	0.42
1:A:344:HIS:HD2	1:A:346:ALA:H	1.68	0.42
1:B:108:ALA:HA	1:B:355:ILE:HD11	2.01	0.42
1:B:360:ALA:HB1	2:B:1407:HEM:HAB	2.00	0.42
1:C:68:PRO:HA	5:C:2002:HOH:O	2.19	0.42
1:C:78:THR:HG23	1:C:312:GLY:HA3	2.01	0.42
1:D:139:ASP:CB	1:D:141:ARG:HB2	2.49	0.42
1:E:174:TRP:O	1:E:177:ALA:HB3	2.20	0.42
1:F:168:ARG:O	1:F:171:PHE:HB2	2.19	0.42
1:J:219:ARG:O	1:J:223:GLU:HG3	2.19	0.42
1:K:60:ARG:O	1:K:64:VAL:HG23	2.19	0.42
1:K:277:ASP:OD1	1:K:365:ARG:HD3	2.19	0.42
1:C:175:THR:CG2	1:C:176:ASP:N	2.82	0.42
1:D:119:LEU:O	1:D:120:ARG:C	2.57	0.42
1:D:325:THR:HA	1:D:326:PRO:HD3	1.94	0.42
1:E:280:VAL:HA	1:E:283:MET:HG3	2.01	0.42
1:J:57:GLY:N	1:J:321:ASP:OD2	2.50	0.42
1:J:61:ALA:HB1	1:J:317:VAL:CG1	2.50	0.42
1:M:150:TRP:O	1:M:153:PRO:HD2	2.20	0.42
1:F:382:VAL:HG22	1:F:383:SER:H	1.84	0.42
1:J:60:ARG:NH1	1:J:305:ASP:HB2	2.35	0.42
1:M:370:ALA:O	1:M:374:ARG:HG3	2.20	0.42
1:P:58:TYR:CD1	1:P:58:TYR:C	2.92	0.42
1:A:168:ARG:O	1:A:171:PHE:HB2	2.19	0.42
1:B:90:HIS:O	1:B:232:GLU:HA	2.19	0.42
1:B:119:LEU:O	1:B:123:VAL:HG23	2.19	0.42
1:C:376:PRO:O	1:C:377:ASP:HB2	2.19	0.42
1:D:115:ARG:HD3	1:D:115:ARG:HA	1.77	0.42
1:D:168:ARG:O	1:D:171:PHE:HB2	2.20	0.42
1:E:203[B]:ASP:OD1	1:E:203[B]:ASP:O	2.37	0.42
1:F:122:ARG:HA	1:F:122:ARG:HD2	1.92	0.42
1:G:60:ARG:HH11	1:G:304:LEU:HD22	1.85	0.42
1:G:243:ALA:HB2	4:G:1410:17Q:H41C	2.00	0.42
1:H:175:THR:O	1:H:179:VAL:HG23	2.20	0.42
1:I:251:LEU:CB	2:I:1407:HEM:HBB1	2.50	0.42
1:J:150:TRP:CZ2	1:J:172:ARG:HB2	2.55	0.42
1:J:197:TYR:OH	1:J:201:LEU:HD13	2.19	0.42
1:K:175:THR:C	1:K:177:ALA:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:164:PRO:HB2	1:L:166:PRO:HD2	2.02	0.42
1:N:161:LEU:HD21	1:N:213:LEU:HD23	2.01	0.42
1:O:259:LEU:O	1:O:266:LEU:HB2	2.20	0.42
1:E:241:LEU:O	1:E:245:HIS:HB2	2.19	0.42
1:F:144:LEU:HD23	1:F:401:LEU:HD23	2.02	0.42
1:H:360:ALA:O	1:H:361:ARG:C	2.56	0.42
1:I:74:TRP:CD2	1:I:81:LEU:HD21	2.55	0.42
1:L:92:MET:O	1:L:100:HIS:HD2	2.02	0.42
1:M:61:ALA:O	1:M:65:LEU:HG	2.19	0.42
1:M:203:ASP:N	1:M:203:ASP:OD1	2.53	0.42
1:N:392:ASN:HA	1:N:393:PRO:HD2	1.92	0.42
1:E:46:THR:HB	1:E:48:GLU:OE2	2.19	0.42
1:F:11:SER:CB	1:F:12:PRO:CD	2.94	0.42
1:H:67:ASP:OD1	1:H:68:PRO:HD2	2.20	0.42
1:K:60:ARG:HH21	1:K:305:ASP:HB2	1.83	0.42
1:K:273:MET:HE1	1:K:276:LEU:HD22	2.02	0.42
1:L:339:ARG:HG3	1:L:341:THR:HG22	2.01	0.42
1:C:243:ALA:HB2	4:C:1410:17Q:C5	2.50	0.42
1:C:344:HIS:CD2	1:C:344:HIS:C	2.94	0.42
1:F:150:TRP:HZ3	1:F:245[A]:HIS:HE1	1.65	0.42
1:H:260:LEU:HD23	1:H:260:LEU:HA	1.87	0.42
1:J:60:ARG:HH22	1:J:305:ASP:HB2	1.85	0.42
1:K:154:ILE:HD12	1:K:154:ILE:HA	1.86	0.42
1:L:67:ASP:HA	1:L:68:PRO:HD3	1.94	0.42
1:P:67:ASP:HA	1:P:68:PRO:HD3	1.77	0.42
1:A:202:ILE:HG23	1:A:218:VAL:HG22	2.02	0.41
1:A:265:GLN:NE2	1:A:337:ILE:H	2.18	0.41
1:B:289:PRO:HG2	2:B:1407:HEM:HMB3	2.02	0.41
1:B:361:ARG:HD3	1:B:365:ARG:NH2	2.35	0.41
1:G:154:ILE:HD12	1:G:154:ILE:HA	1.93	0.41
1:H:110:GLU:HB2	1:H:111:PHE:CD2	2.55	0.41
1:P:25:ALA:CB	1:P:391:PRO:HA	2.50	0.41
1:A:160:LEU:O	1:A:161:LEU:HD23	2.20	0.41
1:C:392:ASN:O	5:C:2038:HOH:O	2.21	0.41
2:H:1407:HEM:HMB2	2:H:1407:HEM:CBB	2.49	0.41
1:B:144:LEU:HD13	1:B:403:ILE:HD13	2.01	0.41
1:B:299:VAL:HG23	1:B:300:GLU:H	1.84	0.41
1:D:98:PRO:HD2	5:D:2017:HOH:O	2.19	0.41
1:G:77:SER:HB2	1:G:297:PHE:CE1	2.55	0.41
1:G:120:ARG:HG3	1:G:366:ILE:HD11	2.02	0.41
1:K:310:PRO:HB2	1:K:313:ASP:OD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:60:ARG:HD3	1:M:60:ARG:HA	1.85	0.41
1:M:104:ARG:NH1	2:M:1407:HEM:O2D	2.53	0.41
1:N:265:GLN:NE2	1:N:337:ILE:H	2.18	0.41
1:A:99:ARG:HG3	1:A:102:ARG:NH2	2.35	0.41
1:B:60:ARG:HA	1:B:60:ARG:HD3	1.89	0.41
1:D:67:ASP:HA	1:D:68:PRO:HD2	1.90	0.41
1:E:175:THR:HG22	1:E:176:ASP:N	2.35	0.41
1:F:292:SER:HB2	1:F:394:MET:HA	2.02	0.41
1:G:257:TYR:CE1	1:G:387:LEU:CD1	3.04	0.41
1:G:392[A]:ASN:OD1	1:G:394:MET:HB2	2.20	0.41
1:J:126:ILE:HD13	1:J:155:THR:CG2	2.49	0.41
1:K:124:GLN:HA	1:K:366:ILE:HG21	2.02	0.41
1:L:29:TYR:CE1	1:L:320:ALA:HB1	2.55	0.41
1:L:67:ASP:OD2	1:L:69:ARG:NH2	2.49	0.41
1:A:236:MET:HA	1:A:239:ILE:HG22	2.01	0.41
1:C:135:LEU:HD21	1:C:375:CYS:SG	2.61	0.41
1:E:244:GLY:HA2	2:E:1407:HEM:C2C	2.55	0.41
1:I:135:LEU:HA	1:I:405:TRP:CZ2	2.56	0.41
1:I:265:GLN:HE21	1:I:337:ILE:HG23	1.85	0.41
1:L:202:ILE:HD13	1:L:233:LEU:HG	2.02	0.41
1:M:36:ARG:HH21	1:M:321:ASP:CG	2.23	0.41
1:O:398:LEU:HD13	1:O:401:LEU:HB2	2.02	0.41
1:C:24:PHE:O	1:C:25:ALA:C	2.59	0.41
1:D:13:PRO:HA	1:D:43:ARG:HB3	2.01	0.41
1:D:150:TRP:CE2	1:D:172:ARG:HD2	2.55	0.41
1:D:390:TYR:HA	1:D:391:PRO:HD3	1.80	0.41
1:F:250:ASN:O	1:F:254:ASN:HB2	2.20	0.41
1:F:356:GLY:O	1:F:357:ALA:C	2.59	0.41
1:H:99:ARG:HG3	1:H:102:ARG:NH2	2.35	0.41
1:I:356:GLY:O	1:I:357:ALA:C	2.59	0.41
1:J:352:HIS:O	1:J:353:PHE:C	2.59	0.41
1:L:111:PHE:CE1	2:L:1407:HEM:HBC1	2.55	0.41
1:L:328:ARG:NH2	1:L:343:GLY:HA3	2.36	0.41
1:M:122:ARG:HE	1:M:126:ILE:HD11	1.85	0.41
1:N:150:TRP:CH2	1:N:172:ARG:HB2	2.55	0.41
1:O:224:ASP:OD2	1:O:227:ARG:HG3	2.21	0.41
1:O:329:PHE:HA	1:O:330:PRO:HD3	1.94	0.41
1:C:239:ILE:O	1:C:243:ALA:HB3	2.20	0.41
1:D:309:ILE:HA	1:D:310:PRO:HD3	1.91	0.41
1:F:150:TRP:HE3	1:F:245[A]:HIS:CE1	2.38	0.41
1:H:265:GLN:HE21	1:H:337:ILE:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:LEU:HD12	1:K:160:LEU:HA	1.85	0.41
1:K:224:ASP:OD2	1:K:227:ARG:HG3	2.20	0.41
1:M:76:ASN:O	1:M:312:GLY:HA2	2.19	0.41
1:P:74:TRP:C	1:P:76:ASN:H	2.24	0.41
1:A:137:ALA:HA	1:A:138:PRO:HD3	1.93	0.41
1:F:344:HIS:CD2	1:F:346:ALA:HB3	2.56	0.41
1:G:223:GLU:O	3:O:1409:SO4:O2	2.38	0.41
1:G:309:ILE:HA	1:G:310:PRO:HD3	1.93	0.41
1:H:150:TRP:CE2	1:H:172:ARG:HD2	2.56	0.41
1:J:10:ALA:O	1:J:43:ARG:HG3	2.20	0.41
1:J:255:GLY:CA	1:J:283:MET:HG2	2.50	0.41
1:O:135:LEU:HA	1:O:405:TRP:CZ2	2.56	0.41
1:A:260:LEU:HD21	1:A:378:LEU:HD23	2.03	0.41
1:D:88:LEU:HD22	1:D:238:HIS:CG	2.55	0.41
1:D:175:THR:C	1:D:177:ALA:N	2.75	0.41
1:D:361:ARG:O	1:D:365:ARG:CG	2.57	0.41
2:D:1407:HEM:HMB1	2:D:1407:HEM:HBB2	2.03	0.41
1:F:229:THR:O	1:F:232:GLU:N	2.52	0.41
1:G:392[B]:ASN:OD1	1:G:392[B]:ASN:N	2.54	0.41
1:H:13:PRO:HA	1:H:43:ARG:HB3	2.02	0.41
1:H:108:ALA:HA	1:H:355:ILE:HD11	2.03	0.41
1:H:150:TRP:HA	1:H:249:VAL:HG22	2.02	0.41
1:I:243:ALA:O	1:I:245:HIS:N	2.50	0.41
1:J:244:GLY:HA2	2:J:1407:HEM:C2C	2.56	0.41
1:K:104:ARG:NH1	2:K:1407:HEM:O2D	2.53	0.41
1:L:203[A]:ASP:HA	1:L:206:ARG:NH1	2.36	0.41
1:M:322:ALA:CB	1:M:345:LEU:HD12	2.51	0.41
1:M:390:TYR:CE1	1:M:399:LYS:HG2	2.56	0.41
1:P:58:TYR:O	1:P:61:ALA:HB3	2.21	0.41
1:P:156:VAL:HG11	1:P:363:GLU:OE2	2.21	0.41
1:D:154:ILE:HD12	1:D:154:ILE:HA	1.92	0.41
1:D:381:ASP:CG	1:D:381:ASP:O	2.58	0.41
1:D:382:VAL:HG22	1:D:383:SER:N	2.36	0.41
1:G:240:LEU:HD23	1:G:240:LEU:HA	1.93	0.41
1:H:143:ASP:O	1:H:147:SER:HB2	2.21	0.41
1:L:154:ILE:HD13	1:L:245:HIS:CE1	2.56	0.41
1:L:269:LEU:HD12	1:L:269:LEU:HA	1.89	0.41
1:L:390:TYR:HA	1:L:391:PRO:HD3	1.80	0.41
1:M:122:ARG:NE	1:M:126:ILE:HD11	2.36	0.41
1:N:32:TYR:HB3	1:N:321:ASP:OD2	2.21	0.41
1:O:12:PRO:HA	1:O:13:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:131:VAL:HG11	1:O:374:ARG:HD3	2.03	0.41
1:B:127:VAL:HG23	1:B:152:LEU:HD13	2.03	0.40
1:D:89:ASN:ND2	5:D:2014:HOH:O	2.52	0.40
1:E:82:THR:HG23	1:E:85:GLU:OE1	2.21	0.40
1:G:289:PRO:HG3	2:G:1407:HEM:HBB2	2.02	0.40
1:I:52:VAL:HG12	1:I:314:THR:HB	2.03	0.40
1:I:157:ILE:HD12	1:I:157:ILE:HA	1.91	0.40
1:J:41:ALA:HA	1:J:54:LEU:O	2.21	0.40
1:N:12:PRO:HA	1:N:13:PRO:HD3	1.79	0.40
1:N:60:ARG:HH12	1:N:305:ASP:N	2.19	0.40
1:P:265:GLN:NE2	1:P:337:ILE:H	2.19	0.40
1:B:78:THR:HG23	1:B:312:GLY:HA3	2.03	0.40
1:C:265:GLN:HE21	1:C:337:ILE:HG12	1.81	0.40
1:C:319:LEU:N	1:C:319:LEU:HD23	2.36	0.40
1:D:171:PHE:HE1	1:D:197:TYR:CE2	2.39	0.40
1:G:239:ILE:CD1	4:G:1410:17Q:H51C	2.52	0.40
1:I:158:SER:O	1:I:162:GLY:N	2.51	0.40
1:I:181:PRO:O	1:I:182:ASP:C	2.59	0.40
1:K:295:TYR:CD2	1:K:314:THR:CG2	3.05	0.40
1:L:92:MET:CE	1:L:104:ARG:HA	2.52	0.40
1:M:165:GLU:HA	1:M:168:ARG:HD2	2.01	0.40
1:P:262:HIS:HB3	1:P:265:GLN:HG3	2.04	0.40
1:D:364:ALA:O	1:D:368:VAL:HG23	2.21	0.40
1:E:99:ARG:HG3	1:E:102:ARG:HH21	1.86	0.40
1:F:11:SER:HB2	1:F:12:PRO:CD	2.41	0.40
1:F:157:ILE:HD12	1:F:157:ILE:HA	1.84	0.40
1:F:228:LEU:CD1	1:F:232:GLU:HB3	2.51	0.40
1:G:295:TYR:CD1	1:G:316[B]:LEU:HD11	2.55	0.40
1:H:177:ALA:CB	1:H:190:ALA:HB2	2.52	0.40
1:K:295:TYR:CD2	1:K:314:THR:HG23	2.56	0.40
1:L:116:VAL:HG13	1:L:362:LEU:HD22	2.02	0.40
1:M:381:ASP:HB2	1:M:404:ARG:HG2	2.03	0.40
1:O:269:LEU:HD23	1:O:372:LEU:HD22	2.03	0.40
1:A:171:PHE:CE2	1:A:194:MET:HE1	2.56	0.40
1:C:390:TYR:HA	1:C:391:PRO:HD3	1.87	0.40
1:D:157:ILE:HD12	1:D:157:ILE:HA	1.94	0.40
2:D:1407:HEM:HBB2	2:D:1407:HEM:CMB	2.51	0.40
1:F:294:THR:HA	1:F:394:MET:HE1	2.04	0.40
1:G:228:LEU:CD1	1:G:232:GLU:HB3	2.50	0.40
1:H:66:ALA:HB2	1:H:349:HIS:CD2	2.57	0.40
1:I:93:LEU:HD21	1:I:294:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:161:LEU:HD13	1:K:241:LEU:HG	2.04	0.40
1:M:15:LEU:O	1:M:44:VAL:HB	2.21	0.40
1:M:127:VAL:HG21	1:M:366:ILE:HG22	2.02	0.40
1:M:280:VAL:HG21	1:M:365:ARG:HG3	2.04	0.40
1:N:277:ASP:N	1:N:277:ASP:OD1	2.54	0.40
1:O:300:GLU:O	1:O:301:PRO:C	2.59	0.40
1:P:251:LEU:CD2	2:P:1407:HEM:HBB1	2.52	0.40
1:A:136:ALA:CB	1:M:268:ALA:HA	2.52	0.40
1:A:239:ILE:HD12	1:A:239:ILE:HA	1.92	0.40
1:A:383:SER:O	1:A:385:GLY:N	2.54	0.40
1:E:44:VAL:O	1:E:51:GLU:HA	2.21	0.40
1:F:145:MET:HE1	1:F:253:ALA:CB	2.52	0.40
1:I:150:TRP:HZ3	1:I:245:HIS:NE2	2.19	0.40
1:L:339:ARG:HH11	1:L:339:ARG:HD3	1.75	0.40
1:M:361:ARG:O	1:M:365:ARG:HD2	2.22	0.40
1:O:93:LEU:HA	2:O:1407:HEM:O1D	2.22	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	394/436 (90%)	370 (94%)	20 (5%)	4 (1%)	15	37
1	B	397/436 (91%)	367 (92%)	29 (7%)	1 (0%)	41	66
1	C	395/436 (91%)	370 (94%)	23 (6%)	2 (0%)	29	54
1	D	397/436 (91%)	366 (92%)	28 (7%)	3 (1%)	19	43
1	E	396/436 (91%)	367 (93%)	26 (7%)	3 (1%)	19	43
1	F	398/436 (91%)	362 (91%)	30 (8%)	6 (2%)	10	26
1	G	398/436 (91%)	373 (94%)	22 (6%)	3 (1%)	19	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	395/436 (91%)	368 (93%)	26 (7%)	1 (0%)	41	66
1	I	396/436 (91%)	363 (92%)	29 (7%)	4 (1%)	15	37
1	J	396/436 (91%)	370 (93%)	24 (6%)	2 (0%)	29	54
1	K	397/436 (91%)	362 (91%)	30 (8%)	5 (1%)	12	30
1	L	397/436 (91%)	357 (90%)	33 (8%)	7 (2%)	8	21
1	M	396/436 (91%)	367 (93%)	22 (6%)	7 (2%)	8	21
1	N	396/436 (91%)	355 (90%)	37 (9%)	4 (1%)	15	37
1	O	395/436 (91%)	343 (87%)	47 (12%)	5 (1%)	12	30
1	P	395/436 (91%)	356 (90%)	35 (9%)	4 (1%)	15	37
All	All	6338/6976 (91%)	5816 (92%)	461 (7%)	61 (1%)	15	37

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL
1	E	179	VAL
1	E	305	ASP
1	F	245[A]	HIS
1	F	245[B]	HIS
1	G	245	HIS
1	I	382	VAL
1	J	183	ASP
1	K	245	HIS
1	L	305	ASP
1	L	382	VAL
1	M	138	PRO
1	M	245	HIS
1	N	14	VAL
1	N	245	HIS
1	O	382	VAL
1	A	179	VAL
1	B	179	VAL
1	C	244	GLY
1	C	245	HIS
1	D	176	ASP
1	F	182	ASP
1	F	305	ASP
1	G	244	GLY
1	I	244	GLY

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Mol	Chain	Res	Type
1	K	134	MET
1	M	301	PRO
1	N	244	GLY
1	P	40	PRO
1	A	245	HIS
1	A	384	PRO
1	F	139	ASP
1	G	181	PRO
1	K	83	GLU
1	K	244	GLY
1	L	286	TYR
1	M	40	PRO
1	O	89	ASN
1	O	191	MET
1	O	354	CYS
1	P	349	HIS
1	D	83	GLU
1	E	244	GLY
1	I	137	ALA
1	J	184	PRO
1	D	173	VAL
1	K	384	PRO
1	L	182	ASP
1	M	263	PRO
1	N	13	PRO
1	P	344	HIS
1	F	384	PRO
1	H	176	ASP
1	L	40	PRO
1	L	303	ASP
1	I	181	PRO
1	L	384	PRO
1	M	337	ILE
1	M	384	PRO
1	O	184	PRO
1	P	47	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/355 (88%)	293 (94%)	19 (6%)	18	41
1	B	316/355 (89%)	298 (94%)	18 (6%)	20	44
1	C	317/355 (89%)	300 (95%)	17 (5%)	22	47
1	D	318/355 (90%)	300 (94%)	18 (6%)	20	44
1	E	317/355 (89%)	304 (96%)	13 (4%)	30	59
1	F	317/355 (89%)	307 (97%)	10 (3%)	39	68
1	G	321/355 (90%)	307 (96%)	14 (4%)	28	56
1	H	315/355 (89%)	298 (95%)	17 (5%)	22	47
1	I	316/355 (89%)	302 (96%)	14 (4%)	28	56
1	J	315/355 (89%)	301 (96%)	14 (4%)	28	56
1	K	318/355 (90%)	302 (95%)	16 (5%)	24	51
1	L	314/355 (88%)	289 (92%)	25 (8%)	12	27
1	M	315/355 (89%)	295 (94%)	20 (6%)	18	40
1	N	316/355 (89%)	304 (96%)	12 (4%)	33	62
1	O	313/355 (88%)	295 (94%)	18 (6%)	20	43
1	P	315/355 (89%)	296 (94%)	19 (6%)	19	42
All	All	5055/5680 (89%)	4791 (95%)	264 (5%)	23	49

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	43	ARG
1	A	50	ASN
1	A	89	ASN
1	A	101	THR
1	A	134	MET
1	A	139	ASP
1	A	141	ARG
1	A	146	GLU
1	A	160	LEU
1	A	205	LYS
1	A	226	SER
1	A	227	ARG
1	A	231	GLU

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Mol	Chain	Res	Type
1	A	270	ARG
1	A	355	ILE
1	A	380	LEU
1	A	382	VAL
1	A	398	LEU
1	B	11	SER
1	B	12	PRO
1	B	43	ARG
1	B	45	ARG
1	B	48	GLU
1	B	50	ASN
1	B	141	ARG
1	B	146	GLU
1	B	150	TRP
1	B	160	LEU
1	B	195	SER
1	B	270	ARG
1	B	303	ASP
1	B	307	THR
1	B	334	ARG
1	B	383	SER
1	B	392	ASN
1	B	404	ARG
1	C	43	ARG
1	C	72	LYS
1	C	101	THR
1	C	115	ARG
1	C	139	ASP
1	C	150	TRP
1	C	175	THR
1	C	178	PHE
1	C	183	ASP
1	C	189	THR
1	C	203	ASP
1	C	239	ILE
1	C	274	THR
1	C	297	PHE
1	C	307	THR
1	C	341	THR
1	C	372	LEU
1	D	43	ARG
1	D	45	ARG

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Mol	Chain	Res	Type
1	D	54	LEU
1	D	85	GLU
1	D	89	ASN
1	D	105	LYS
1	D	116	VAL
1	D	160	LEU
1	D	175	THR
1	D	178	PHE
1	D	195	SER
1	D	206	ARG
1	D	239	ILE
1	D	245	HIS
1	D	247	THR
1	D	292	SER
1	D	316	LEU
1	D	355	ILE
1	E	43	ARG
1	E	45	ARG
1	E	50	ASN
1	E	116	VAL
1	E	150	TRP
1	E	160	LEU
1	E	175	THR
1	E	230	SER
1	E	246	GLU
1	E	292	SER
1	E	298	PRO
1	E	334	ARG
1	E	372	LEU
1	F	43	ARG
1	F	82	THR
1	F	89	ASN
1	F	150	TRP
1	F	160	LEU
1	F	231	GLU
1	F	297	PHE
1	F	299	VAL
1	F	339	ARG
1	F	388	VAL
1	G	43	ARG
1	G	50[A]	ASN
1	G	50[B]	ASN

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Mol	Chain	Res	Type
1	G	81	LEU
1	G	147	SER
1	G	150	TRP
1	G	175	THR
1	G	176	ASP
1	G	233	LEU
1	G	247	THR
1	G	305	ASP
1	G	334	ARG
1	G	355	ILE
1	G	382	VAL
1	H	43	ARG
1	H	50	ASN
1	H	89	ASN
1	H	114	ARG
1	H	139	ASP
1	H	150	TRP
1	H	160	LEU
1	H	183	ASP
1	H	186	GLN
1	H	195	SER
1	H	241	LEU
1	H	245	HIS
1	H	299	VAL
1	H	303	ASP
1	H	328	ARG
1	H	339	ARG
1	H	344	HIS
1	I	43	ARG
1	I	56	VAL
1	I	89	ASN
1	I	139	ASP
1	I	141	ARG
1	I	150	TRP
1	I	171	PHE
1	I	182	ASP
1	I	189	THR
1	I	195	SER
1	I	247	THR
1	I	261	SER
1	I	380	LEU
1	I	382	VAL

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Mol	Chain	Res	Type
1	J	11	SER
1	J	43	ARG
1	J	48	GLU
1	J	60	ARG
1	J	79	THR
1	J	85	GLU
1	J	113	MET
1	J	139	ASP
1	J	160	LEU
1	J	161	LEU
1	J	195	SER
1	J	334	ARG
1	J	338	ARG
1	J	404	ARG
1	K	43	ARG
1	K	48	GLU
1	K	89	ASN
1	K	95	SER
1	K	101	THR
1	K	150	TRP
1	K	160	LEU
1	K	176	ASP
1	K	178	PHE
1	K	247	THR
1	K	248	THR
1	K	313	ASP
1	K	328	ARG
1	K	334	ARG
1	K	339	ARG
1	K	403	ILE
1	L	43	ARG
1	L	50	ASN
1	L	56	VAL
1	L	60	ARG
1	L	78	THR
1	L	79	THR
1	L	89	ASN
1	L	95	SER
1	L	116	VAL
1	L	139	ASP
1	L	147	SER
1	L	150	TRP

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Mol	Chain	Res	Type
1	L	175	THR
1	L	183	ASP
1	L	186	GLN
1	L	189	THR
1	L	195	SER
1	L	264	ASP
1	L	304	LEU
1	L	305	ASP
1	L	307	THR
1	L	308	VAL
1	L	382	VAL
1	L	383	SER
1	L	396	ARG
1	M	23	ASP
1	M	43	ARG
1	M	45	ARG
1	M	48	GLU
1	M	89	ASN
1	M	113	MET
1	M	139	ASP
1	M	150	TRP
1	M	178	PHE
1	M	199	SER
1	M	203	ASP
1	M	204	SER
1	M	214	LEU
1	M	220	THR
1	M	230	SER
1	M	274	THR
1	M	334	ARG
1	M	340	ASP
1	M	369	ARG
1	M	396	ARG
1	N	43	ARG
1	N	56	VAL
1	N	89	ASN
1	N	115	ARG
1	N	150	TRP
1	N	183	ASP
1	N	242	VAL
1	N	331	ASP
1	N	339	ARG

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Mol	Chain	Res	Type
1	N	383	SER
1	N	388	VAL
1	N	404	ARG
1	O	11	SER
1	O	14	VAL
1	O	23	ASP
1	O	43	ARG
1	O	48	GLU
1	O	101	THR
1	O	150	TRP
1	O	175	THR
1	O	188	GLN
1	O	204	SER
1	O	230	SER
1	O	241	LEU
1	O	316	LEU
1	O	339	ARG
1	O	369	ARG
1	O	375	CYS
1	O	382	VAL
1	O	404	ARG
1	P	23	ASP
1	P	56	VAL
1	P	78	THR
1	P	89	ASN
1	P	95	SER
1	P	114	ARG
1	P	139	ASP
1	P	150	TRP
1	P	171	PHE
1	P	175	THR
1	P	176	ASP
1	P	189	THR
1	P	195	SER
1	P	239	ILE
1	P	270	ARG
1	P	324	ARG
1	P	334	ARG
1	P	338	ARG
1	P	401	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	50	ASN
1	A	238	HIS
1	A	265	GLN
1	A	344	HIS
1	B	188	GLN
1	B	265	GLN
1	B	344	HIS
1	C	22	GLN
1	C	188	GLN
1	C	238	HIS
1	C	245	HIS
1	C	265	GLN
1	C	344	HIS
1	D	22	GLN
1	D	89	ASN
1	D	90	HIS
1	D	124	GLN
1	D	188	GLN
1	D	245	HIS
1	D	265	GLN
1	D	344	HIS
1	E	22	GLN
1	E	188	GLN
1	E	265	GLN
1	E	344	HIS
1	F	265	GLN
1	F	344	HIS
1	F	349	HIS
1	G	22	GLN
1	G	124	GLN
1	G	188	GLN
1	G	238	HIS
1	G	245	HIS
1	G	265	GLN
1	G	344	HIS
1	H	89	ASN
1	H	245	HIS
1	H	265	GLN
1	H	344	HIS
1	H	349	HIS
1	I	238	HIS
1	I	245	HIS

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Mol	Chain	Res	Type
1	I	265	GLN
1	I	344	HIS
1	I	349	HIS
1	J	188	GLN
1	J	245	HIS
1	J	250	ASN
1	J	265	GLN
1	J	344	HIS
1	J	349	HIS
1	K	22	GLN
1	K	245	HIS
1	K	344	HIS
1	L	50	ASN
1	L	265	GLN
1	L	344	HIS
1	M	22	GLN
1	M	188	GLN
1	M	265	GLN
1	M	344	HIS
1	N	50	ASN
1	N	188	GLN
1	N	245	HIS
1	N	265	GLN
1	N	344	HIS
1	O	245	HIS
1	O	265	GLN
1	O	344	HIS
1	P	22	GLN
1	P	188	GLN
1	P	265	GLN
1	P	344	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	H	1408	-	4,4,4	0.48	0	6,6,6	0.52	0
4	17Q	G	1410	-	21,21,21	0.47	0	21,23,23	0.68	0
3	SO4	A	1408	-	4,4,4	0.27	0	6,6,6	0.53	0
2	HEM	K	1407	1	41,50,50	1.86	5 (12%)	45,82,82	1.61	11 (24%)
3	SO4	B	1408	-	4,4,4	0.27	0	6,6,6	0.33	0
2	HEM	B	1407	1	41,50,50	1.89	6 (14%)	45,82,82	1.89	12 (26%)
3	SO4	O	1408	-	4,4,4	0.55	0	6,6,6	0.60	0
2	HEM	H	1407	1	41,50,50	1.96	8 (19%)	45,82,82	1.50	6 (13%)
2	HEM	A	1407	1	41,50,50	1.91	5 (12%)	45,82,82	1.69	11 (24%)
3	SO4	J	1408	-	4,4,4	0.60	0	6,6,6	0.47	0
4	17Q	C	1410	-	21,21,21	0.30	0	21,23,23	0.97	2 (9%)
2	HEM	M	1407	1	41,50,50	2.06	7 (17%)	45,82,82	1.67	8 (17%)
2	HEM	L	1407	1	41,50,50	1.85	4 (9%)	45,82,82	1.59	10 (22%)
2	HEM	I	1407	1	41,50,50	1.95	9 (21%)	45,82,82	1.70	10 (22%)
2	HEM	F	1407	1	41,50,50	1.98	9 (21%)	45,82,82	1.75	9 (20%)
3	SO4	I	1409	-	4,4,4	0.23	0	6,6,6	0.38	0
2	HEM	G	1407	1	41,50,50	1.97	5 (12%)	45,82,82	1.75	7 (15%)
3	SO4	I	1408	-	4,4,4	0.68	0	6,6,6	0.77	0
2	HEM	N	1407	1	41,50,50	1.91	6 (14%)	45,82,82	1.48	9 (20%)
2	HEM	C	1407	1	41,50,50	2.07	7 (17%)	45,82,82	1.79	11 (24%)
3	SO4	F	1408	-	4,4,4	0.51	0	6,6,6	0.52	0
3	SO4	B	1409	-	4,4,4	0.26	0	6,6,6	0.23	0
2	HEM	J	1407	1	41,50,50	1.93	6 (14%)	45,82,82	1.43	6 (13%)
2	HEM	O	1407	1	41,50,50	1.96	7 (17%)	45,82,82	1.67	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	O	1409	-	4,4,4	0.48	0	6,6,6	0.88	0
2	HEM	P	1407	1	41,50,50	1.95	8 (19%)	45,82,82	1.77	13 (28%)
2	HEM	D	1407	1	41,50,50	1.92	9 (21%)	45,82,82	1.45	7 (15%)
3	SO4	D	1408	-	4,4,4	0.67	0	6,6,6	0.79	0
2	HEM	E	1407	1	41,50,50	1.88	7 (17%)	45,82,82	1.71	10 (22%)
3	SO4	H	1409	-	4,4,4	0.29	0	6,6,6	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	17Q	C	1410	-	-	14/23/23/23	1/1/1/1
4	17Q	G	1410	-	-	14/23/23/23	1/1/1/1
2	HEM	I	1407	1	-	1/12/54/54	-
2	HEM	M	1407	1	-	4/12/54/54	-
2	HEM	F	1407	1	-	0/12/54/54	-
2	HEM	H	1407	1	-	2/12/54/54	-
2	HEM	A	1407	1	-	2/12/54/54	-
2	HEM	G	1407	1	-	2/12/54/54	-
2	HEM	J	1407	1	-	2/12/54/54	-
2	HEM	K	1407	1	-	4/12/54/54	-
2	HEM	B	1407	1	-	2/12/54/54	-
2	HEM	N	1407	1	-	0/12/54/54	-
2	HEM	O	1407	1	-	1/12/54/54	-
2	HEM	P	1407	1	-	2/12/54/54	-
2	HEM	D	1407	1	-	2/12/54/54	-
2	HEM	E	1407	1	-	2/12/54/54	-
2	HEM	C	1407	1	-	2/12/54/54	-
2	HEM	L	1407	1	-	2/12/54/54	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1407	HEM	C3D-C2D	8.28	1.54	1.36
2	M	1407	HEM	C3D-C2D	8.20	1.54	1.36
2	P	1407	HEM	C3D-C2D	7.88	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1407	HEM	C3D-C2D	7.85	1.53	1.36
2	O	1407	HEM	C3D-C2D	7.73	1.53	1.36
2	F	1407	HEM	C3D-C2D	7.69	1.53	1.36
2	E	1407	HEM	C3D-C2D	7.68	1.53	1.36
2	G	1407	HEM	C3D-C2D	7.65	1.53	1.36
2	I	1407	HEM	C3D-C2D	7.43	1.52	1.36
2	D	1407	HEM	C3D-C2D	7.42	1.52	1.36
2	N	1407	HEM	C3D-C2D	7.41	1.52	1.36
2	J	1407	HEM	C3D-C2D	7.38	1.52	1.36
2	K	1407	HEM	C3D-C2D	7.36	1.52	1.36
2	H	1407	HEM	C3D-C2D	7.34	1.52	1.36
2	L	1407	HEM	C3D-C2D	7.25	1.52	1.36
2	B	1407	HEM	C3D-C2D	6.93	1.51	1.36
2	C	1407	HEM	C3C-C2C	-5.46	1.32	1.40
2	L	1407	HEM	C3C-C2C	-5.07	1.33	1.40
2	M	1407	HEM	C3C-C2C	-5.02	1.33	1.40
2	G	1407	HEM	C3C-C2C	-4.96	1.33	1.40
2	N	1407	HEM	C3C-C2C	-4.94	1.33	1.40
2	F	1407	HEM	C3C-C2C	-4.93	1.33	1.40
2	H	1407	HEM	C3C-C2C	-4.52	1.34	1.40
2	O	1407	HEM	C3C-C2C	-4.36	1.34	1.40
2	A	1407	HEM	C3C-C2C	-4.34	1.34	1.40
2	B	1407	HEM	C3C-C2C	-4.18	1.34	1.40
2	I	1407	HEM	C3C-CAC	4.15	1.56	1.47
2	J	1407	HEM	C3C-C2C	-4.13	1.34	1.40
2	K	1407	HEM	C3C-C2C	-4.10	1.34	1.40
2	B	1407	HEM	C3C-CAC	4.10	1.56	1.47
2	J	1407	HEM	C3C-CAC	4.08	1.56	1.47
2	P	1407	HEM	C3C-C2C	-3.93	1.34	1.40
2	H	1407	HEM	C3C-CAC	3.92	1.55	1.47
2	G	1407	HEM	C3C-CAC	3.86	1.55	1.47
2	D	1407	HEM	C3C-C2C	-3.73	1.35	1.40
2	E	1407	HEM	C3C-C2C	-3.73	1.35	1.40
2	D	1407	HEM	C3C-CAC	3.71	1.55	1.47
2	M	1407	HEM	C3C-CAC	3.68	1.55	1.47
2	P	1407	HEM	C3C-CAC	3.60	1.55	1.47
2	K	1407	HEM	C3C-CAC	3.59	1.55	1.47
2	C	1407	HEM	CAB-C3B	3.57	1.57	1.47
2	N	1407	HEM	C3C-CAC	3.53	1.55	1.47
2	A	1407	HEM	C3C-CAC	3.50	1.55	1.47
2	F	1407	HEM	C3C-CAC	3.48	1.54	1.47
2	B	1407	HEM	FE-ND	3.33	2.13	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1407	HEM	C3C-CAC	3.28	1.54	1.47
2	M	1407	HEM	CAA-C2A	3.26	1.56	1.52
2	C	1407	HEM	C3C-CAC	3.25	1.54	1.47
2	I	1407	HEM	C3C-C2C	-3.14	1.36	1.40
2	L	1407	HEM	C3C-CAC	3.13	1.54	1.47
2	E	1407	HEM	C3C-CAC	3.11	1.54	1.47
2	K	1407	HEM	CAB-C3B	3.10	1.55	1.47
2	B	1407	HEM	CAB-C3B	3.05	1.55	1.47
2	P	1407	HEM	FE-NB	2.99	2.11	1.96
2	D	1407	HEM	FE-ND	2.93	2.11	1.96
2	D	1407	HEM	CAB-C3B	2.92	1.55	1.47
2	I	1407	HEM	FE-NB	2.90	2.11	1.96
2	A	1407	HEM	CAB-C3B	2.88	1.55	1.47
2	G	1407	HEM	CAA-C2A	2.87	1.56	1.52
2	G	1407	HEM	CAB-C3B	2.87	1.55	1.47
2	H	1407	HEM	CAA-C2A	2.85	1.56	1.52
2	O	1407	HEM	FE-ND	2.77	2.10	1.96
2	J	1407	HEM	FE-ND	2.69	2.10	1.96
2	I	1407	HEM	FE-ND	2.67	2.10	1.96
2	N	1407	HEM	CAB-C3B	2.65	1.54	1.47
2	O	1407	HEM	CAB-C3B	2.63	1.54	1.47
2	I	1407	HEM	CAB-C3B	2.55	1.54	1.47
2	J	1407	HEM	CAA-C2A	2.50	1.55	1.52
2	F	1407	HEM	CAB-C3B	2.49	1.54	1.47
2	L	1407	HEM	CAB-C3B	2.49	1.54	1.47
2	C	1407	HEM	CAA-C2A	2.42	1.55	1.52
2	F	1407	HEM	CMB-C2B	2.42	1.55	1.50
2	F	1407	HEM	FE-ND	2.39	2.08	1.96
2	H	1407	HEM	FE-ND	2.38	2.08	1.96
2	H	1407	HEM	CAB-C3B	2.35	1.53	1.47
2	P	1407	HEM	CAA-C2A	2.34	1.55	1.52
2	F	1407	HEM	CAA-C2A	2.34	1.55	1.52
2	J	1407	HEM	CAB-C3B	2.33	1.53	1.47
2	E	1407	HEM	CAA-C2A	2.32	1.55	1.52
2	I	1407	HEM	CMD-C2D	2.30	1.55	1.50
2	F	1407	HEM	CMD-C2D	2.30	1.55	1.50
2	O	1407	HEM	CMD-C2D	2.29	1.55	1.50
2	D	1407	HEM	CMB-C2B	2.27	1.55	1.50
2	C	1407	HEM	C4D-ND	-2.26	1.36	1.40
2	E	1407	HEM	FE-ND	2.26	2.08	1.96
2	N	1407	HEM	FE-ND	2.24	2.08	1.96
2	N	1407	HEM	CAA-C2A	2.22	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1407	HEM	CAB-C3B	2.21	1.53	1.47
2	P	1407	HEM	CAB-C3B	2.21	1.53	1.47
2	C	1407	HEM	CMD-C2D	2.21	1.55	1.50
2	P	1407	HEM	FE-ND	2.21	2.07	1.96
2	M	1407	HEM	CAB-C3B	2.21	1.53	1.47
2	P	1407	HEM	C3B-C2B	-2.19	1.32	1.37
2	E	1407	HEM	CMC-C2C	2.17	1.56	1.51
2	A	1407	HEM	FE-ND	2.17	2.07	1.96
2	M	1407	HEM	FE-NB	2.14	2.07	1.96
2	K	1407	HEM	CMD-C2D	2.13	1.55	1.50
2	B	1407	HEM	CMB-C2B	2.12	1.55	1.50
2	I	1407	HEM	CMA-C3A	2.06	1.55	1.51
2	M	1407	HEM	CMB-C2B	2.03	1.55	1.50
2	D	1407	HEM	CAA-C2A	2.03	1.55	1.52
2	I	1407	HEM	CAA-C2A	2.03	1.55	1.52
2	O	1407	HEM	CMA-C3A	2.03	1.55	1.51
2	H	1407	HEM	C1A-NA	2.03	1.40	1.36
2	H	1407	HEM	CMC-C2C	2.02	1.56	1.51
2	F	1407	HEM	CMA-C3A	2.01	1.55	1.51
2	D	1407	HEM	C1B-NB	-2.00	1.36	1.40
2	D	1407	HEM	C4D-ND	-2.00	1.36	1.40

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1407	HEM	C4D-ND-C1D	6.02	111.29	105.07
2	P	1407	HEM	C4D-ND-C1D	5.95	111.21	105.07
2	A	1407	HEM	C4D-ND-C1D	5.64	110.89	105.07
2	O	1407	HEM	C4D-ND-C1D	5.63	110.89	105.07
2	F	1407	HEM	C4D-ND-C1D	5.33	110.58	105.07
2	M	1407	HEM	C4D-ND-C1D	5.25	110.50	105.07
2	K	1407	HEM	C4D-ND-C1D	5.18	110.42	105.07
2	B	1407	HEM	C4D-ND-C1D	5.06	110.30	105.07
2	B	1407	HEM	C4C-CHD-C1D	4.99	129.15	122.56
2	H	1407	HEM	C4D-ND-C1D	4.98	110.21	105.07
2	C	1407	HEM	C4D-ND-C1D	4.91	110.15	105.07
2	E	1407	HEM	C4D-ND-C1D	4.71	109.94	105.07
2	J	1407	HEM	C4D-ND-C1D	4.64	109.86	105.07
2	I	1407	HEM	C4D-ND-C1D	4.53	109.75	105.07
2	L	1407	HEM	C4D-ND-C1D	4.49	109.71	105.07
2	N	1407	HEM	C4D-ND-C1D	4.41	109.63	105.07
2	P	1407	HEM	C4C-CHD-C1D	4.33	128.27	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1407	HEM	C2C-C3C-C4C	4.23	109.85	106.90
2	F	1407	HEM	C4B-CHC-C1C	4.03	127.88	122.56
2	L	1407	HEM	C4C-CHD-C1D	3.98	127.82	122.56
2	D	1407	HEM	C4D-ND-C1D	3.95	109.15	105.07
2	A	1407	HEM	CBA-CAA-C2A	-3.87	106.01	112.62
2	I	1407	HEM	CMD-C2D-C1D	3.78	130.79	125.04
2	C	1407	HEM	C1D-C2D-C3D	-3.65	103.12	106.96
2	F	1407	HEM	CMD-C2D-C1D	3.63	130.57	125.04
2	H	1407	HEM	C4A-C3A-C2A	3.48	109.42	107.00
2	B	1407	HEM	C1B-NB-C4B	3.41	108.59	105.07
2	C	1407	HEM	C3B-C2B-C1B	3.40	109.00	106.49
2	B	1407	HEM	CAD-CBD-CGD	-3.39	106.31	113.60
2	G	1407	HEM	C1B-NB-C4B	3.39	108.57	105.07
2	F	1407	HEM	CBD-CAD-C3D	-3.34	103.36	112.63
2	I	1407	HEM	CBD-CAD-C3D	-3.29	103.48	112.63
2	C	1407	HEM	CBD-CAD-C3D	-3.27	103.55	112.63
2	G	1407	HEM	C4B-CHC-C1C	3.26	126.86	122.56
2	E	1407	HEM	C1D-C2D-C3D	-3.25	103.54	106.96
2	G	1407	HEM	CBD-CAD-C3D	-3.25	103.60	112.63
2	O	1407	HEM	CMA-C3A-C4A	-3.25	123.47	128.46
2	D	1407	HEM	C4C-CHD-C1D	3.23	126.81	122.56
2	I	1407	HEM	C4C-CHD-C1D	3.21	126.79	122.56
2	E	1407	HEM	CMD-C2D-C1D	3.18	129.88	125.04
2	O	1407	HEM	C4C-CHD-C1D	3.16	126.73	122.56
2	M	1407	HEM	CAD-C3D-C4D	3.07	130.01	124.66
2	L	1407	HEM	CHD-C1D-ND	3.07	127.76	124.43
2	I	1407	HEM	C1D-C2D-C3D	-3.06	103.74	106.96
2	H	1407	HEM	C4C-CHD-C1D	2.97	126.48	122.56
2	M	1407	HEM	C4B-CHC-C1C	2.97	126.47	122.56
2	C	1407	HEM	CHD-C1D-ND	2.96	127.65	124.43
2	G	1407	HEM	CHD-C1D-ND	2.91	127.59	124.43
2	M	1407	HEM	C1B-NB-C4B	2.91	108.07	105.07
2	J	1407	HEM	CAD-C3D-C4D	2.89	129.71	124.66
2	E	1407	HEM	C4C-CHD-C1D	2.89	126.38	122.56
2	C	1407	HEM	C1B-NB-C4B	2.88	108.05	105.07
2	H	1407	HEM	C4B-CHC-C1C	2.86	126.33	122.56
2	A	1407	HEM	C4C-CHD-C1D	2.85	126.31	122.56
2	C	1407	HEM	CHB-C1B-NB	2.83	127.88	124.38
2	L	1407	HEM	CBD-CAD-C3D	-2.82	104.78	112.63
2	C	1407	HEM	CHD-C1D-C2D	-2.81	120.59	124.98
2	B	1407	HEM	CAA-CBA-CGA	-2.81	105.89	113.76
2	K	1407	HEM	C2C-C3C-C4C	2.80	108.85	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1407	HEM	CHC-C4B-NB	2.72	127.38	124.43
2	I	1407	HEM	CAD-C3D-C4D	2.69	129.36	124.66
2	B	1407	HEM	CBD-CAD-C3D	-2.69	105.16	112.63
2	O	1407	HEM	CAD-C3D-C4D	2.68	129.35	124.66
2	B	1407	HEM	C4A-C3A-C2A	2.64	108.83	107.00
2	N	1407	HEM	C1D-C2D-C3D	-2.64	104.18	106.96
2	C	1407	HEM	C4C-CHD-C1D	2.63	126.03	122.56
2	P	1407	HEM	CAD-C3D-C4D	2.61	129.22	124.66
2	F	1407	HEM	C2C-C3C-C4C	2.59	108.71	106.90
2	O	1407	HEM	C1D-C2D-C3D	-2.57	104.25	106.96
2	N	1407	HEM	CHB-C1B-NB	2.57	127.55	124.38
2	P	1407	HEM	CHD-C1D-ND	2.56	127.21	124.43
2	C	1407	HEM	CMB-C2B-C1B	-2.56	121.14	125.04
4	C	1410	17Q	C12-C13-N	-2.56	106.87	113.79
2	N	1407	HEM	C3B-C2B-C1B	2.54	108.37	106.49
2	M	1407	HEM	CBA-CAA-C2A	-2.53	108.30	112.62
2	B	1407	HEM	CMD-C2D-C1D	2.53	128.89	125.04
2	N	1407	HEM	CMD-C2D-C1D	2.51	128.87	125.04
2	A	1407	HEM	CMA-C3A-C4A	-2.49	124.63	128.46
2	O	1407	HEM	CMD-C2D-C1D	2.49	128.83	125.04
2	D	1407	HEM	C1B-NB-C4B	2.48	107.64	105.07
2	O	1407	HEM	CMC-C2C-C3C	2.46	129.28	124.68
2	L	1407	HEM	CAD-C3D-C4D	2.45	128.95	124.66
2	K	1407	HEM	C1B-NB-C4B	2.45	107.60	105.07
2	E	1407	HEM	CMA-C3A-C4A	-2.45	124.70	128.46
2	D	1407	HEM	O1A-CGA-CBA	-2.44	115.24	123.08
2	F	1407	HEM	C1D-C2D-C3D	-2.44	104.39	106.96
2	E	1407	HEM	CBD-CAD-C3D	-2.44	105.85	112.63
2	J	1407	HEM	C1D-C2D-C3D	-2.43	104.40	106.96
2	A	1407	HEM	O1A-CGA-CBA	-2.43	115.29	123.08
2	G	1407	HEM	C4C-CHD-C1D	2.39	125.71	122.56
2	N	1407	HEM	C4B-CHC-C1C	2.37	125.69	122.56
2	K	1407	HEM	O2A-CGA-CBA	2.36	121.63	114.03
2	K	1407	HEM	CHA-C4D-ND	2.36	127.30	124.38
2	P	1407	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
2	B	1407	HEM	CAD-C3D-C4D	2.36	128.78	124.66
2	P	1407	HEM	O1A-CGA-CBA	-2.34	115.55	123.08
2	F	1407	HEM	C1B-NB-C4B	2.33	107.48	105.07
2	L	1407	HEM	CHC-C4B-NB	2.32	126.95	124.43
2	P	1407	HEM	CBA-CAA-C2A	-2.31	108.68	112.62
2	P	1407	HEM	C1B-NB-C4B	2.31	107.46	105.07
2	A	1407	HEM	O2A-CGA-CBA	2.31	121.44	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1407	HEM	CAD-CBD-CGD	-2.31	108.64	113.60
2	H	1407	HEM	C1B-NB-C4B	2.29	107.44	105.07
2	D	1407	HEM	CBD-CAD-C3D	-2.28	106.28	112.63
2	D	1407	HEM	C1D-C2D-C3D	-2.27	104.57	106.96
2	K	1407	HEM	C4B-CHC-C1C	2.26	125.54	122.56
2	K	1407	HEM	CMD-C2D-C1D	2.25	128.47	125.04
2	K	1407	HEM	C4C-CHD-C1D	2.25	125.52	122.56
2	I	1407	HEM	CHC-C4B-C3B	2.24	128.00	124.57
2	M	1407	HEM	CAD-CBD-CGD	-2.24	108.79	113.60
2	P	1407	HEM	C4B-CHC-C1C	2.24	125.51	122.56
2	J	1407	HEM	C4C-CHD-C1D	2.23	125.50	122.56
2	B	1407	HEM	C3B-C2B-C1B	2.23	108.14	106.49
2	M	1407	HEM	O2A-CGA-CBA	2.22	121.15	114.03
2	A	1407	HEM	C2C-C3C-C4C	2.20	108.44	106.90
2	A	1407	HEM	C4B-CHC-C1C	2.19	125.45	122.56
2	K	1407	HEM	CBD-CAD-C3D	-2.19	106.54	112.63
2	B	1407	HEM	CBA-CAA-C2A	-2.19	108.89	112.62
2	I	1407	HEM	C1B-NB-C4B	2.18	107.32	105.07
2	F	1407	HEM	O2A-CGA-CBA	2.17	121.01	114.03
2	I	1407	HEM	CAA-CBA-CGA	-2.17	107.68	113.76
2	L	1407	HEM	C4B-C3B-C2B	2.17	108.84	107.11
2	C	1407	HEM	CMD-C2D-C3D	2.16	131.99	126.12
2	N	1407	HEM	C1B-NB-C4B	2.16	107.31	105.07
2	P	1407	HEM	C3B-C2B-C1B	2.16	108.09	106.49
2	N	1407	HEM	C4C-CHD-C1D	2.16	125.41	122.56
2	M	1407	HEM	C2C-C3C-C4C	2.15	108.40	106.90
2	J	1407	HEM	C4A-C3A-C2A	2.15	108.49	107.00
2	L	1407	HEM	C2C-C3C-C4C	2.14	108.40	106.90
2	P	1407	HEM	C4A-C3A-C2A	2.14	108.48	107.00
2	A	1407	HEM	C1B-NB-C4B	2.14	107.28	105.07
4	C	1410	17Q	C6-C7-C8	-2.13	106.92	114.64
2	L	1407	HEM	CAA-CBA-CGA	-2.13	107.79	113.76
2	P	1407	HEM	CBD-CAD-C3D	-2.12	106.75	112.63
2	K	1407	HEM	C1D-C2D-C3D	-2.12	104.73	106.96
2	E	1407	HEM	C1B-NB-C4B	2.11	107.25	105.07
2	L	1407	HEM	C1B-NB-C4B	2.10	107.25	105.07
2	O	1407	HEM	O2A-CGA-CBA	2.10	120.77	114.03
2	F	1407	HEM	CMA-C3A-C4A	-2.08	125.26	128.46
2	P	1407	HEM	O2A-CGA-CBA	2.07	120.68	114.03
2	N	1407	HEM	CHC-C4B-NB	2.07	126.68	124.43
2	G	1407	HEM	O2A-CGA-CBA	2.05	120.61	114.03
2	E	1407	HEM	CBB-CAB-C3B	-2.05	117.43	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1407	HEM	C4A-C3A-C2A	2.04	108.42	107.00
2	A	1407	HEM	C4D-C3D-C2D	-2.04	103.92	106.90
2	O	1407	HEM	C4B-CHC-C1C	2.04	125.25	122.56
2	A	1407	HEM	C3C-C4C-NC	-2.04	107.09	110.94
2	B	1407	HEM	O1D-CGD-CBD	-2.04	116.54	123.08
2	I	1407	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
2	H	1407	HEM	O2D-CGD-CBD	2.01	120.49	114.03
2	D	1407	HEM	CAA-CBA-CGA	-2.00	108.14	113.76

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1407	HEM	C2B-C3B-CAB-CBB
2	J	1407	HEM	C4B-C3B-CAB-CBB
2	P	1407	HEM	C2B-C3B-CAB-CBB
2	P	1407	HEM	C4B-C3B-CAB-CBB
4	C	1410	17Q	C7-C8-O-C9
4	C	1410	17Q	C6-C7-C8-O
4	G	1410	17Q	C7-C8-O-C9
4	C	1410	17Q	C2-C1-C19-C18
4	C	1410	17Q	C1-C2-C3-C4
4	G	1410	17Q	C11-C12-C13-N
4	G	1410	17Q	C11-C10-C9-O
4	C	1410	17Q	C6-C7-C8-C16
4	G	1410	17Q	C19-C1-C2-C3
4	C	1410	17Q	C19-C1-C2-C3
4	G	1410	17Q	C2-C3-C4-C5
4	G	1410	17Q	C1-C2-C3-C4
4	C	1410	17Q	C16-C17-C18-C19
4	C	1410	17Q	C2-C3-C4-C5
4	G	1410	17Q	C10-C9-O-C8
4	C	1410	17Q	C9-C10-C11-C12
4	C	1410	17Q	C4-C5-C6-C7
4	G	1410	17Q	C17-C18-C19-C1
2	M	1407	HEM	C2B-C3B-CAB-CBB
4	G	1410	17Q	C3-C4-C5-C6
4	G	1410	17Q	C9-C10-C11-C12
4	G	1410	17Q	C2-C1-C19-C18
4	G	1410	17Q	C16-C17-C18-C19
4	G	1410	17Q	C10-C11-C12-C13
4	C	1410	17Q	C17-C16-C8-C7

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Mol	Chain	Res	Type	Atoms
2	M	1407	HEM	C4B-C3B-CAB-CBB
4	C	1410	17Q	C17-C16-C8-O
2	K	1407	HEM	C2B-C3B-CAB-CBB
4	C	1410	17Q	C5-C6-C7-C8
2	K	1407	HEM	CAA-CBA-CGA-O1A
2	K	1407	HEM	CAA-CBA-CGA-O2A
2	G	1407	HEM	CAA-CBA-CGA-O2A
2	M	1407	HEM	CAA-CBA-CGA-O2A
2	L	1407	HEM	CAA-CBA-CGA-O2A
2	B	1407	HEM	CAA-CBA-CGA-O2A
2	E	1407	HEM	CAA-CBA-CGA-O2A
2	M	1407	HEM	CAA-CBA-CGA-O1A
2	E	1407	HEM	CAA-CBA-CGA-O1A
2	G	1407	HEM	CAA-CBA-CGA-O1A
2	L	1407	HEM	CAA-CBA-CGA-O1A
4	C	1410	17Q	C17-C18-C19-C1
2	C	1407	HEM	C2B-C3B-CAB-CBB
2	B	1407	HEM	CAA-CBA-CGA-O1A
2	K	1407	HEM	C4B-C3B-CAB-CBB
4	G	1410	17Q	C6-C7-C8-O
2	H	1407	HEM	CAA-CBA-CGA-O2A
2	O	1407	HEM	CAA-CBA-CGA-O2A
2	A	1407	HEM	CAA-CBA-CGA-O2A
2	D	1407	HEM	CAA-CBA-CGA-O2A
2	H	1407	HEM	CAA-CBA-CGA-O1A
2	A	1407	HEM	CAA-CBA-CGA-O1A
2	D	1407	HEM	CAA-CBA-CGA-O1A
2	I	1407	HEM	CAA-CBA-CGA-O2A
2	C	1407	HEM	CAA-CBA-CGA-O2A

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8
4	G	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8

22 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1410	17Q	5	0
3	A	1408	SO4	2	0
2	K	1407	HEM	3	0

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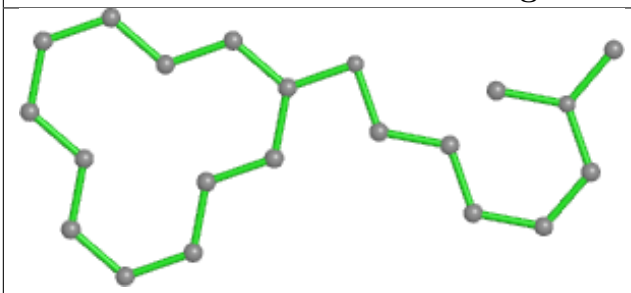
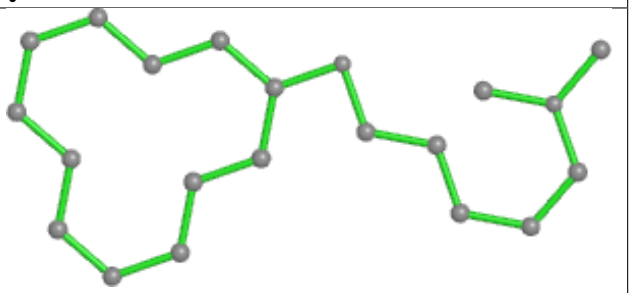
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1407	HEM	6	0
2	H	1407	HEM	7	0
2	A	1407	HEM	1	0
4	C	1410	17Q	6	0
2	M	1407	HEM	5	0
2	L	1407	HEM	4	0
2	I	1407	HEM	5	0
2	F	1407	HEM	3	0
2	G	1407	HEM	6	0
2	N	1407	HEM	7	0
2	C	1407	HEM	6	0
3	F	1408	SO4	1	0
2	J	1407	HEM	4	0
2	O	1407	HEM	4	0
3	O	1409	SO4	1	0
2	P	1407	HEM	5	0
2	D	1407	HEM	8	0
2	E	1407	HEM	5	0
3	H	1409	SO4	1	0

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

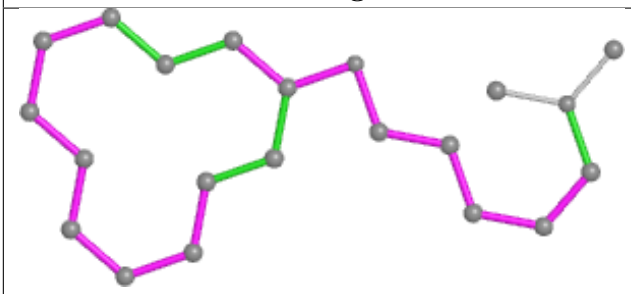
Ligand 17Q G 1410



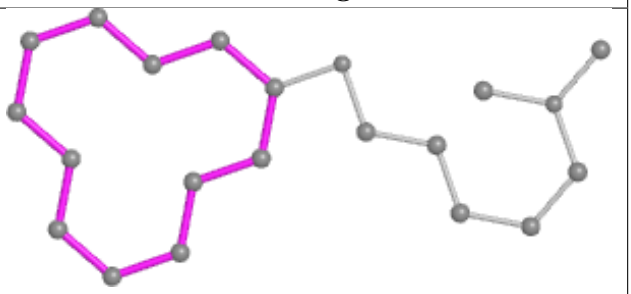
Bond lengths



Bond angles

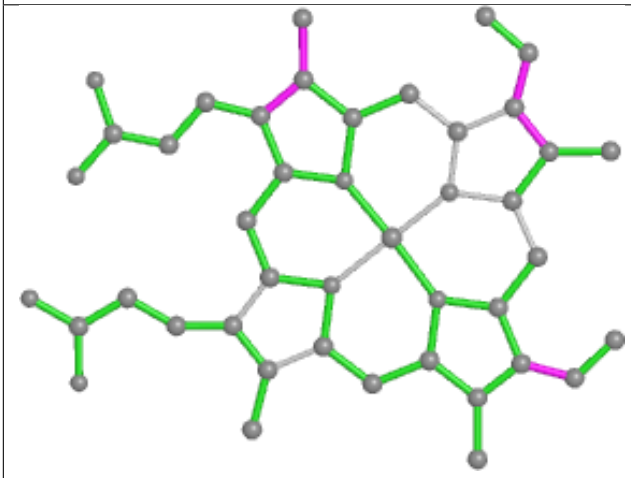


Torsions

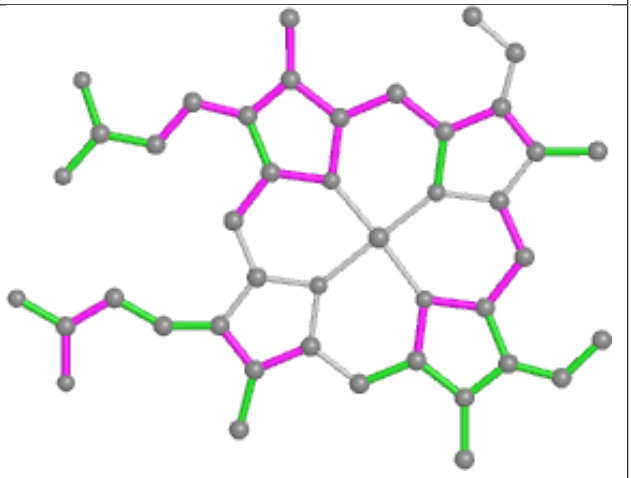


Rings

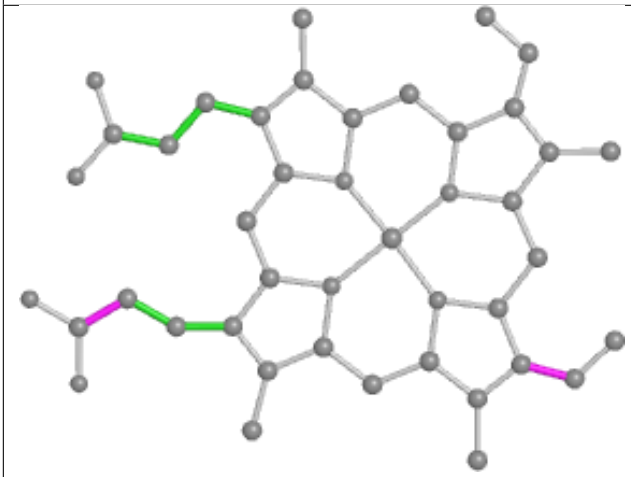
Ligand HEM K 1407



Bond lengths



Bond angles



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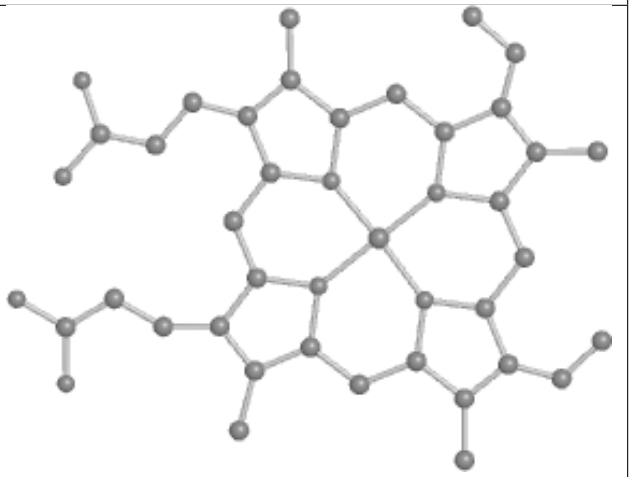
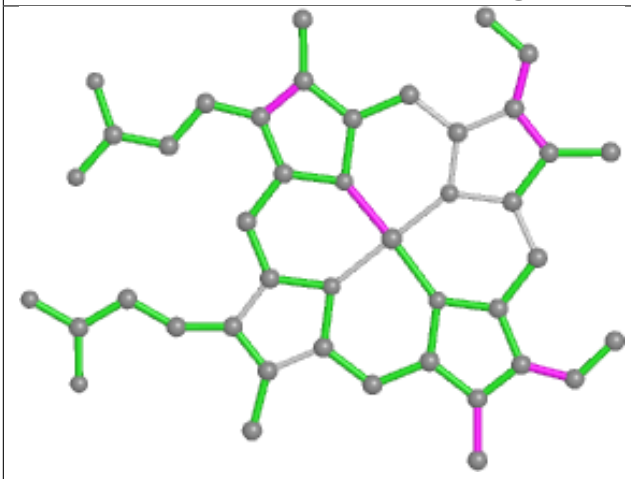
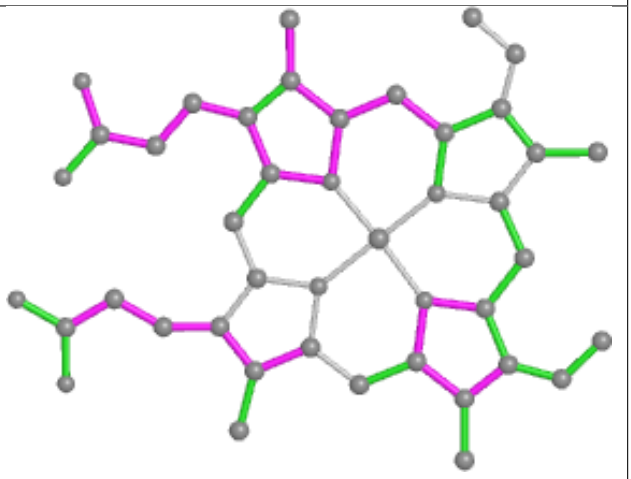


Rings

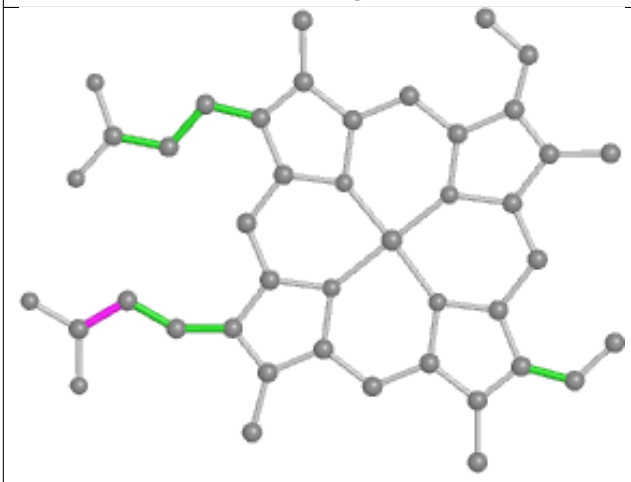
Ligand HEM B 1407



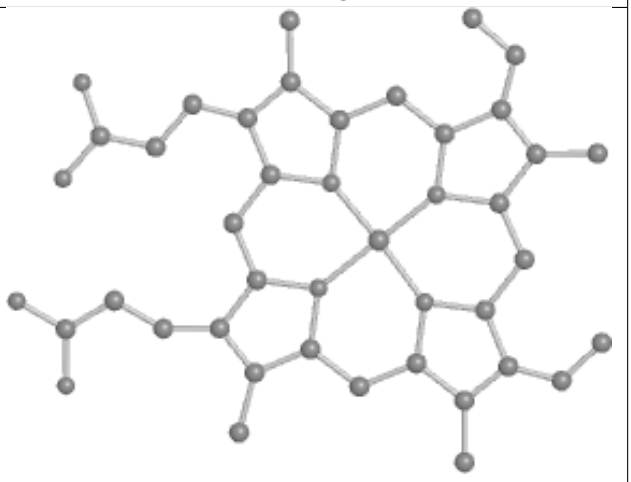
Bond lengths



Bond angles

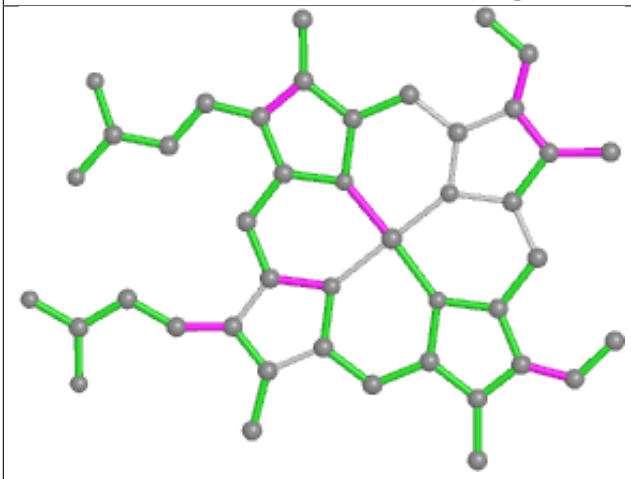


Torsions

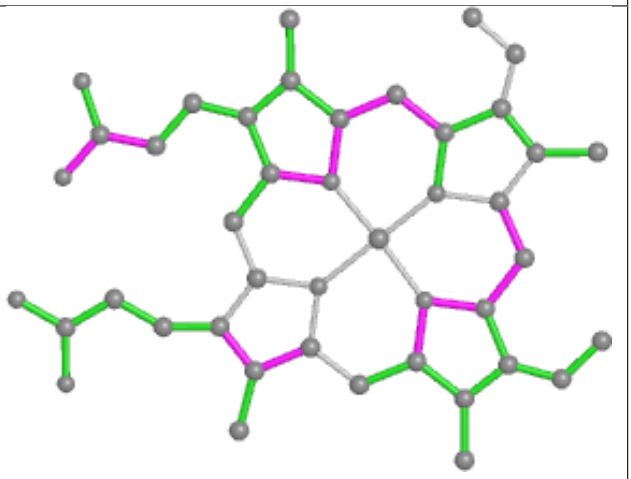


Rings

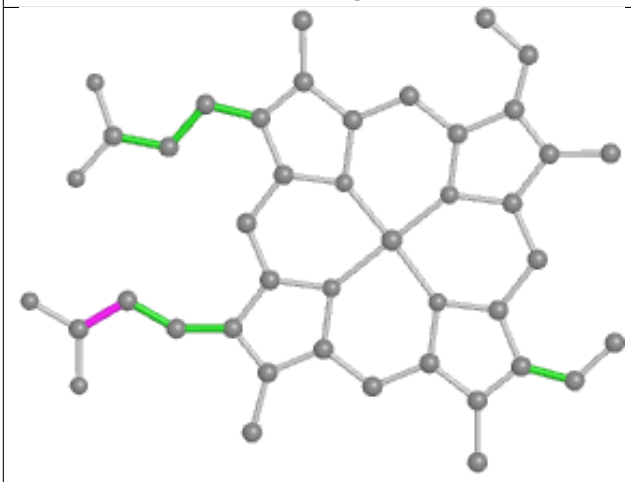
Ligand HEM H 1407



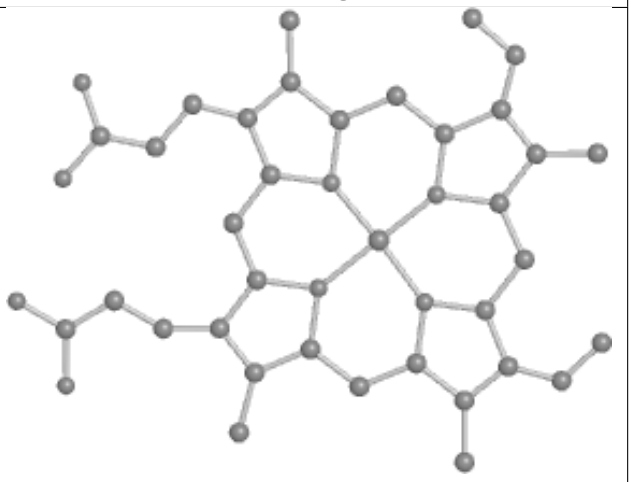
Bond lengths



Bond angles

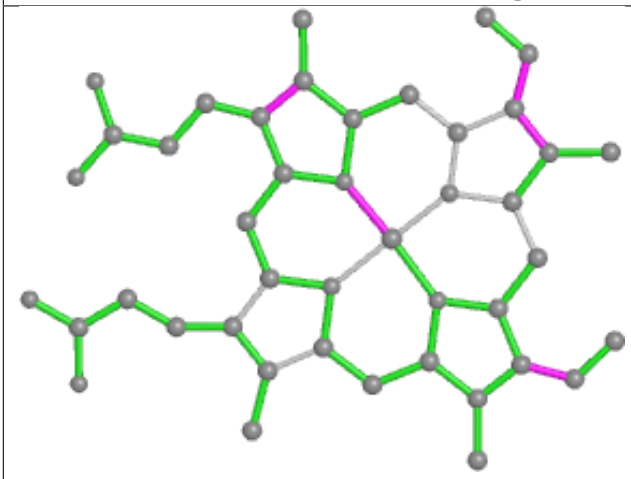


Torsions

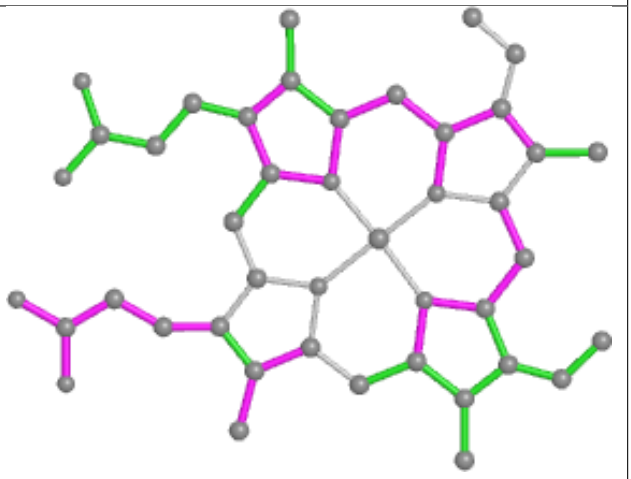


Rings

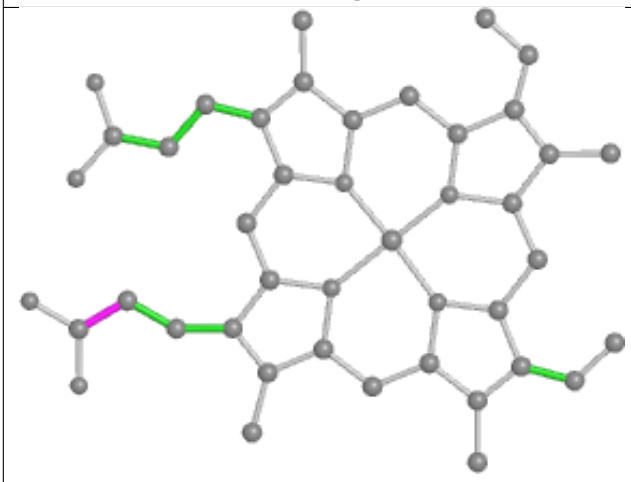
Ligand HEM A 1407



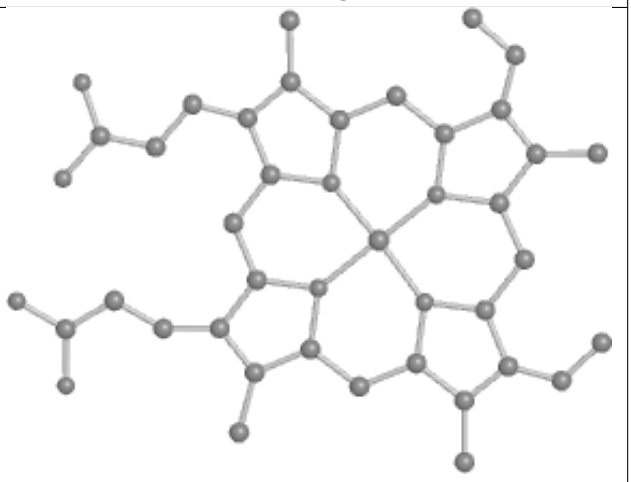
Bond lengths



Bond angles

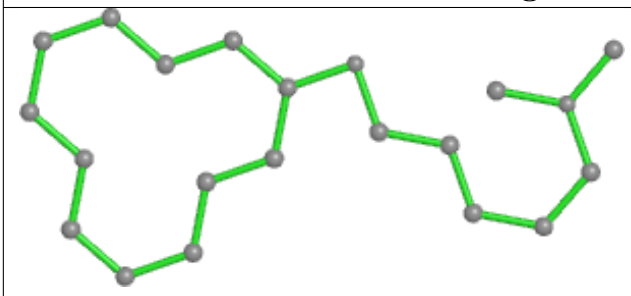


Torsions

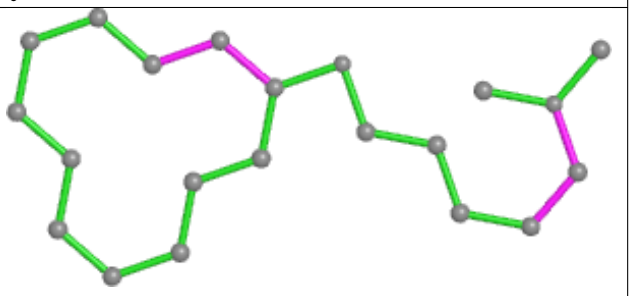


Rings

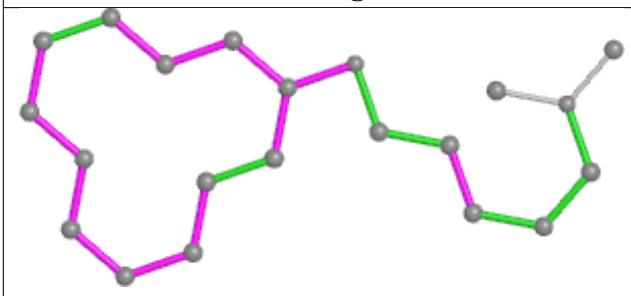
Ligand 17Q C 1410



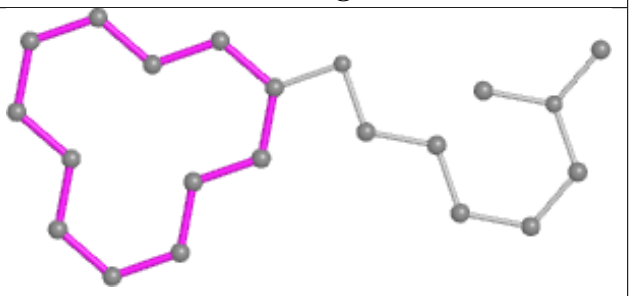
Bond lengths



Bond angles

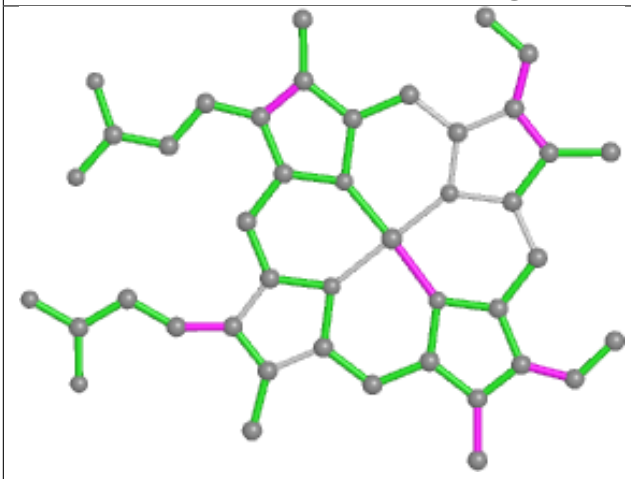


Torsions



Rings

Ligand HEM M 1407



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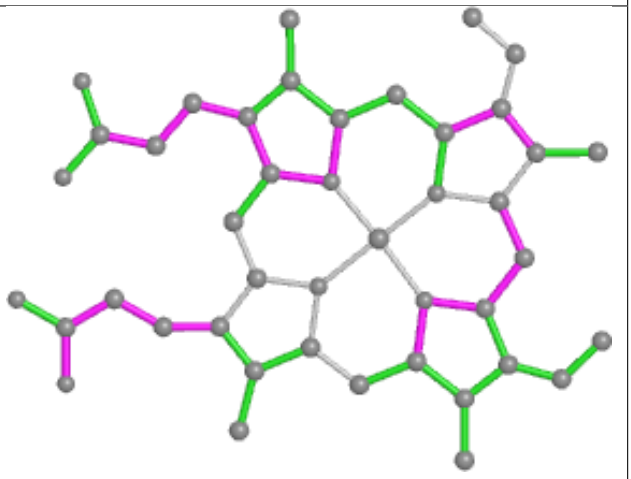
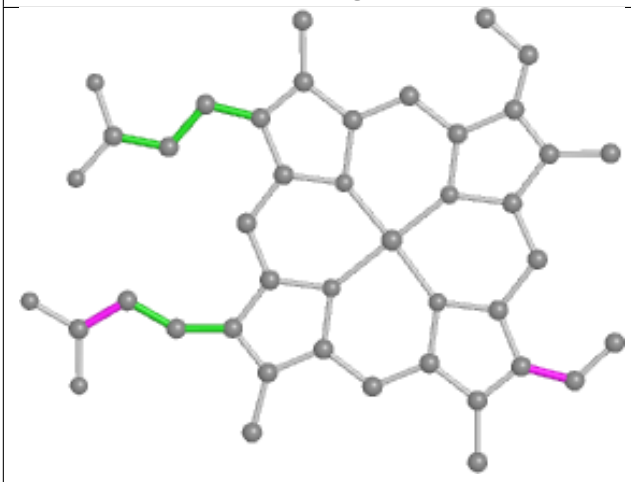


Bond angles



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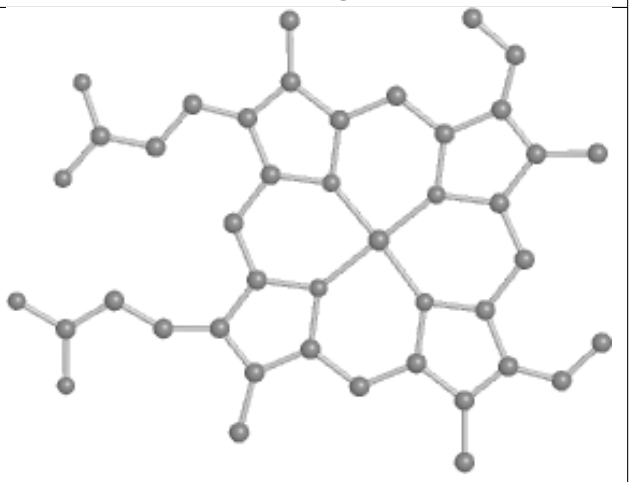
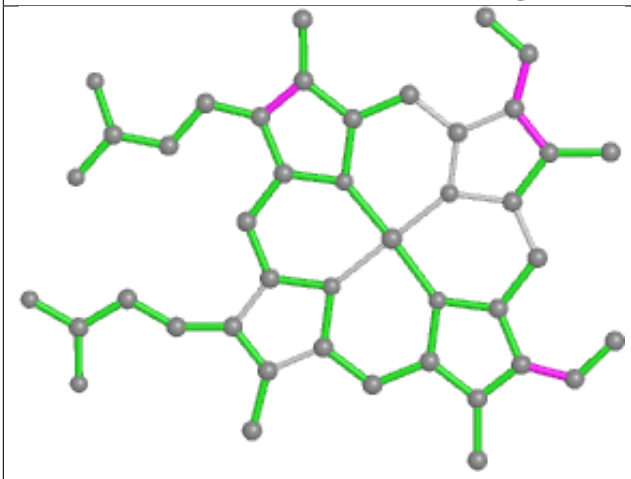


Rings

Ligand HEM L 1407



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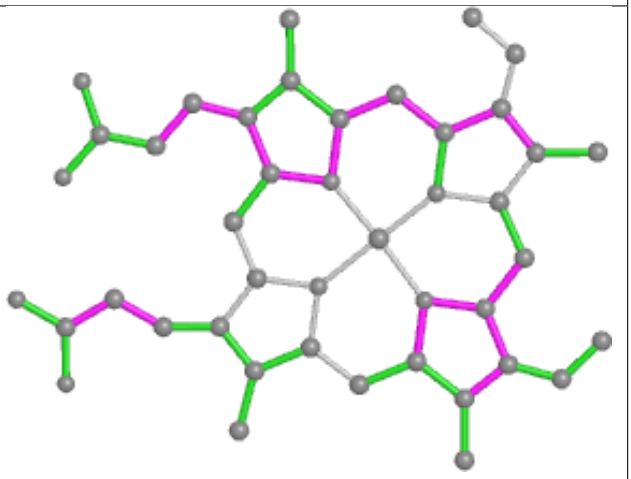
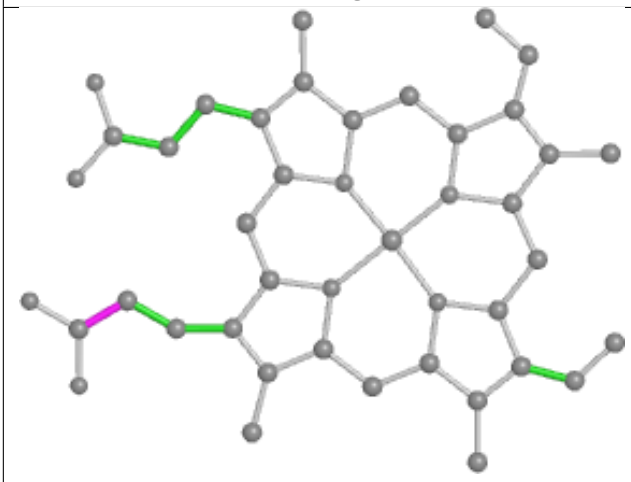


Bond angles



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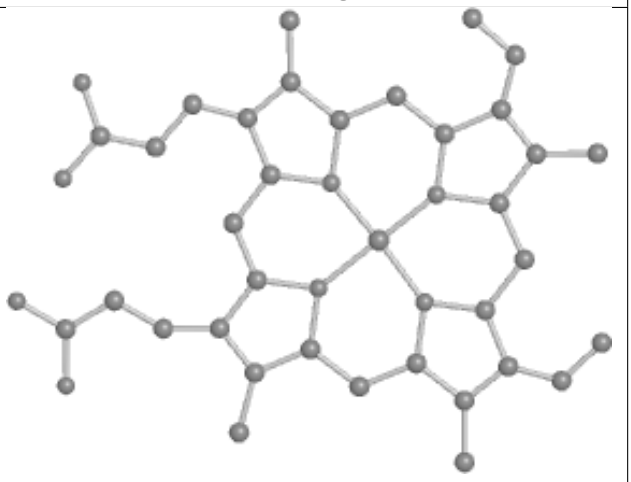
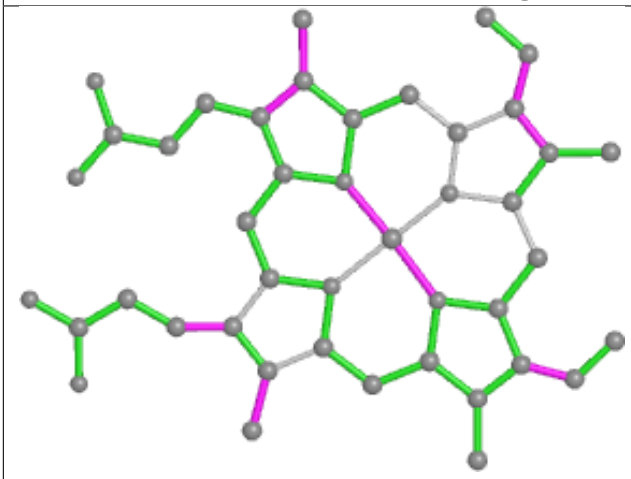


Rings

Ligand HEM I 1407



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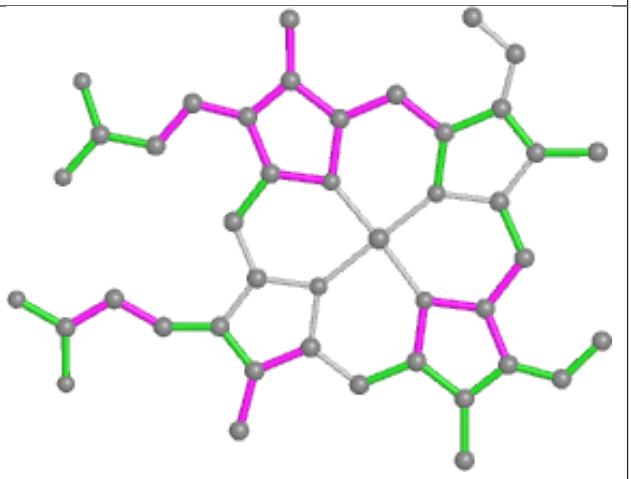

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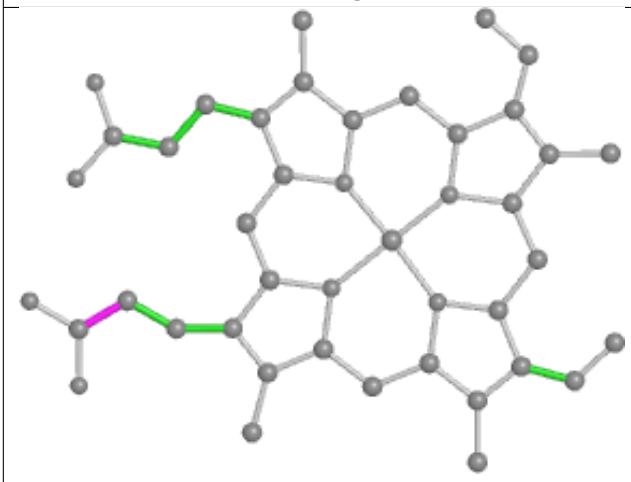

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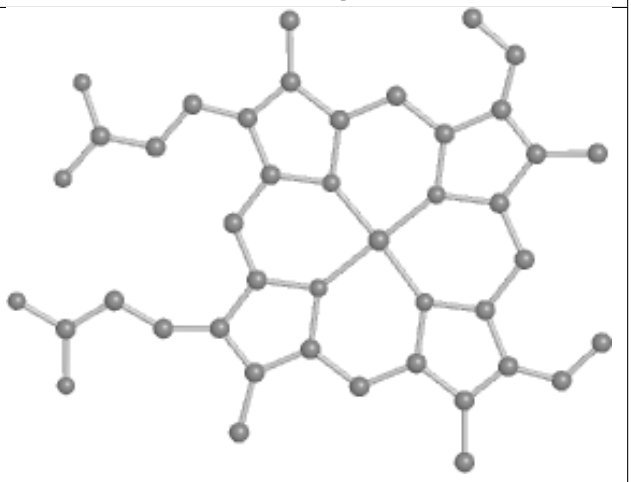
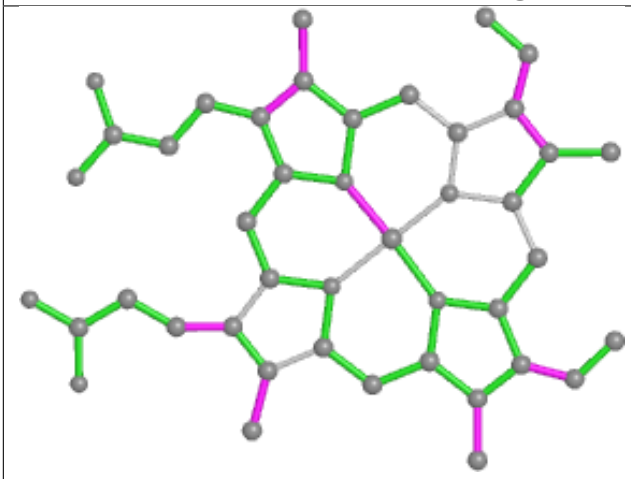
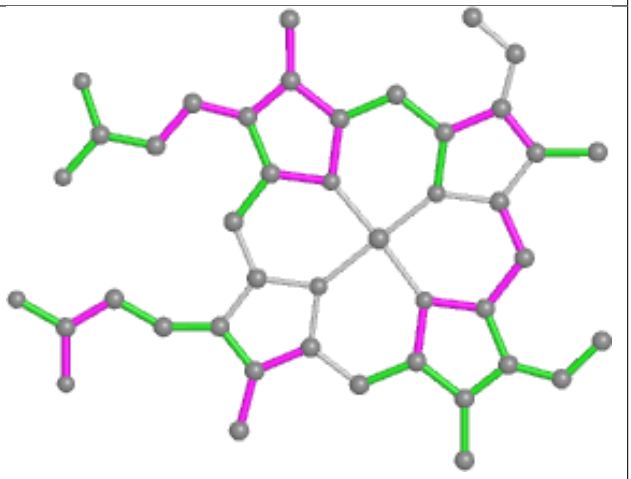


Rings

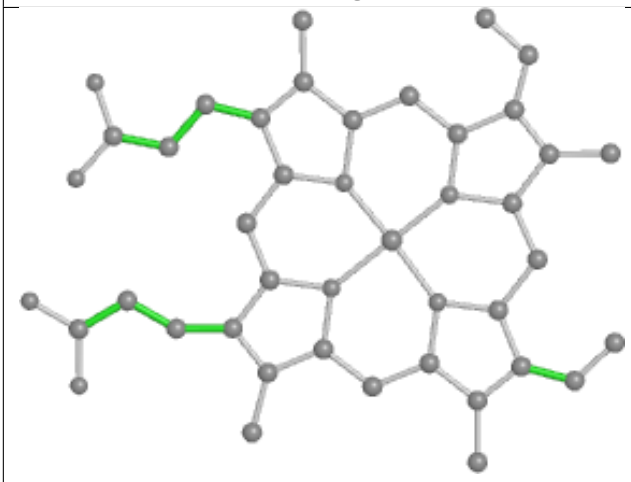
Ligand HEM F 1407



Bond lengths



Bond angles



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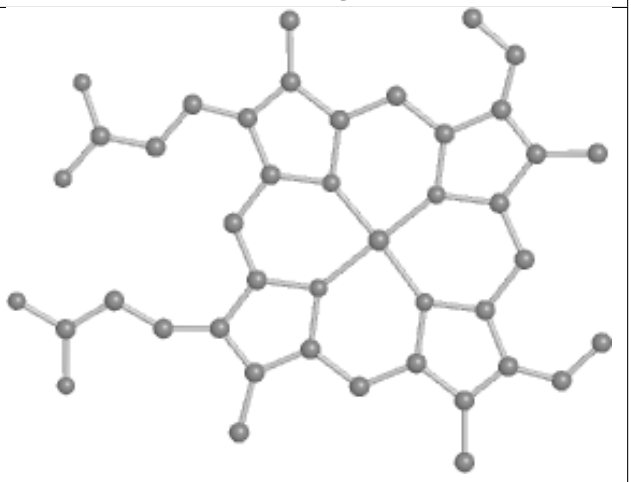
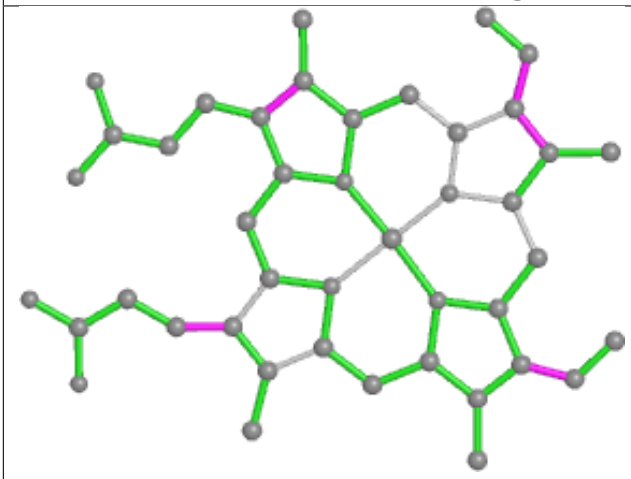
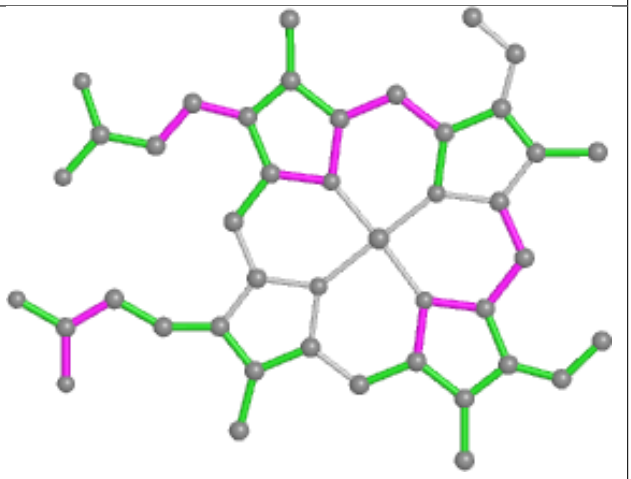


Rings

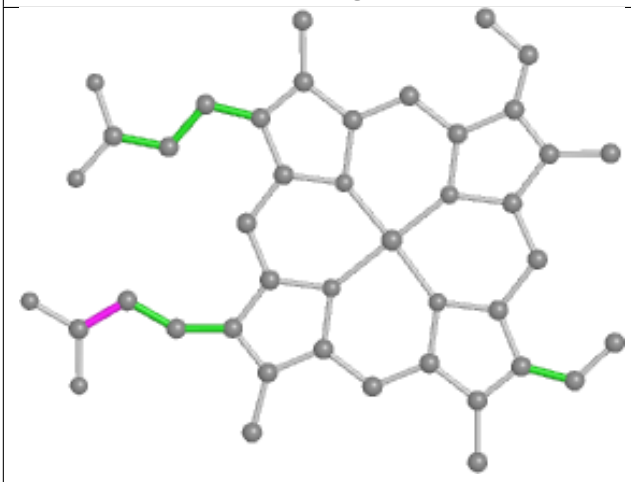
Ligand HEM G 1407



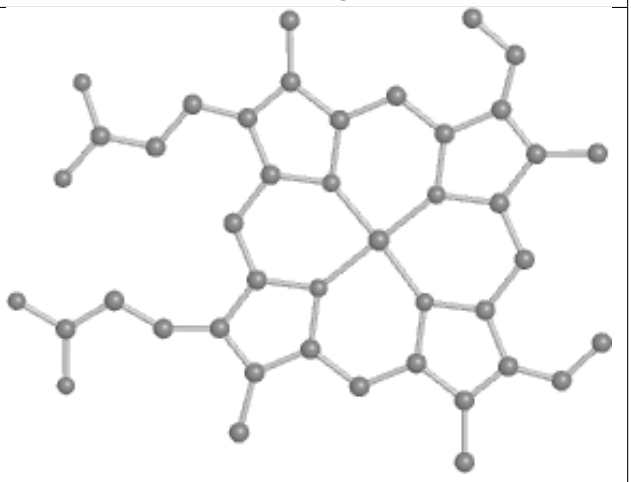
Bond lengths



Bond angles

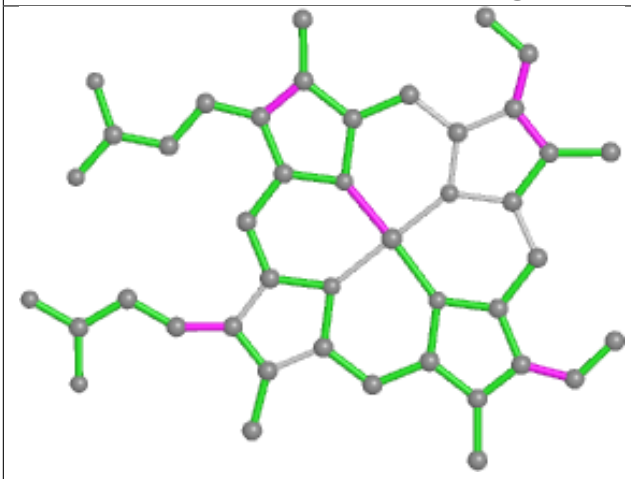


Torsions

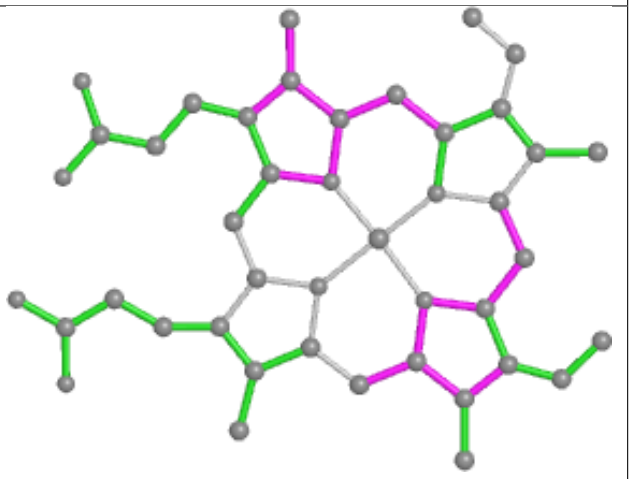


Rings

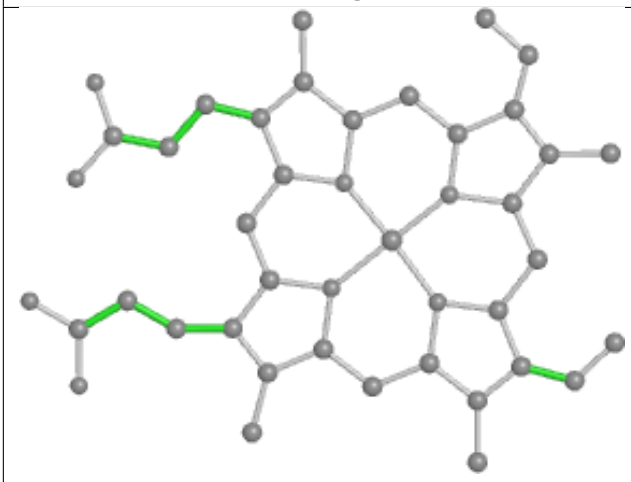
Ligand HEM N 1407



Bond lengths



Bond angles



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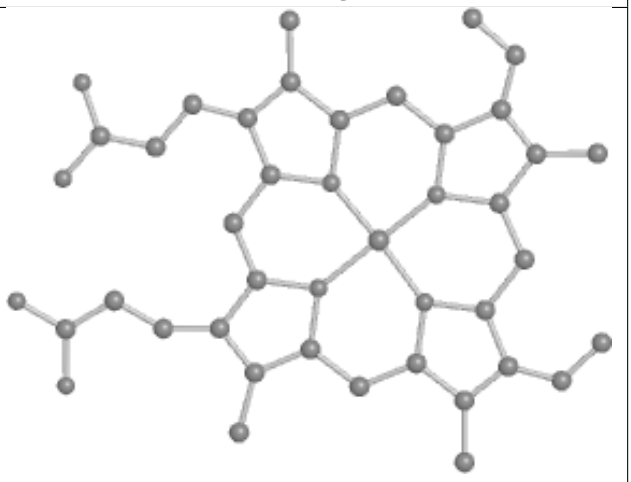
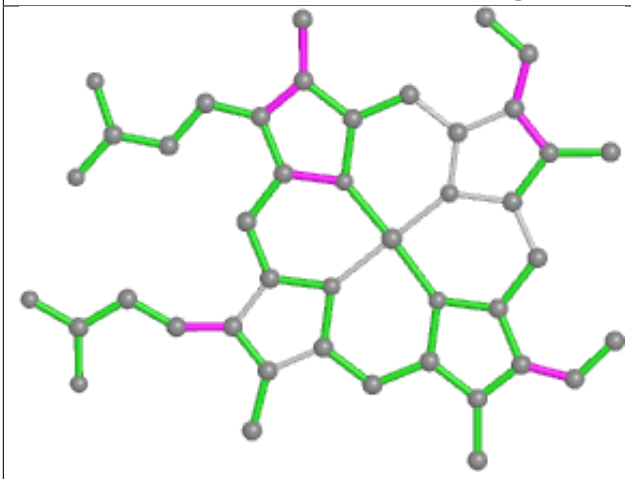
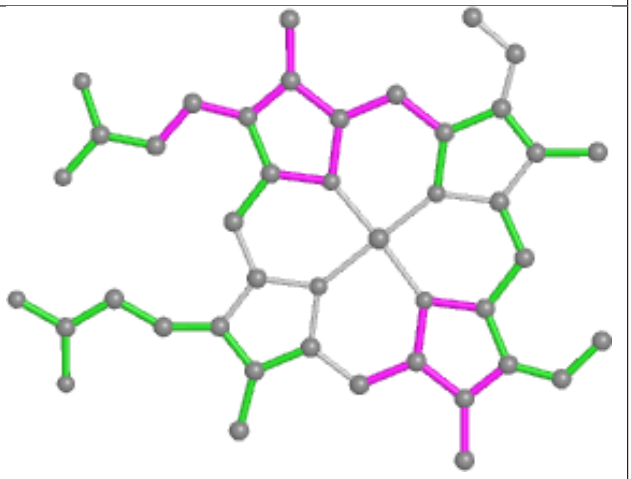


Rings

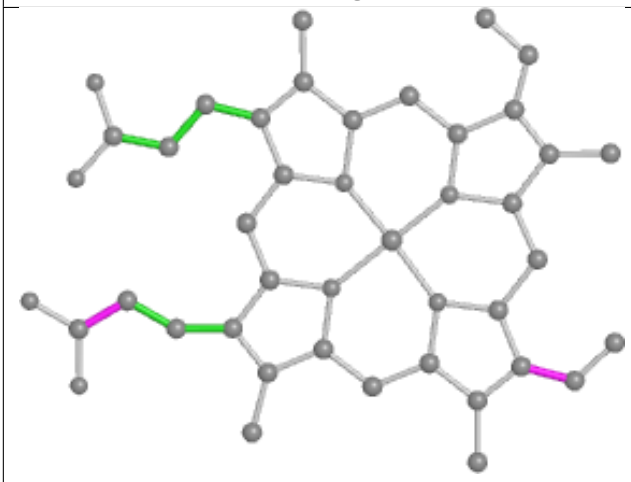
Ligand HEM C 1407



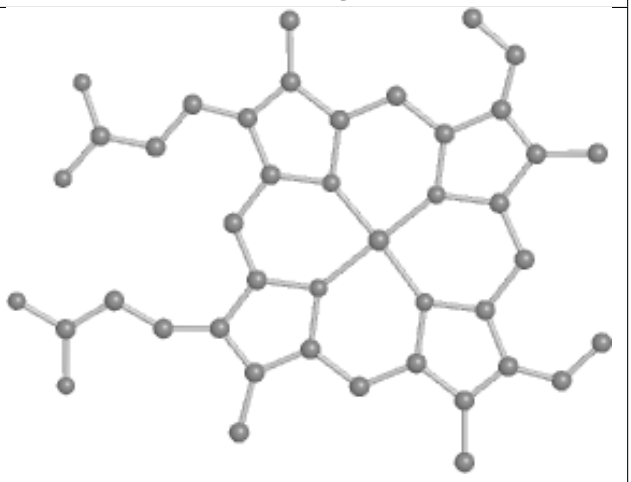
Bond lengths



Bond angles

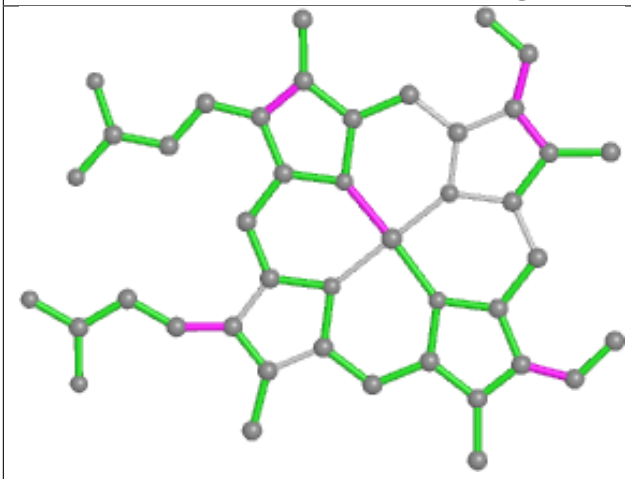


Torsions

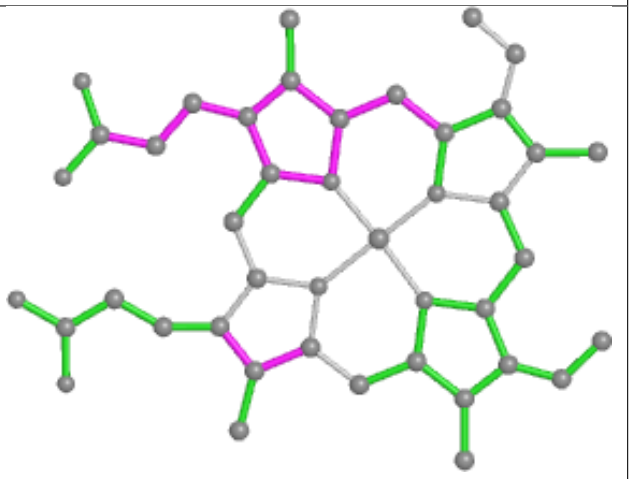


Rings

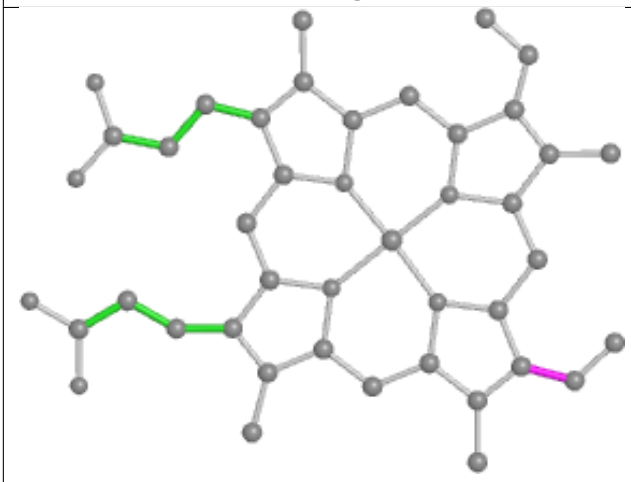
Ligand HEM J 1407



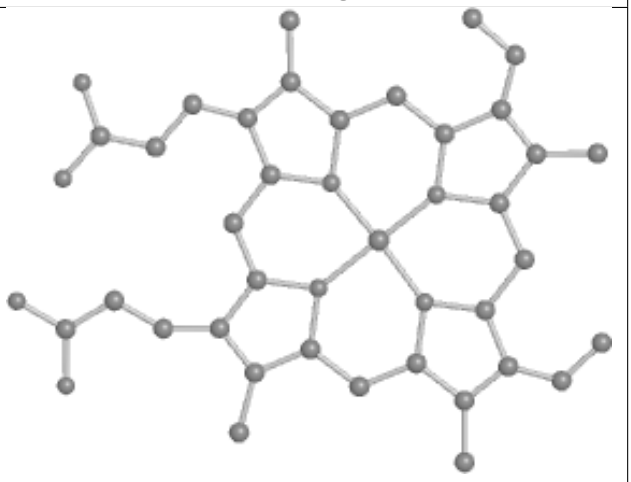
Bond lengths



Bond angles

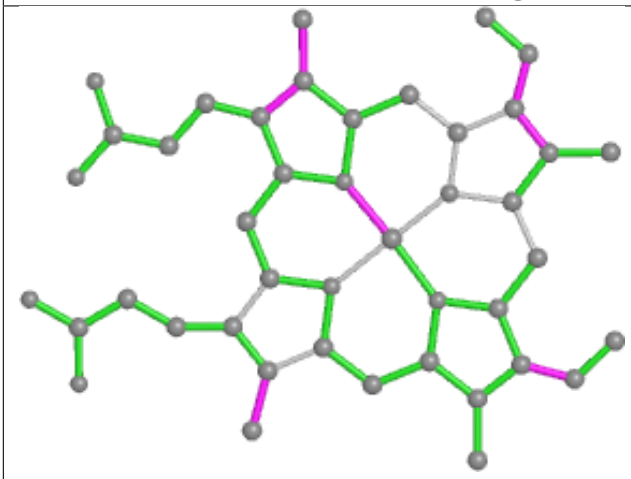


Torsions

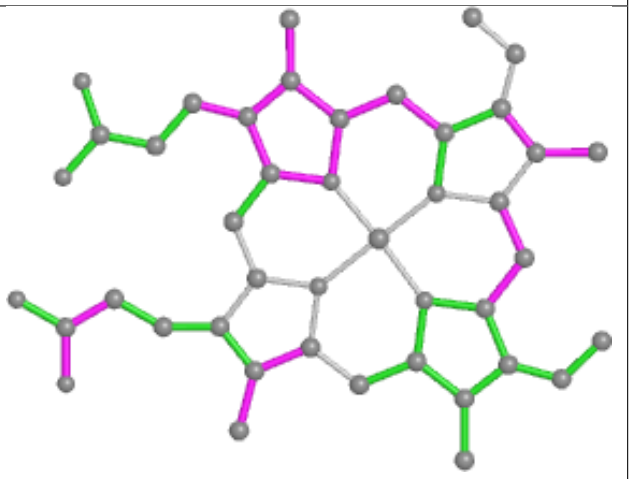


Rings

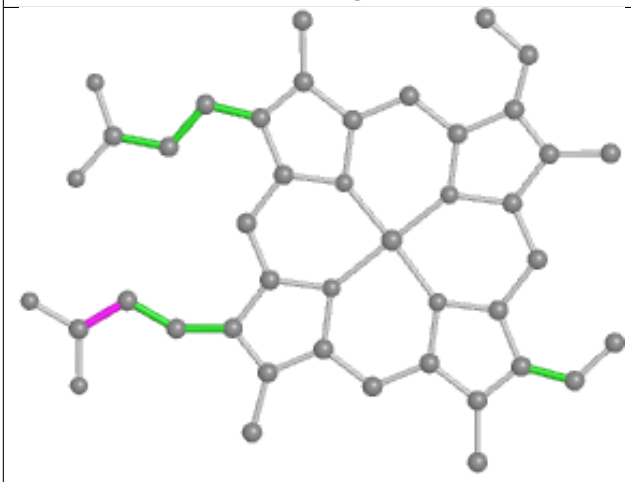
Ligand HEM O 1407



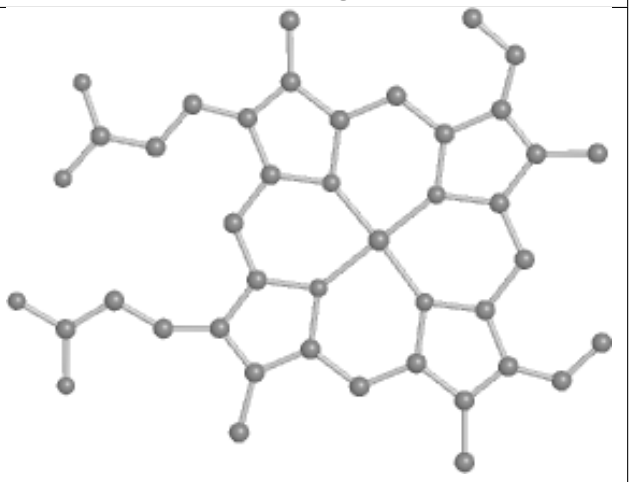
Bond lengths



Bond angles

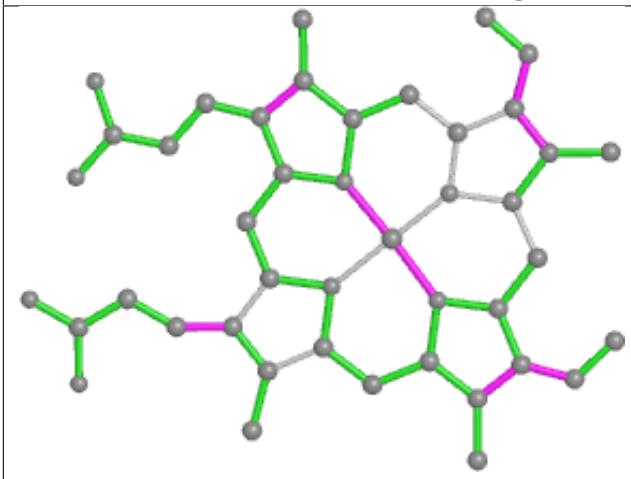


Torsions

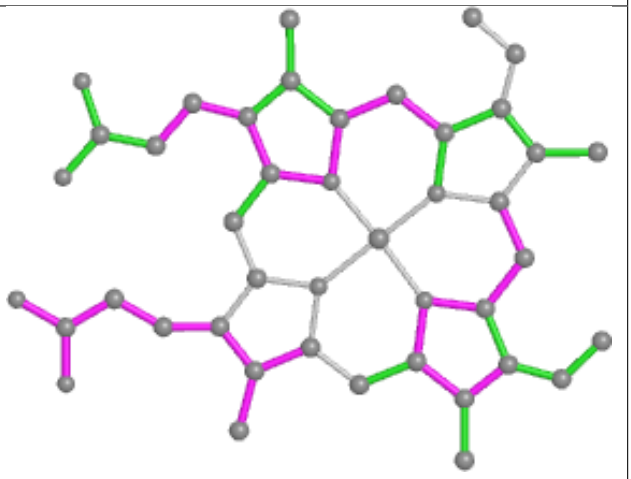


Rings

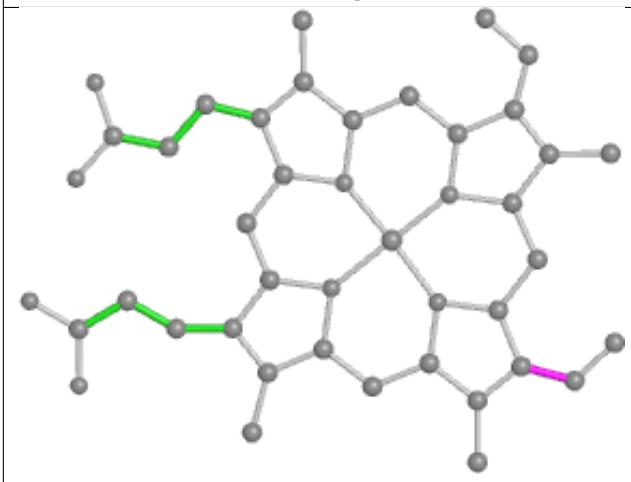
Ligand HEM P 1407



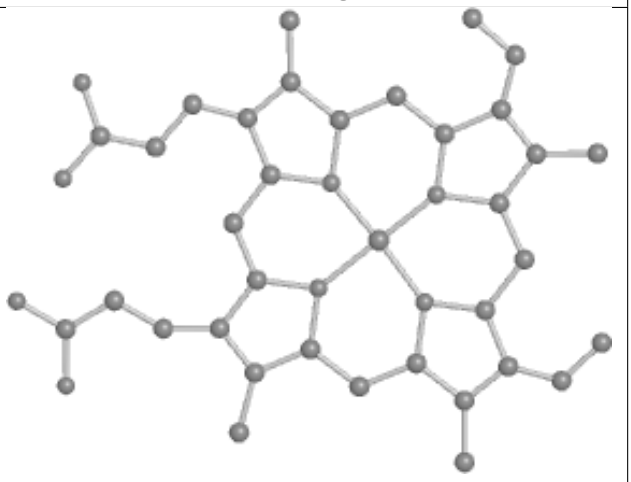
Bond lengths



Bond angles

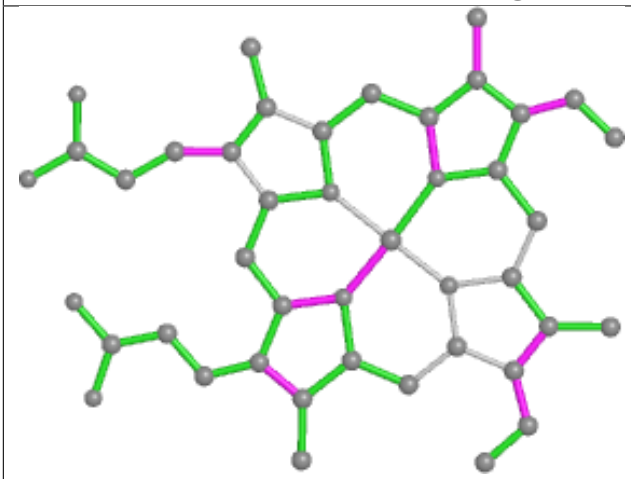


Torsions

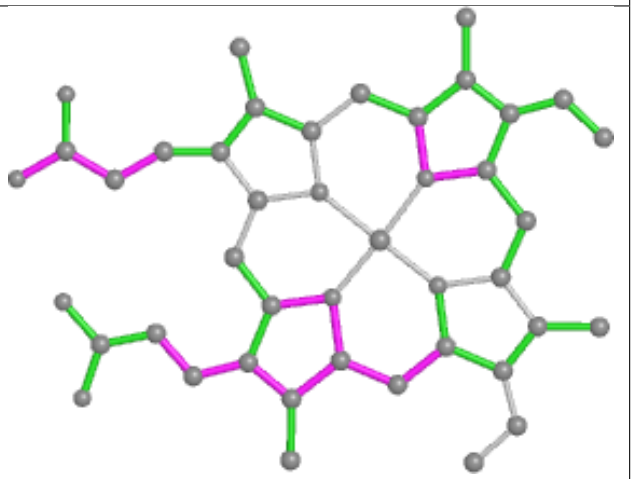


Rings

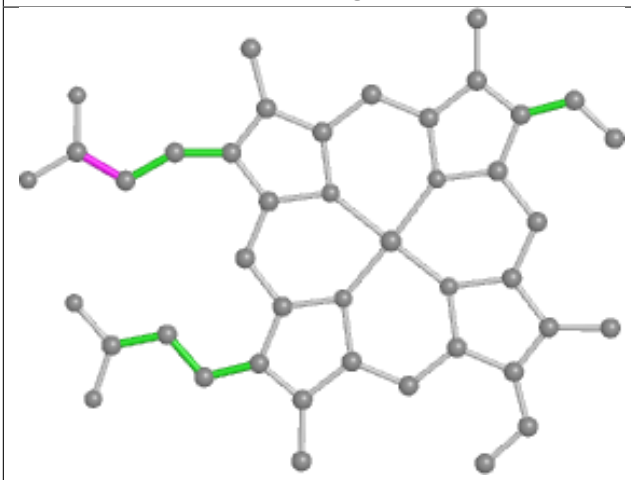
Ligand HEM D 1407



Bond lengths



Bond angles



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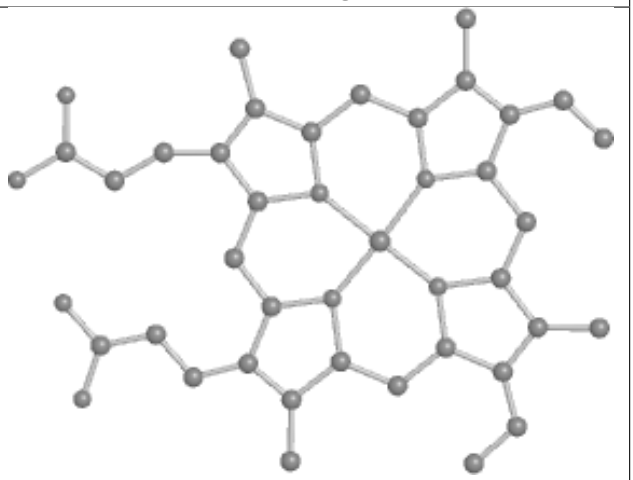
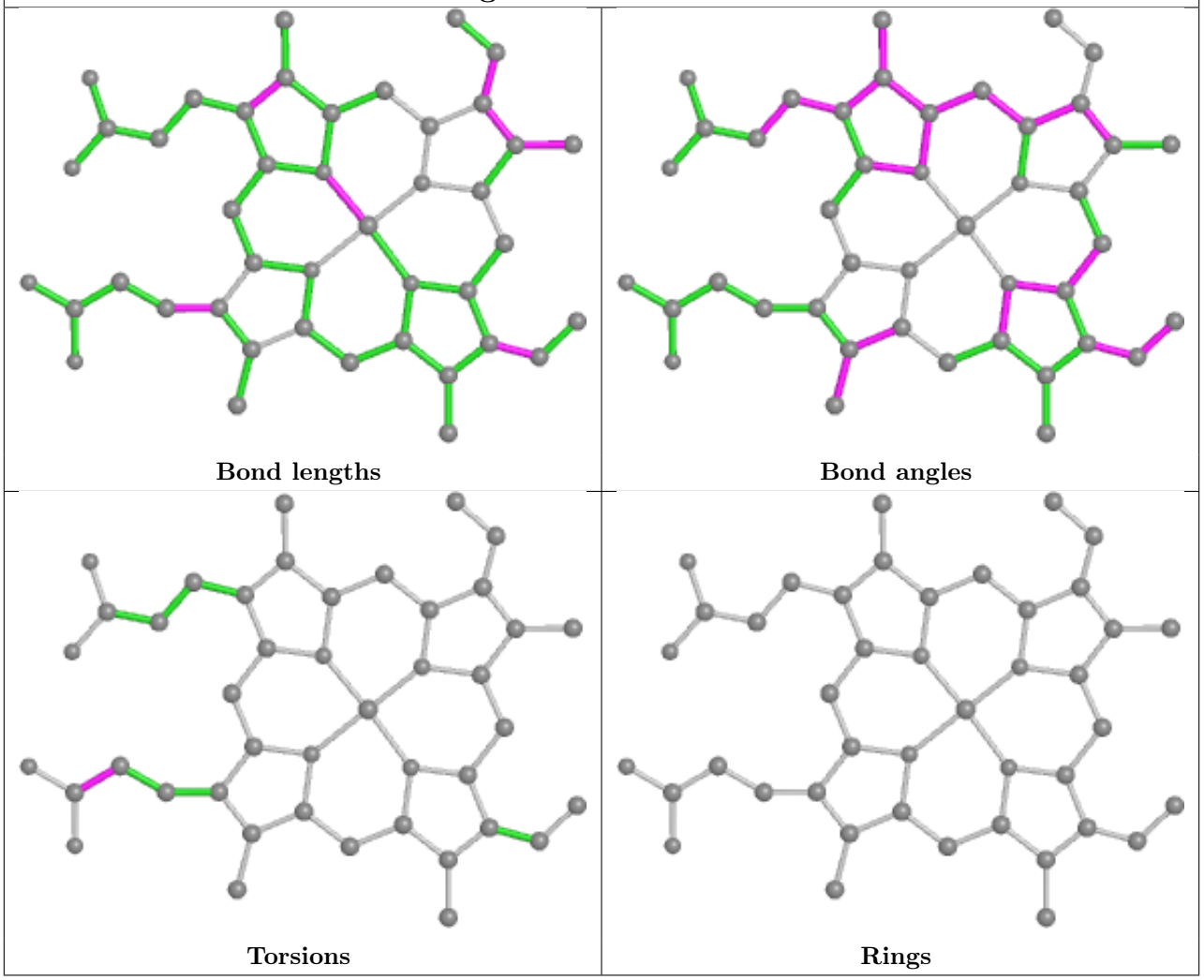


Rings

Ligand HEM E 1407



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	396/436 (90%)	-0.56	0 100 100	17, 33, 55, 71	0
1	B	397/436 (91%)	-0.48	2 (0%) 91 92	20, 35, 57, 76	0
1	C	396/436 (90%)	-0.54	0 100 100	16, 33, 55, 73	0
1	D	397/436 (91%)	-0.49	1 (0%) 94 95	18, 32, 55, 81	0
1	E	397/436 (91%)	-0.47	3 (0%) 86 87	16, 33, 55, 73	0
1	F	396/436 (90%)	-0.47	1 (0%) 94 95	16, 39, 66, 84	0
1	G	396/436 (90%)	-0.54	0 100 100	19, 35, 52, 61	0
1	H	396/436 (90%)	-0.46	3 (0%) 86 87	18, 35, 61, 87	0
1	I	396/436 (90%)	-0.45	2 (0%) 91 92	20, 38, 66, 79	0
1	J	397/436 (91%)	-0.42	1 (0%) 94 95	21, 42, 68, 91	0
1	K	397/436 (91%)	-0.34	1 (0%) 94 95	25, 46, 72, 90	0
1	L	397/436 (91%)	-0.26	2 (0%) 91 92	21, 50, 86, 99	0
1	M	397/436 (91%)	-0.17	5 (1%) 77 78	30, 53, 85, 91	0
1	N	397/436 (91%)	0.09	16 (4%) 38 37	34, 72, 116, 158	0
1	O	397/436 (91%)	0.04	18 (4%) 33 31	28, 57, 105, 133	0
1	P	396/436 (90%)	0.30	32 (8%) 12 10	29, 78, 129, 155	0
All	All	6345/6976 (90%)	-0.33	87 (1%) 75 77	16, 41, 91, 158	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	184	PRO	8.3
1	O	179	VAL	6.6
1	O	180	PHE	6.3
1	O	10	ALA	5.5
1	N	10	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	P	385	GLY	4.8
1	P	184	PRO	4.7
1	O	11	SER	4.7
1	P	13	PRO	4.5
1	P	180	PHE	4.4
1	O	185	ALA	4.4
1	O	377	ASP	4.4
1	O	13	PRO	4.3
1	P	375	CYS	4.1
1	P	377	ASP	4.1
1	N	37	ALA	4.0
1	P	269	LEU	3.9
1	P	380	LEU	3.8
1	P	32	TYR	3.6
1	N	271	ALA	3.6
1	H	382	VAL	3.6
1	N	24	PHE	3.5
1	P	23	ASP	3.5
1	N	23	ASP	3.5
1	P	257	TYR	3.5
1	O	178	PHE	3.5
1	M	37	ALA	3.5
1	O	14	VAL	3.4
1	I	179	VAL	3.4
1	O	384	PRO	3.2
1	P	381	ASP	3.1
1	P	267	ALA	3.1
1	N	180	PHE	3.1
1	P	384	PRO	3.1
1	M	10	ALA	3.0
1	P	24	PHE	3.0
1	D	10	ALA	3.0
1	O	187	ALA	2.9
1	P	382	VAL	2.9
1	L	180	PHE	2.9
1	P	31	THR	2.8
1	P	378	LEU	2.8
1	B	10	ALA	2.7
1	O	385	GLY	2.7
1	P	37	ALA	2.6
1	N	54	LEU	2.6
1	P	305	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	144	LEU	2.5
1	P	56	VAL	2.5
1	B	182	ASP	2.5
1	M	266	LEU	2.5
1	O	12	PRO	2.5
1	J	10	ALA	2.5
1	I	173	VAL	2.4
1	N	377	ASP	2.4
1	E	180	PHE	2.4
1	K	263	PRO	2.4
1	L	376	PRO	2.4
1	N	131	VAL	2.4
1	P	393	PRO	2.4
1	P	12	PRO	2.4
1	N	269	LEU	2.3
1	M	150	TRP	2.3
1	P	295	TYR	2.3
1	E	182	ASP	2.3
1	N	14	VAL	2.2
1	H	181	PRO	2.2
1	O	172	ARG	2.2
1	N	11	SER	2.1
1	N	181	PRO	2.1
1	P	318	VAL	2.1
1	O	86	ALA	2.1
1	P	273	MET	2.1
1	N	270	ARG	2.1
1	P	304	LEU	2.1
1	O	181	PRO	2.1
1	P	246	GLU	2.1
1	H	180	PHE	2.1
1	M	383	SER	2.1
1	P	329	PHE	2.1
1	N	15	LEU	2.1
1	F	179	VAL	2.1
1	P	266	LEU	2.1
1	N	371	LEU	2.0
1	E	10	ALA	2.0
1	P	308	VAL	2.0
1	P	376	PRO	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	17Q	C	1410	21/21	0.86	0.29	53,57,60,60	0
4	17Q	G	1410	21/21	0.90	0.27	39,49,55,55	0
3	SO4	D	1408	5/5	0.91	0.16	37,37,39,40	0
3	SO4	H	1408	5/5	0.95	0.18	42,42,44,45	0
3	SO4	I	1408	5/5	0.95	0.24	39,41,42,43	0
3	SO4	J	1408	5/5	0.95	0.20	41,42,42,43	0
3	SO4	O	1409	5/5	0.95	0.19	39,39,40,40	0
3	SO4	B	1408	5/5	0.95	0.16	61,62,63,63	0
3	SO4	A	1408	5/5	0.95	0.10	41,42,43,43	0
3	SO4	H	1409	5/5	0.96	0.13	38,39,40,40	0
3	SO4	F	1408	5/5	0.96	0.15	38,39,40,41	0
2	HEM	P	1407	43/43	0.96	0.16	36,46,51,54	0
3	SO4	O	1408	5/5	0.97	0.18	41,41,42,42	0
2	HEM	E	1407	43/43	0.97	0.13	13,18,21,23	0
2	HEM	I	1407	43/43	0.97	0.14	23,25,29,31	0
2	HEM	O	1407	43/43	0.97	0.14	29,33,38,41	0
3	SO4	B	1409	5/5	0.98	0.12	49,49,51,51	0
2	HEM	D	1407	43/43	0.98	0.12	13,18,22,23	0
2	HEM	J	1407	43/43	0.98	0.15	26,28,31,32	0
2	HEM	K	1407	43/43	0.98	0.13	21,25,27,29	0
2	HEM	L	1407	43/43	0.98	0.13	19,24,27,31	0
2	HEM	M	1407	43/43	0.98	0.12	18,23,26,31	0
2	HEM	N	1407	43/43	0.98	0.13	29,33,44,49	0
2	HEM	B	1407	43/43	0.98	0.12	19,25,27,29	0
2	HEM	F	1407	43/43	0.98	0.14	17,22,24,26	0
2	HEM	G	1407	43/43	0.98	0.13	17,23,24,28	0
2	HEM	H	1407	43/43	0.98	0.14	15,19,21,22	0

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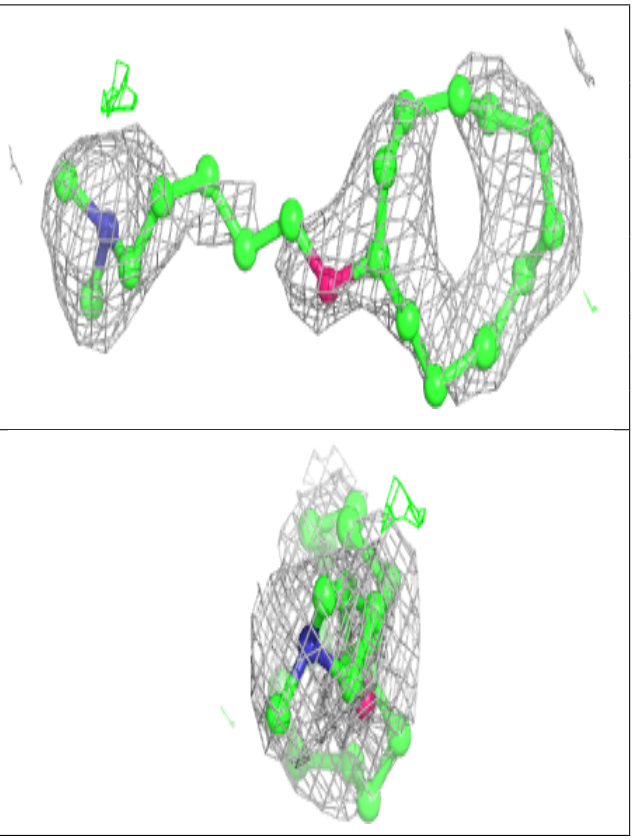
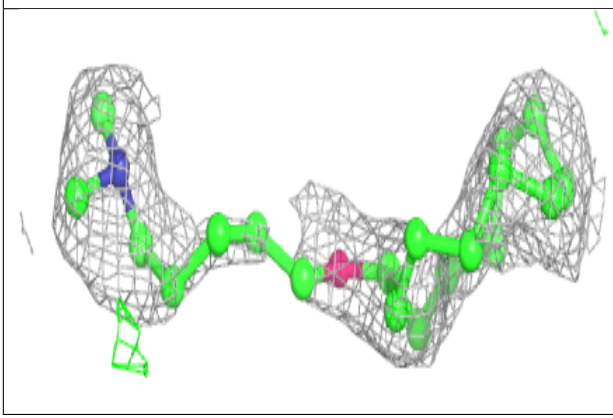
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	I	1409	5/5	0.99	0.05	53,54,55,55	0
2	HEM	C	1407	43/43	0.99	0.14	12,14,19,24	0
2	HEM	A	1407	43/43	0.99	0.12	14,20,24,28	0

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 17Q C 1410:

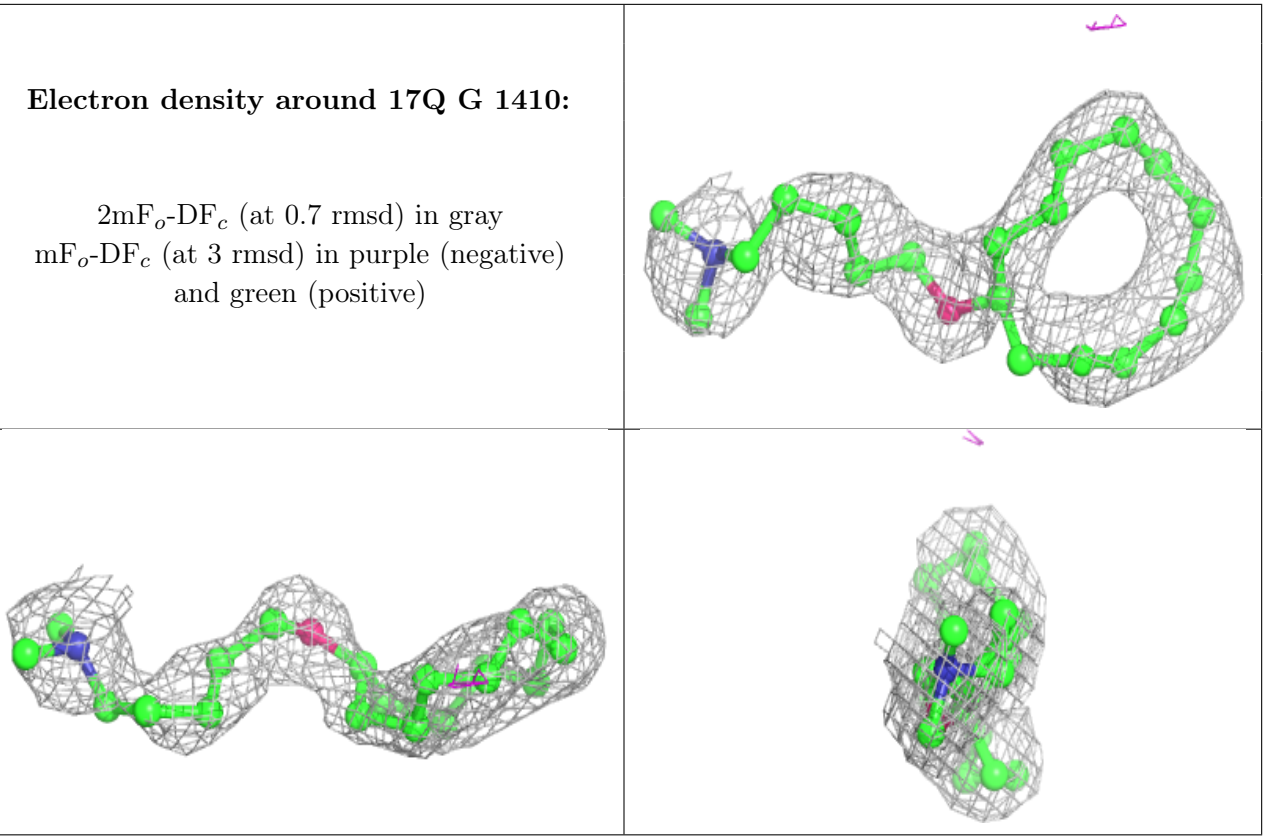
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





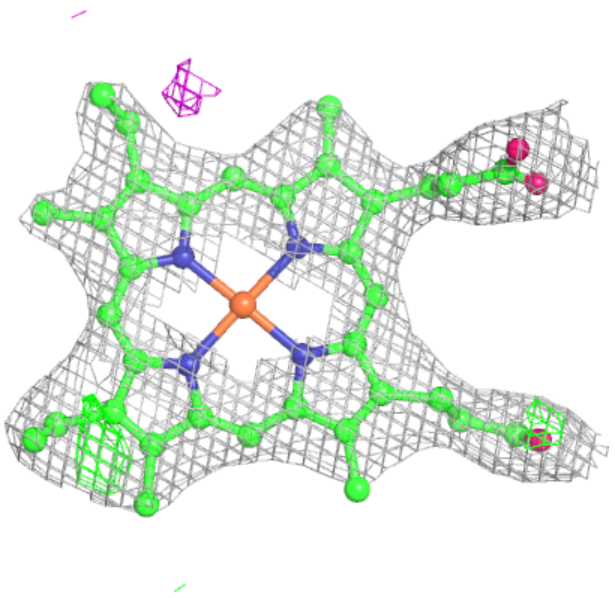
Electron density around 17Q G 1410:

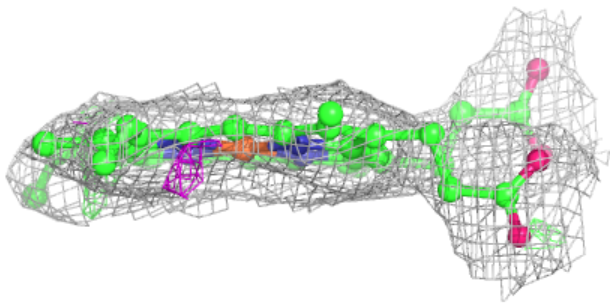
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

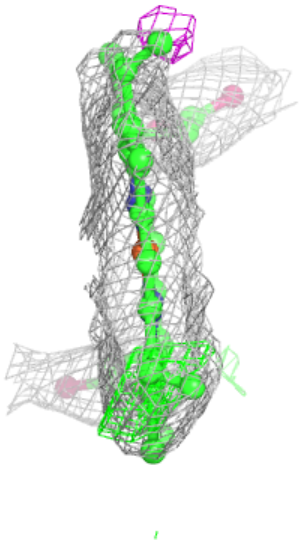


Electron density around HEM P 1407:

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

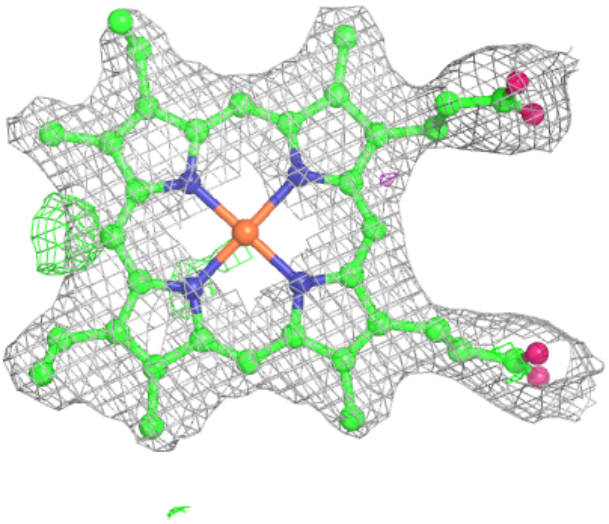


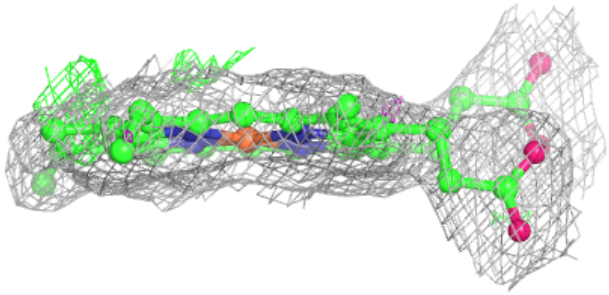


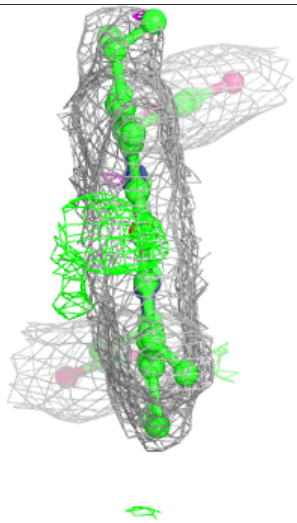


Electron density around HEM E 1407:

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

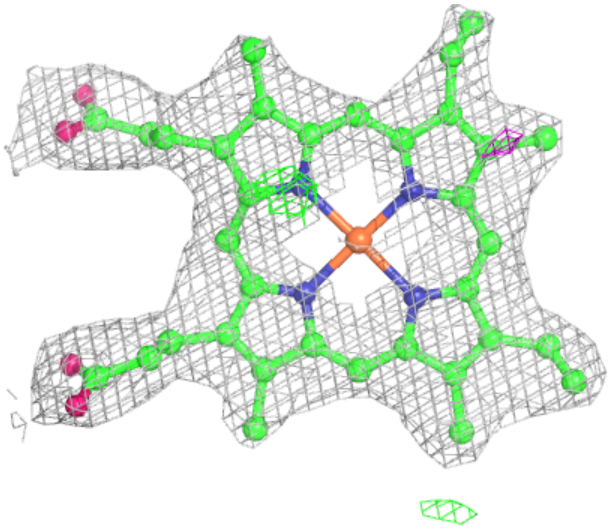


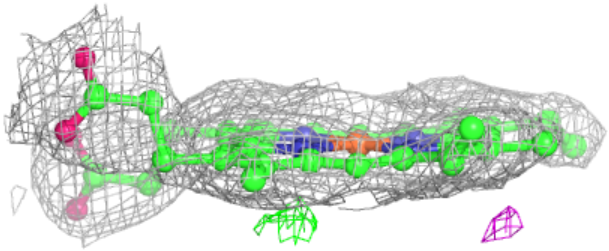


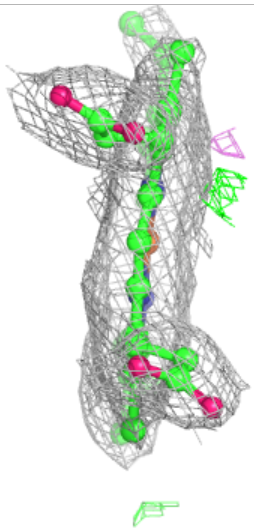


Electron density around HEM I 1407:

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

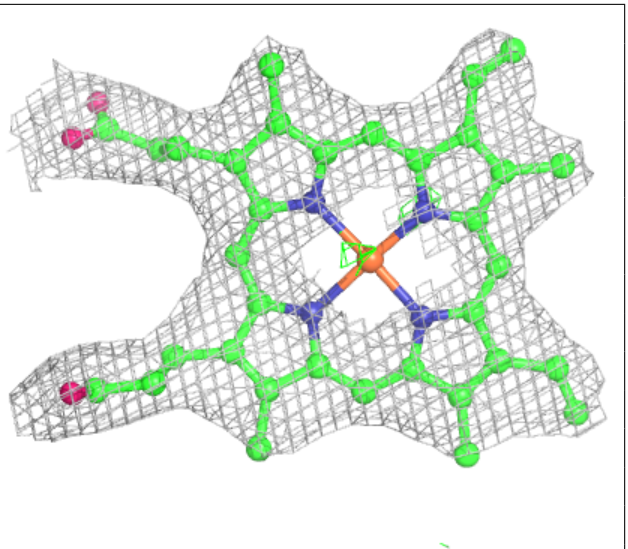


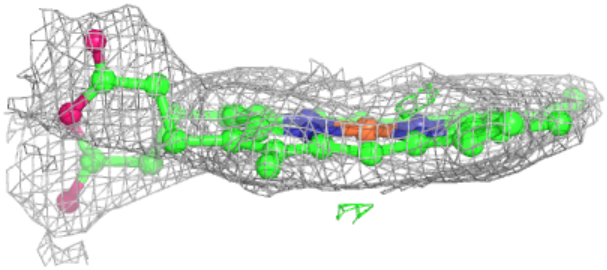


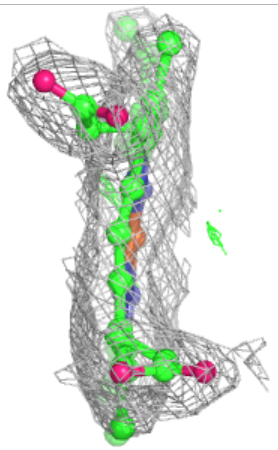


Electron density around HEM O 1407:

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

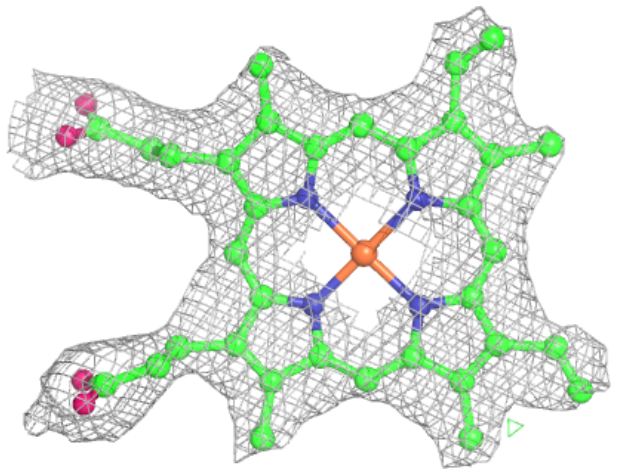


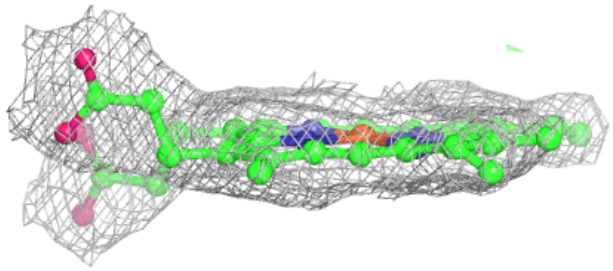


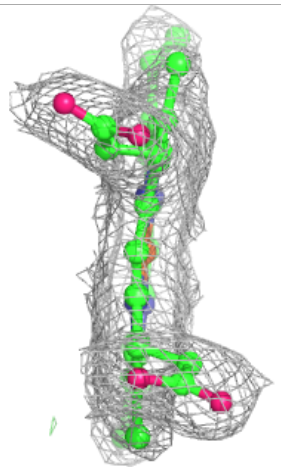


Electron density around HEM D 1407:

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

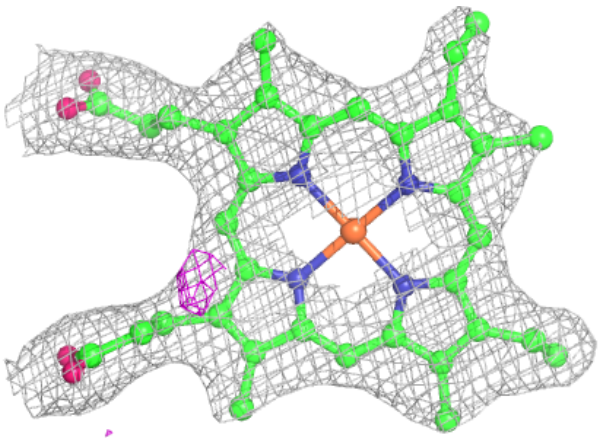


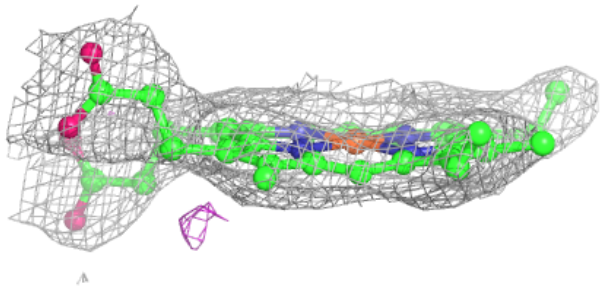


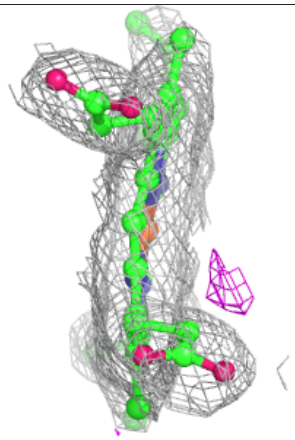


Electron density around HEM J 1407:

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

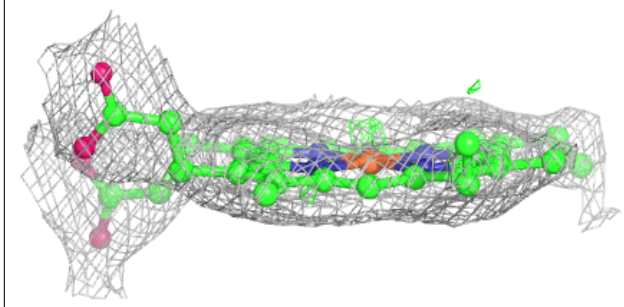


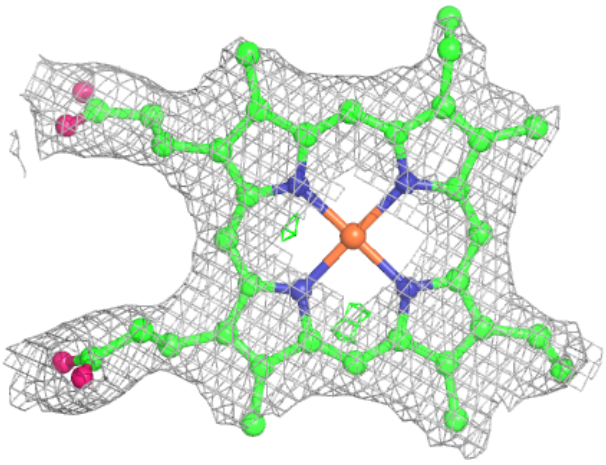


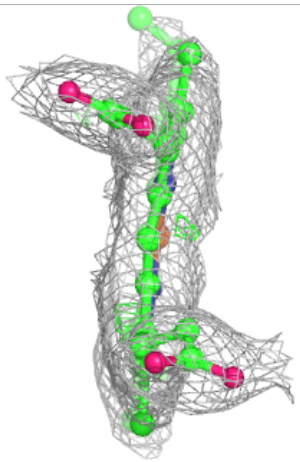


Electron density around HEM K 1407:

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

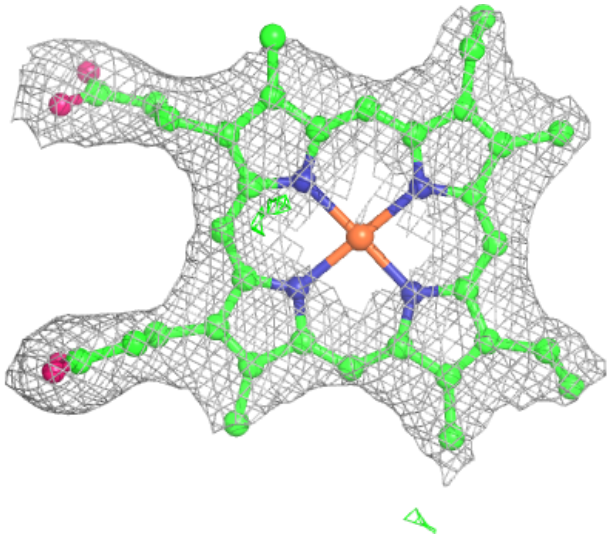


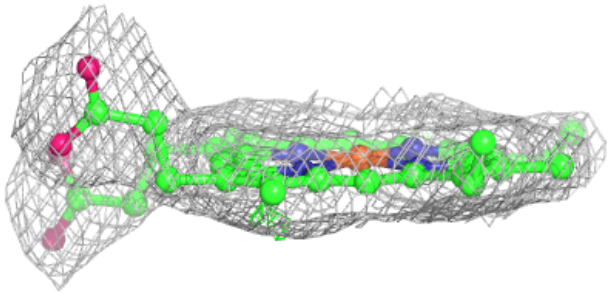


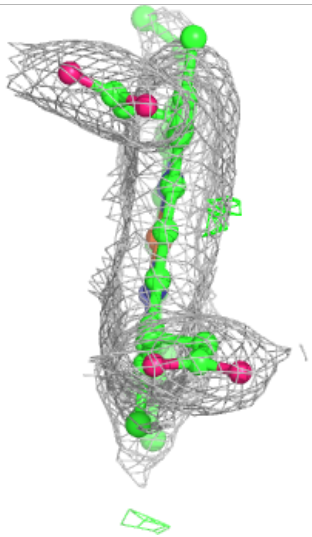


Electron density around HEM L 1407:

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

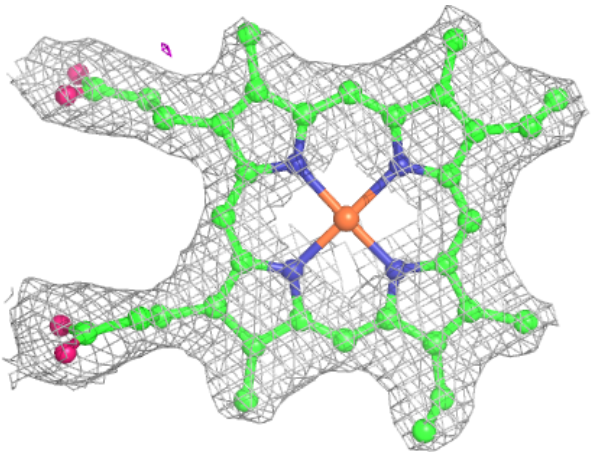


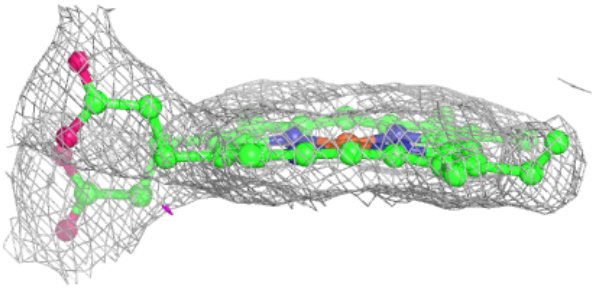


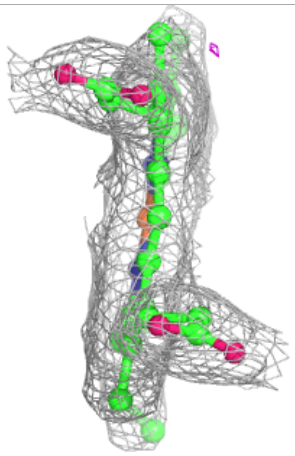


Electron density around HEM M 1407:

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

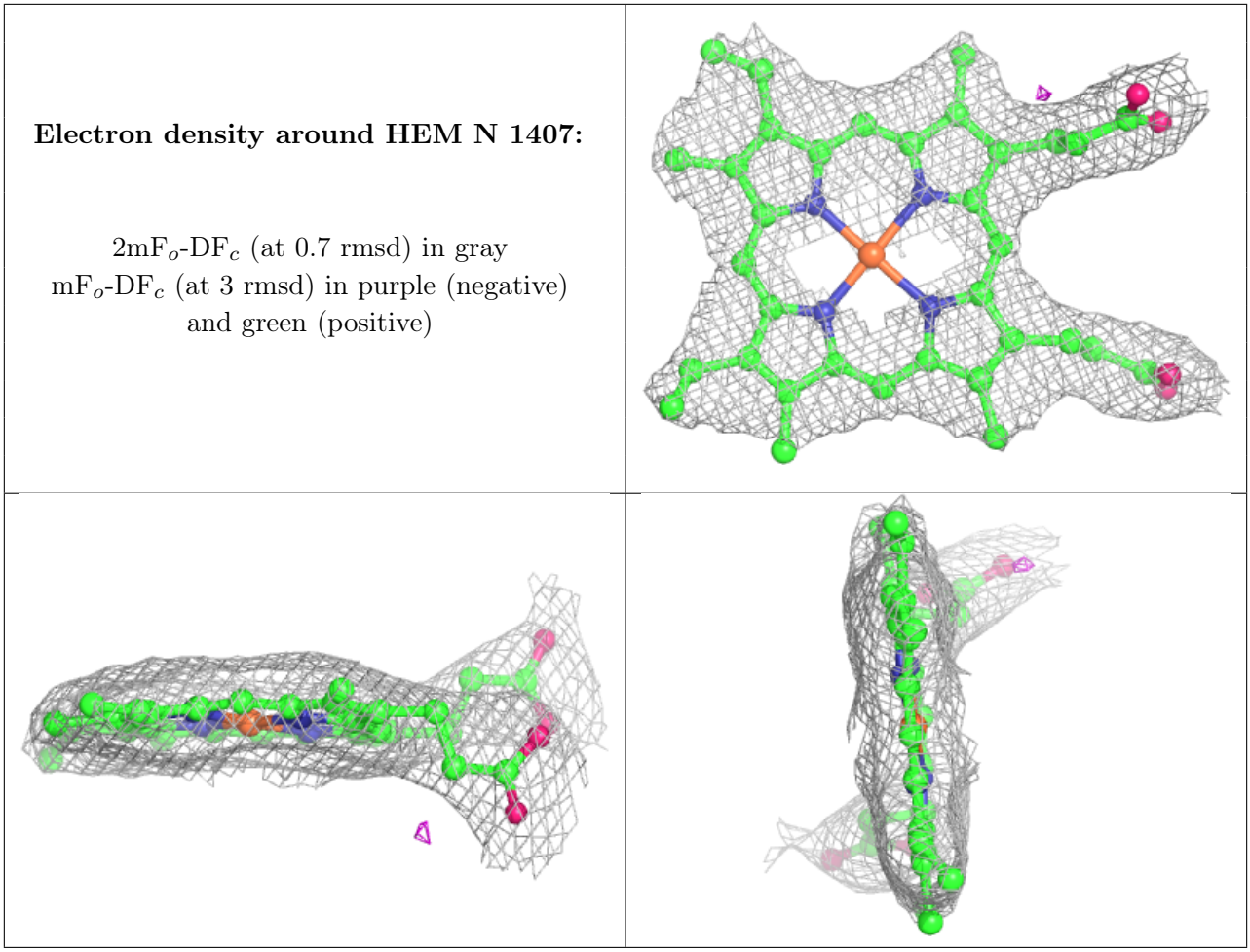






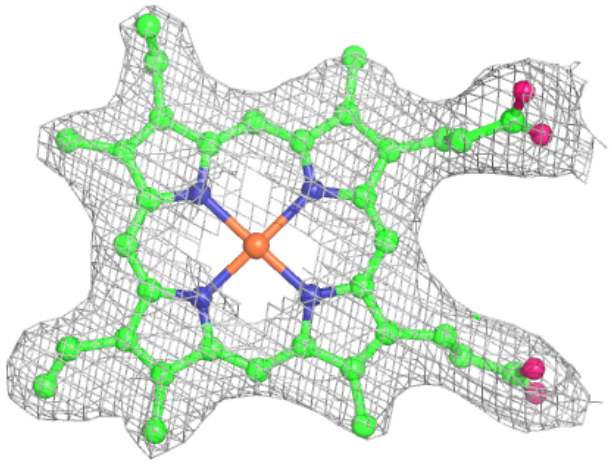
Electron density around HEM N 1407:

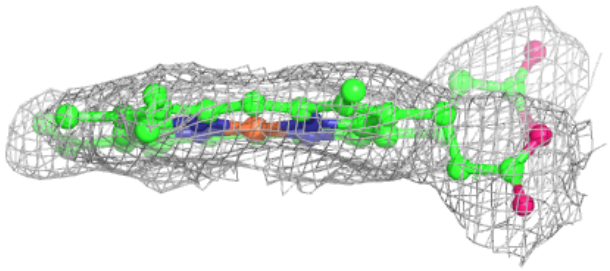
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

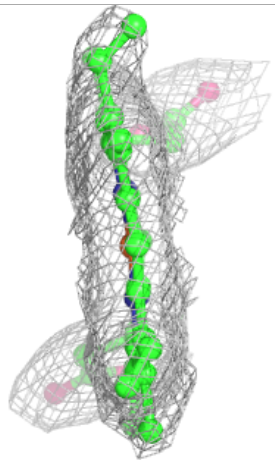


Electron density around HEM B 1407:

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

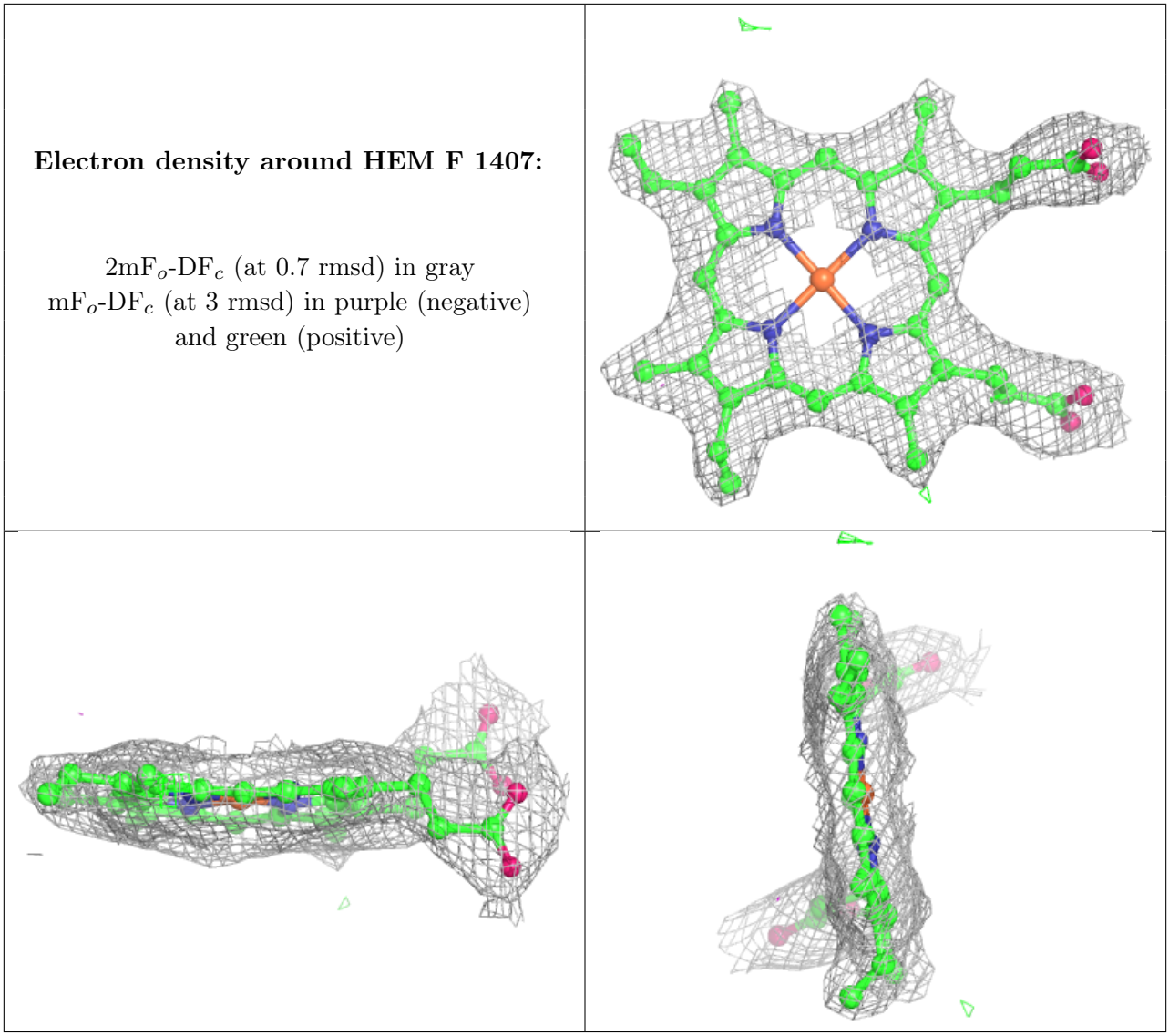






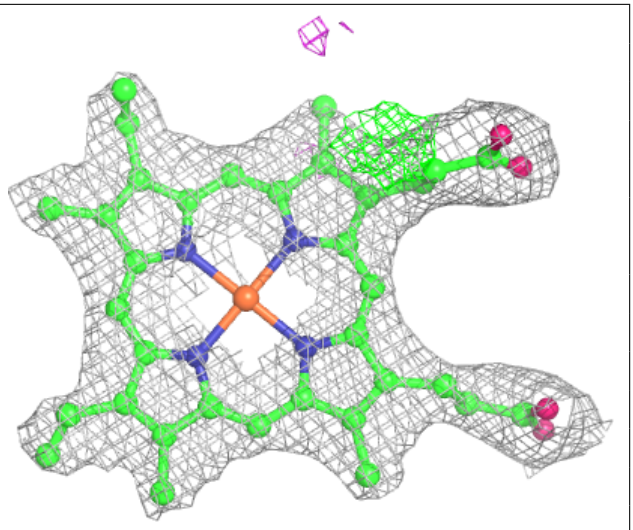
Electron density around HEM F 1407:

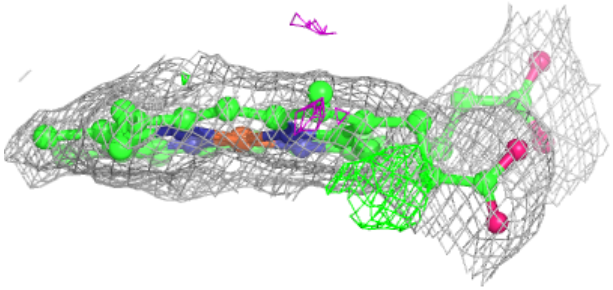
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

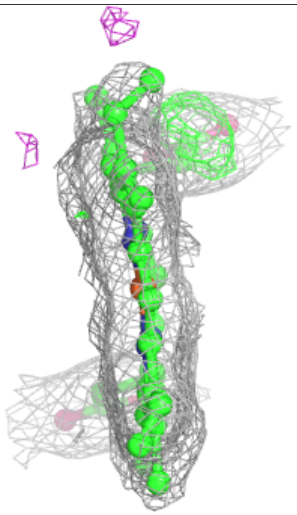


Electron density around HEM G 1407:

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

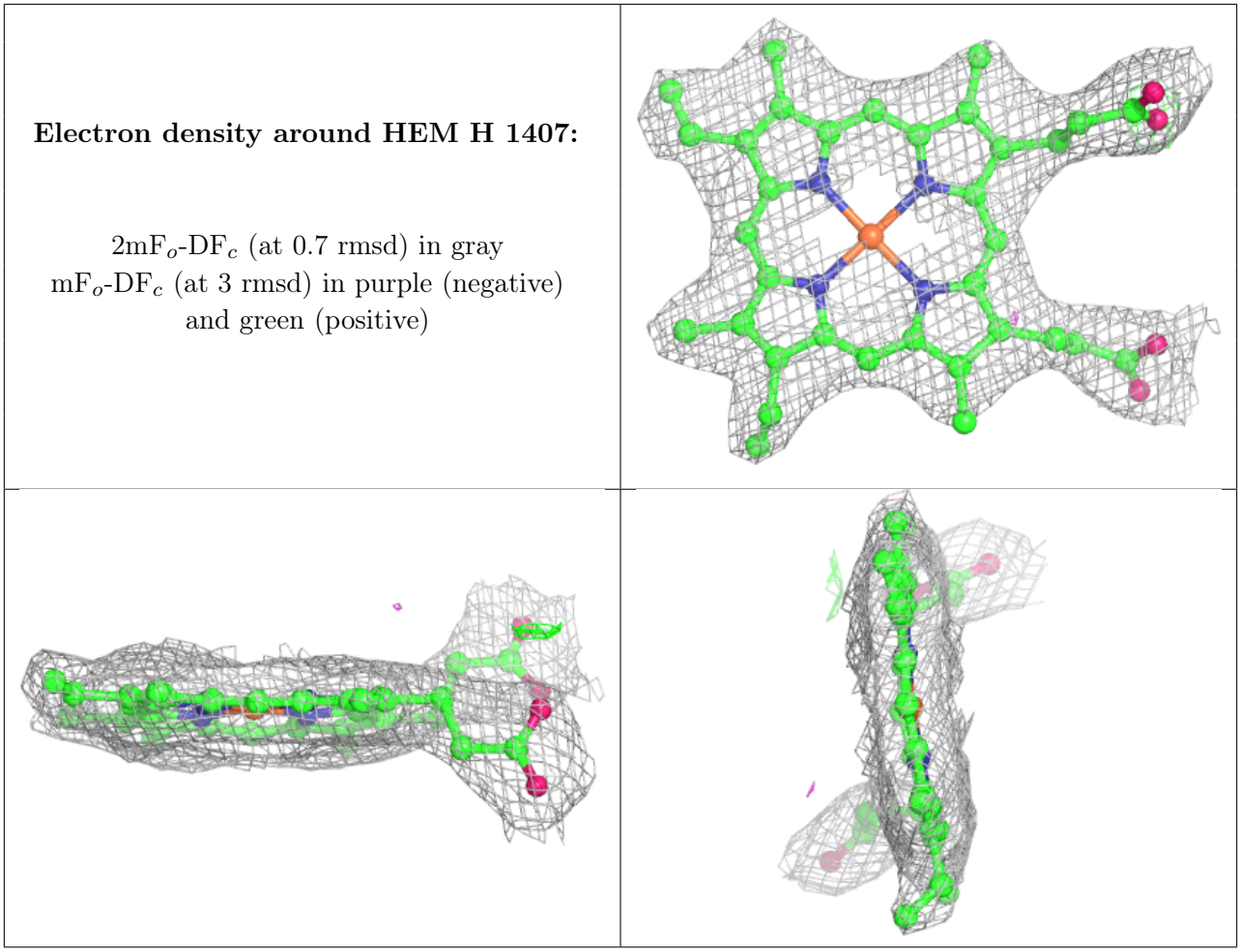






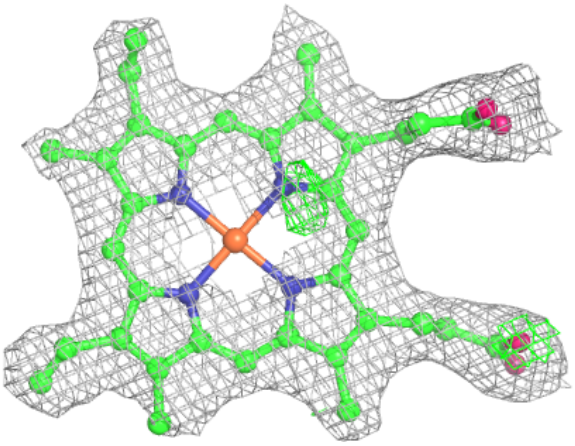
Electron density around HEM H 1407:

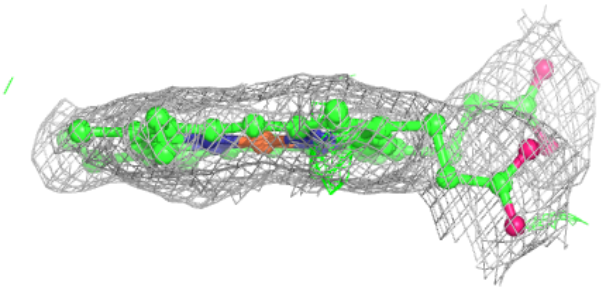
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

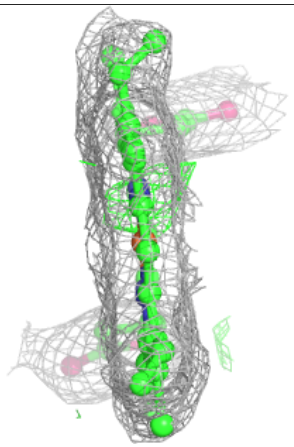


Electron density around HEM C 1407:

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

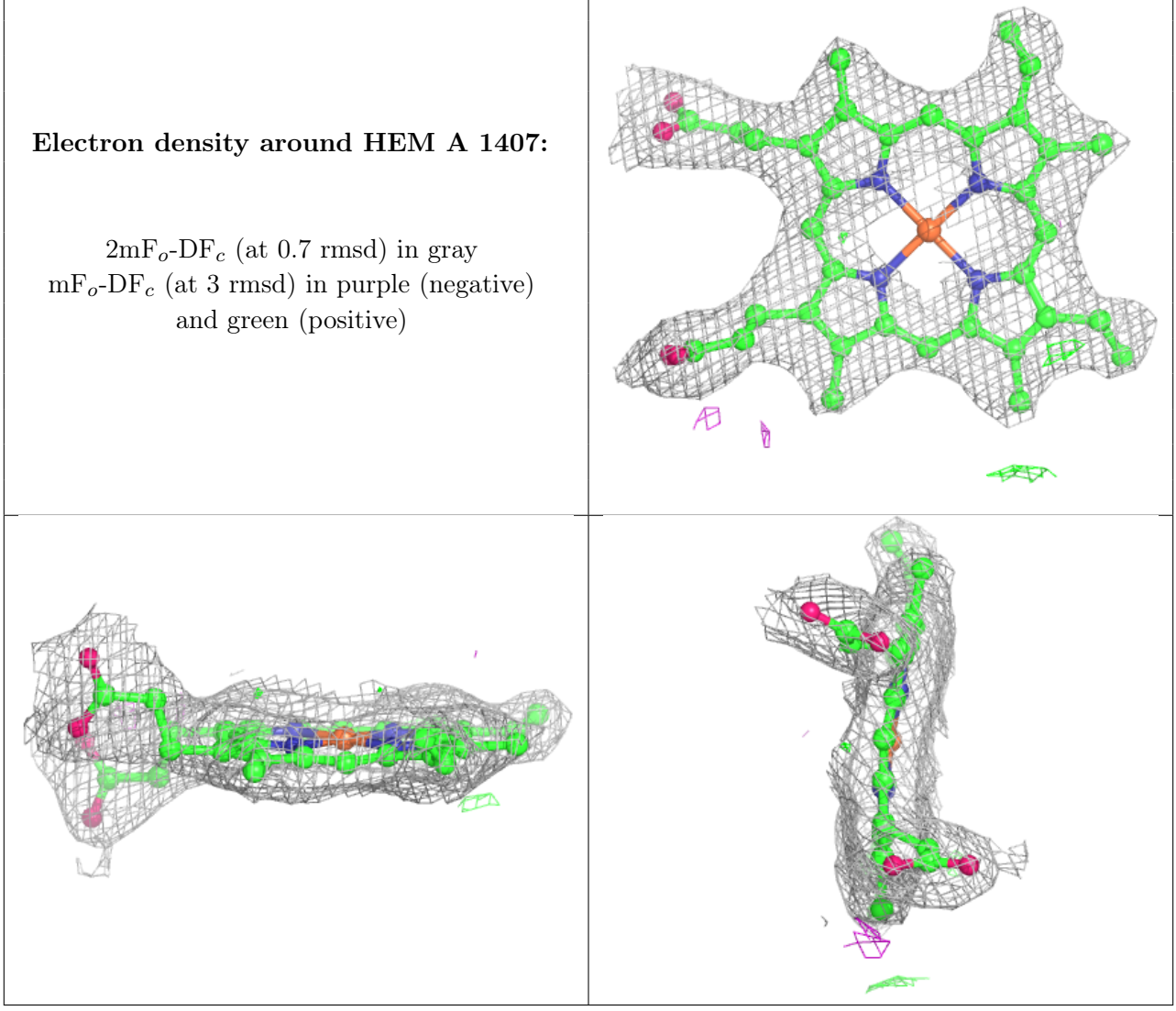






Electron density around HEM A 1407:

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



6.5 Other polymers (i)

There are no such residues in this entry.