Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2024 – 12:59 pm BST

PDB ID	:	4ZGX
Title	:	Structure of aldosterone synthase (CYP11B2) in complex with (+)-(R)-N-(4-(4-chloro-3-fluorophenyl)-5,6,7,8-tetrahydroisoquinolin-8-yl)propionamide
Authors	:	Kuglstatter, A.; Joseph, C.
Deposited on	:	2015-04-24
Resolution	:	3.20 Å(reported)

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

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

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

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

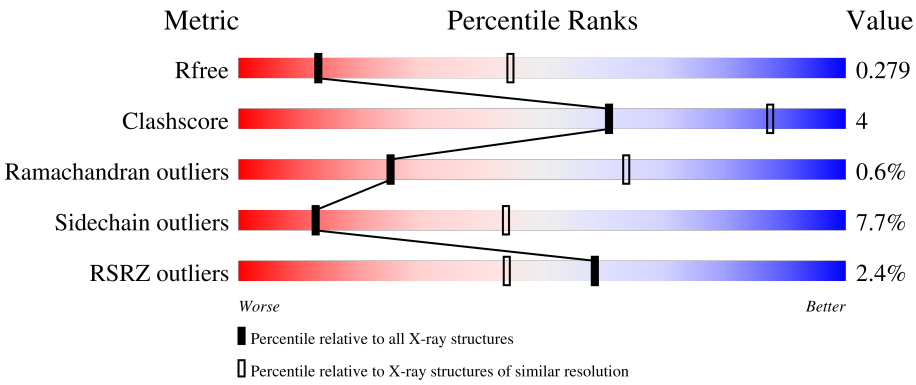
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	489	80% 13% • 5%
1	B	489	.% 83% 11% • 5%
1	C	489	.% 81% 12% • 5%
1	D	489	.% 79% 14% • 5%
1	E	489	2% 82% 11% • 6%

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Mol	Chain	Length	Quality of chain
1	F	489	2% 79% 14% • 5%
1	G	489	4% 80% 12% • 5%
1	H	489	4% 78% 15% • 5%
1	I	489	4% 76% 16% • 6%
1	J	489	4% 78% 15% • 5%
1	K	489	% 79% 13% • 6%
1	L	489	3% 77% 17% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 46675 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 11B2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3774	2439	666	649	20	0	0	0
1	B	465	3774	2439	666	649	20	0	0	0
1	C	465	3774	2439	666	649	20	0	0	0
1	D	465	3774	2439	666	649	20	0	0	0
1	E	459	3731	2412	658	641	20	0	0	0
1	F	464	3770	2437	665	648	20	0	0	0
1	G	465	3774	2439	666	649	20	0	0	0
1	H	465	3774	2439	666	649	20	0	0	0
1	I	458	3721	2406	655	640	20	0	0	0
1	J	463	3762	2431	664	647	20	0	0	0
1	K	461	3737	2416	657	644	20	0	0	0
1	L	462	3747	2422	661	644	20	0	0	0

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP P19099
A	25	ALA	-	expression tag	UNP P19099
A	26	THR	-	expression tag	UNP P19099
A	27	LYS	-	expression tag	UNP P19099
A	504	GLY	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	505	GLY	-	expression tag	UNP P19099
A	506	ARG	-	expression tag	UNP P19099
A	507	HIS	-	expression tag	UNP P19099
A	508	HIS	-	expression tag	UNP P19099
A	509	HIS	-	expression tag	UNP P19099
A	510	HIS	-	expression tag	UNP P19099
A	511	HIS	-	expression tag	UNP P19099
A	512	HIS	-	expression tag	UNP P19099
B	24	MET	-	expression tag	UNP P19099
B	25	ALA	-	expression tag	UNP P19099
B	26	THR	-	expression tag	UNP P19099
B	27	LYS	-	expression tag	UNP P19099
B	504	GLY	-	expression tag	UNP P19099
B	505	GLY	-	expression tag	UNP P19099
B	506	ARG	-	expression tag	UNP P19099
B	507	HIS	-	expression tag	UNP P19099
B	508	HIS	-	expression tag	UNP P19099
B	509	HIS	-	expression tag	UNP P19099
B	510	HIS	-	expression tag	UNP P19099
B	511	HIS	-	expression tag	UNP P19099
B	512	HIS	-	expression tag	UNP P19099
C	24	MET	-	expression tag	UNP P19099
C	25	ALA	-	expression tag	UNP P19099
C	26	THR	-	expression tag	UNP P19099
C	27	LYS	-	expression tag	UNP P19099
C	504	GLY	-	expression tag	UNP P19099
C	505	GLY	-	expression tag	UNP P19099
C	506	ARG	-	expression tag	UNP P19099
C	507	HIS	-	expression tag	UNP P19099
C	508	HIS	-	expression tag	UNP P19099
C	509	HIS	-	expression tag	UNP P19099
C	510	HIS	-	expression tag	UNP P19099
C	511	HIS	-	expression tag	UNP P19099
C	512	HIS	-	expression tag	UNP P19099
D	24	MET	-	expression tag	UNP P19099
D	25	ALA	-	expression tag	UNP P19099
D	26	THR	-	expression tag	UNP P19099
D	27	LYS	-	expression tag	UNP P19099
D	504	GLY	-	expression tag	UNP P19099
D	505	GLY	-	expression tag	UNP P19099
D	506	ARG	-	expression tag	UNP P19099
D	507	HIS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
D	508	HIS	-	expression tag	UNP P19099
D	509	HIS	-	expression tag	UNP P19099
D	510	HIS	-	expression tag	UNP P19099
D	511	HIS	-	expression tag	UNP P19099
D	512	HIS	-	expression tag	UNP P19099
E	24	MET	-	expression tag	UNP P19099
E	25	ALA	-	expression tag	UNP P19099
E	26	THR	-	expression tag	UNP P19099
E	27	LYS	-	expression tag	UNP P19099
E	504	GLY	-	expression tag	UNP P19099
E	505	GLY	-	expression tag	UNP P19099
E	506	ARG	-	expression tag	UNP P19099
E	507	HIS	-	expression tag	UNP P19099
E	508	HIS	-	expression tag	UNP P19099
E	509	HIS	-	expression tag	UNP P19099
E	510	HIS	-	expression tag	UNP P19099
E	511	HIS	-	expression tag	UNP P19099
E	512	HIS	-	expression tag	UNP P19099
F	24	MET	-	expression tag	UNP P19099
F	25	ALA	-	expression tag	UNP P19099
F	26	THR	-	expression tag	UNP P19099
F	27	LYS	-	expression tag	UNP P19099
F	504	GLY	-	expression tag	UNP P19099
F	505	GLY	-	expression tag	UNP P19099
F	506	ARG	-	expression tag	UNP P19099
F	507	HIS	-	expression tag	UNP P19099
F	508	HIS	-	expression tag	UNP P19099
F	509	HIS	-	expression tag	UNP P19099
F	510	HIS	-	expression tag	UNP P19099
F	511	HIS	-	expression tag	UNP P19099
F	512	HIS	-	expression tag	UNP P19099
G	24	MET	-	expression tag	UNP P19099
G	25	ALA	-	expression tag	UNP P19099
G	26	THR	-	expression tag	UNP P19099
G	27	LYS	-	expression tag	UNP P19099
G	504	GLY	-	expression tag	UNP P19099
G	505	GLY	-	expression tag	UNP P19099
G	506	ARG	-	expression tag	UNP P19099
G	507	HIS	-	expression tag	UNP P19099
G	508	HIS	-	expression tag	UNP P19099
G	509	HIS	-	expression tag	UNP P19099
G	510	HIS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
G	511	HIS	-	expression tag	UNP P19099
G	512	HIS	-	expression tag	UNP P19099
H	24	MET	-	expression tag	UNP P19099
H	25	ALA	-	expression tag	UNP P19099
H	26	THR	-	expression tag	UNP P19099
H	27	LYS	-	expression tag	UNP P19099
H	504	GLY	-	expression tag	UNP P19099
H	505	GLY	-	expression tag	UNP P19099
H	506	ARG	-	expression tag	UNP P19099
H	507	HIS	-	expression tag	UNP P19099
H	508	HIS	-	expression tag	UNP P19099
H	509	HIS	-	expression tag	UNP P19099
H	510	HIS	-	expression tag	UNP P19099
H	511	HIS	-	expression tag	UNP P19099
H	512	HIS	-	expression tag	UNP P19099
I	24	MET	-	expression tag	UNP P19099
I	25	ALA	-	expression tag	UNP P19099
I	26	THR	-	expression tag	UNP P19099
I	27	LYS	-	expression tag	UNP P19099
I	504	GLY	-	expression tag	UNP P19099
I	505	GLY	-	expression tag	UNP P19099
I	506	ARG	-	expression tag	UNP P19099
I	507	HIS	-	expression tag	UNP P19099
I	508	HIS	-	expression tag	UNP P19099
I	509	HIS	-	expression tag	UNP P19099
I	510	HIS	-	expression tag	UNP P19099
I	511	HIS	-	expression tag	UNP P19099
I	512	HIS	-	expression tag	UNP P19099
J	24	MET	-	expression tag	UNP P19099
J	25	ALA	-	expression tag	UNP P19099
J	26	THR	-	expression tag	UNP P19099
J	27	LYS	-	expression tag	UNP P19099
J	504	GLY	-	expression tag	UNP P19099
J	505	GLY	-	expression tag	UNP P19099
J	506	ARG	-	expression tag	UNP P19099
J	507	HIS	-	expression tag	UNP P19099
J	508	HIS	-	expression tag	UNP P19099
J	509	HIS	-	expression tag	UNP P19099
J	510	HIS	-	expression tag	UNP P19099
J	511	HIS	-	expression tag	UNP P19099
J	512	HIS	-	expression tag	UNP P19099
K	24	MET	-	expression tag	UNP P19099

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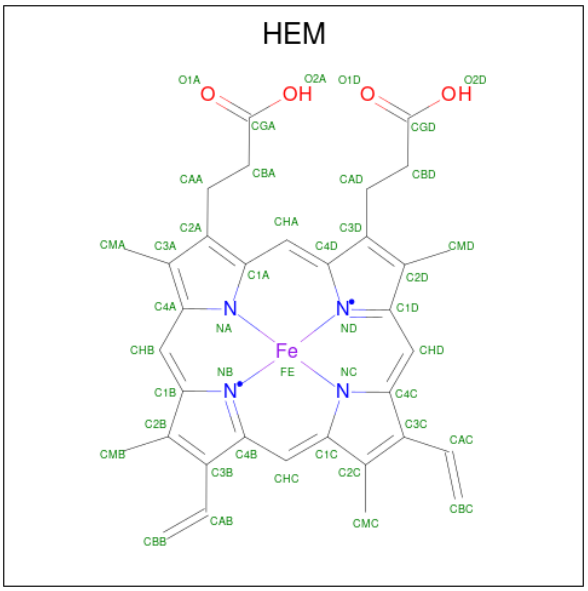
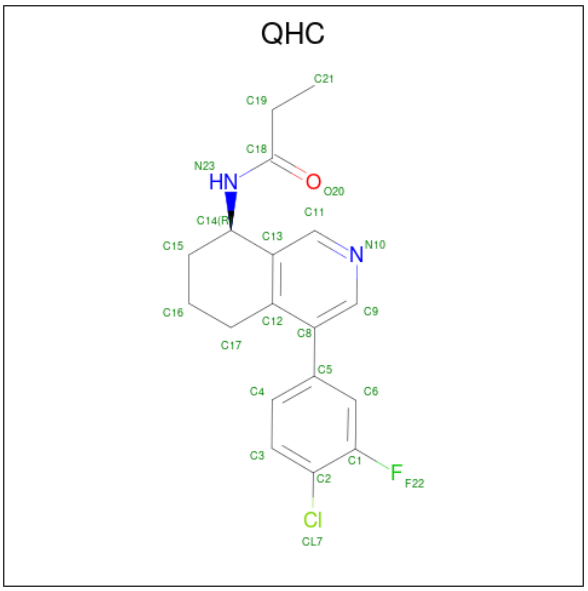
Chain	Residue	Modelled	Actual	Comment	Reference
K	25	ALA	-	expression tag	UNP P19099
K	26	THR	-	expression tag	UNP P19099
K	27	LYS	-	expression tag	UNP P19099
K	504	GLY	-	expression tag	UNP P19099
K	505	GLY	-	expression tag	UNP P19099
K	506	ARG	-	expression tag	UNP P19099
K	507	HIS	-	expression tag	UNP P19099
K	508	HIS	-	expression tag	UNP P19099
K	509	HIS	-	expression tag	UNP P19099
K	510	HIS	-	expression tag	UNP P19099
K	511	HIS	-	expression tag	UNP P19099
K	512	HIS	-	expression tag	UNP P19099
L	24	MET	-	expression tag	UNP P19099
L	25	ALA	-	expression tag	UNP P19099
L	26	THR	-	expression tag	UNP P19099
L	27	LYS	-	expression tag	UNP P19099
L	504	GLY	-	expression tag	UNP P19099
L	505	GLY	-	expression tag	UNP P19099
L	506	ARG	-	expression tag	UNP P19099
L	507	HIS	-	expression tag	UNP P19099
L	508	HIS	-	expression tag	UNP P19099
L	509	HIS	-	expression tag	UNP P19099
L	510	HIS	-	expression tag	UNP P19099
L	511	HIS	-	expression tag	UNP P19099
L	512	HIS	-	expression tag	UNP P19099

- 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0
2	C	1	43	34	1	4	4	0	0
2	D	1	43	34	1	4	4	0	0
2	E	1	43	34	1	4	4	0	0
2	F	1	43	34	1	4	4	0	0
2	G	1	43	34	1	4	4	0	0
2	H	1	43	34	1	4	4	0	0
2	I	1	43	34	1	4	4	0	0
2	J	1	43	34	1	4	4	0	0
2	K	1	43	34	1	4	4	0	0
2	L	1	43	34	1	4	4	0	0

- Molecule 3 is N-[(8R)-4-(4-chloro-3-fluorophenyl)-5,6,7,8-tetrahydroisoquinolin-8-yl]propanamide (three-letter code: QHC) (formula: $C_{18}H_{18}ClFN_2O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
3	A	1	23	18	1	1	2	1	0	0
3	B	1	23	18	1	1	2	1	0	0
3	C	1	23	18	1	1	2	1	0	0
3	D	1	23	18	1	1	2	1	0	0
3	E	1	23	18	1	1	2	1	0	0
3	F	1	23	18	1	1	2	1	0	0
3	I	1	23	18	1	1	2	1	0	0
3	J	1	23	18	1	1	2	1	0	0
3	K	1	23	18	1	1	2	1	0	0
3	L	1	23	18	1	1	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	108	108	108	0	0
4	B	81	81	81	0	0

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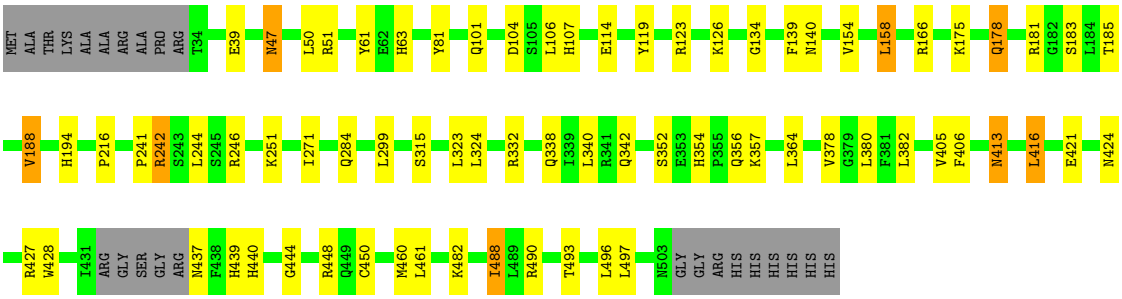
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	64	64	64	0	0
			Total	O		
4	D	100	100	100	0	0
			Total	O		
4	E	54	54	54	0	0
			Total	O		
4	F	73	73	73	0	0
			Total	O		
4	G	45	45	45	0	0
			Total	O		
4	H	68	68	68	0	0
			Total	O		
4	I	54	54	54	0	0
			Total	O		
4	J	50	50	50	0	0
			Total	O		
4	K	53	53	53	0	0
			Total	O		
4	L	67	67	67	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.

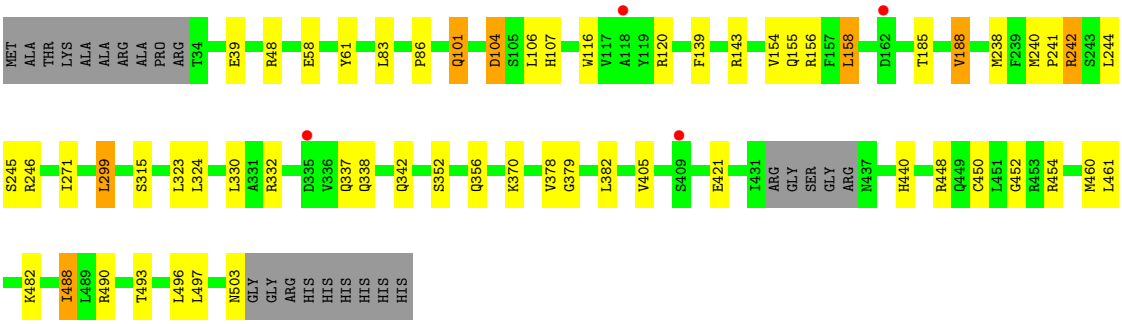
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain A:



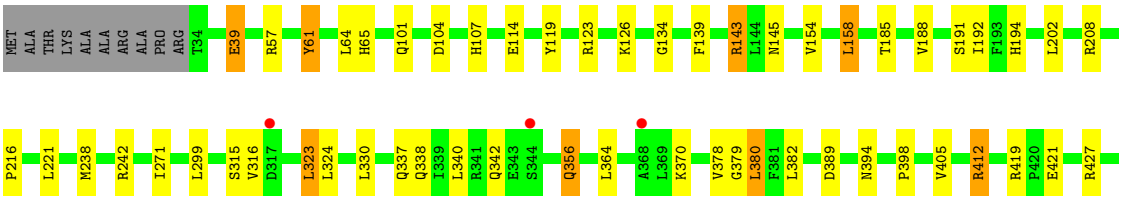
• Molecule 1: Cytochrome P450 11B2, mitochondrial

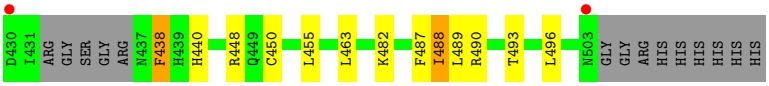
Chain B:



• Molecule 1: Cytochrome P450 11B2, mitochondrial

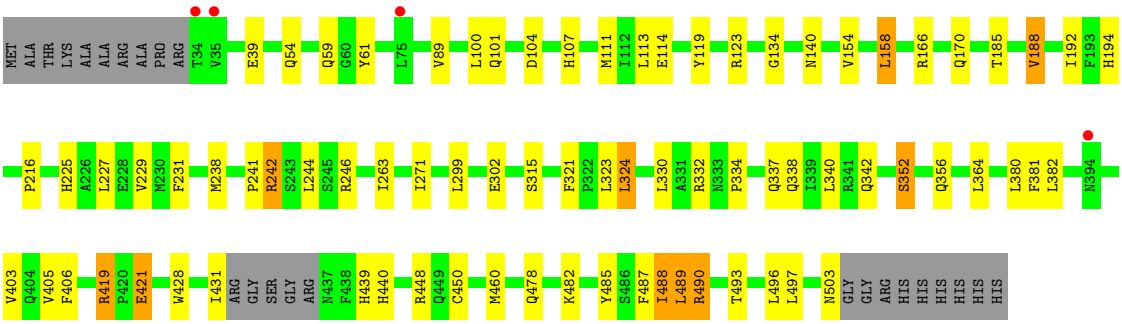
Chain C:





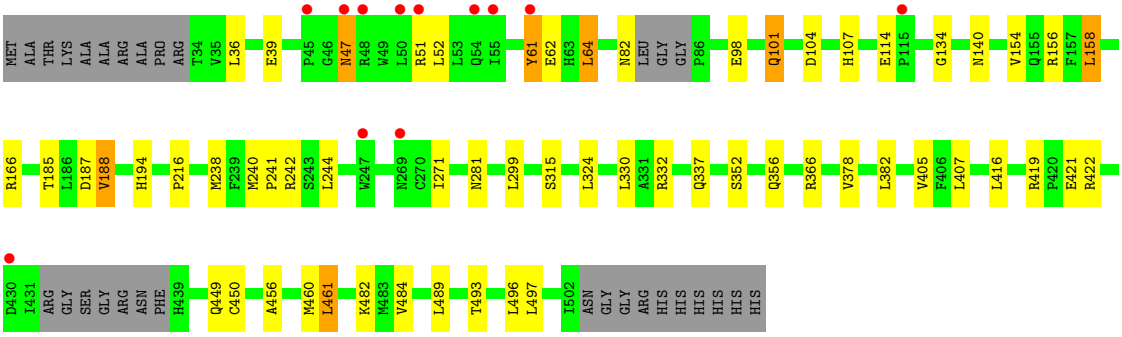
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain D:



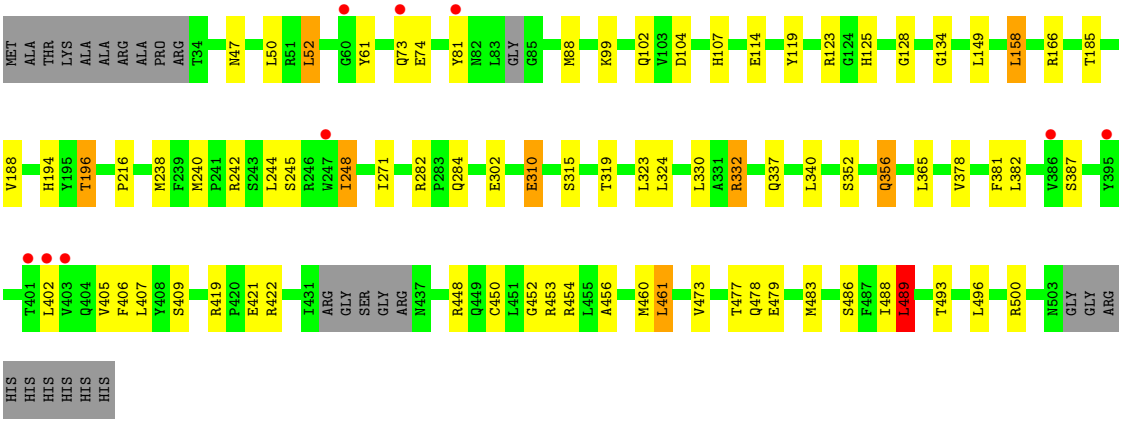
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain E:



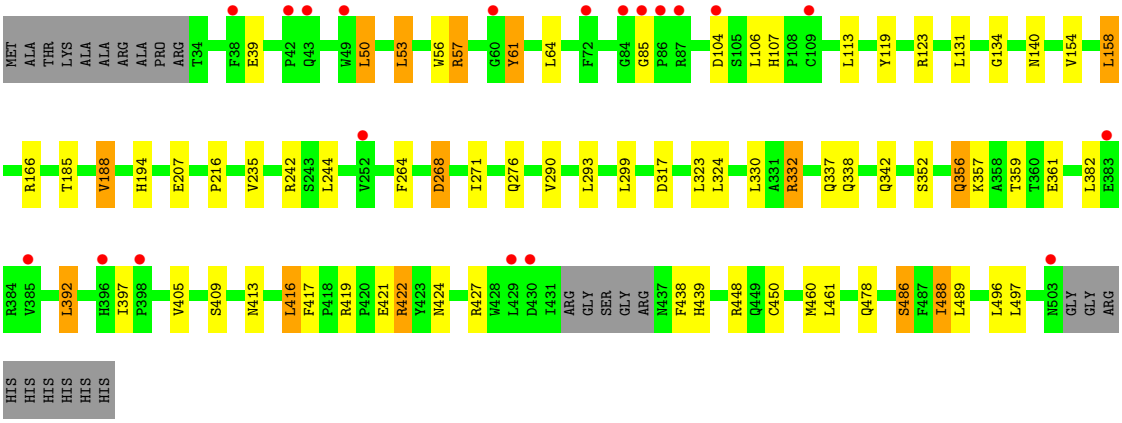
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain F:



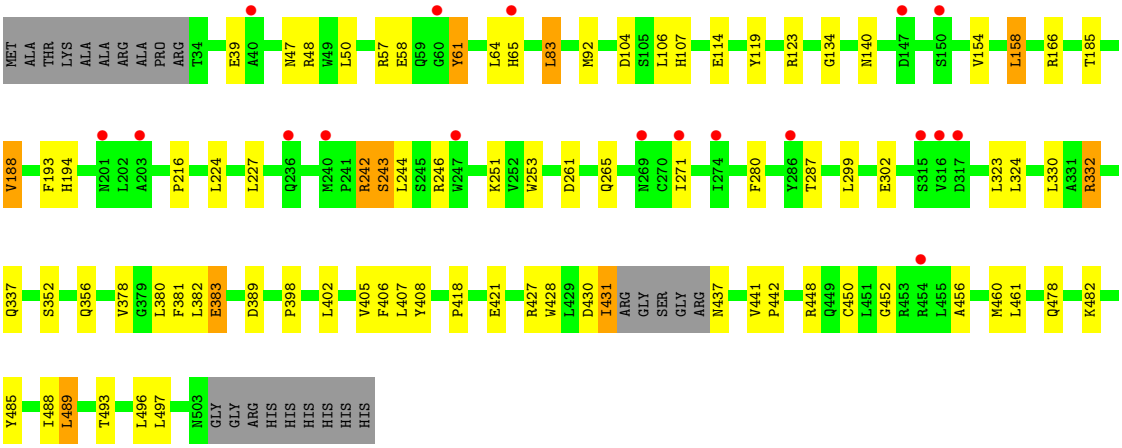
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain G:



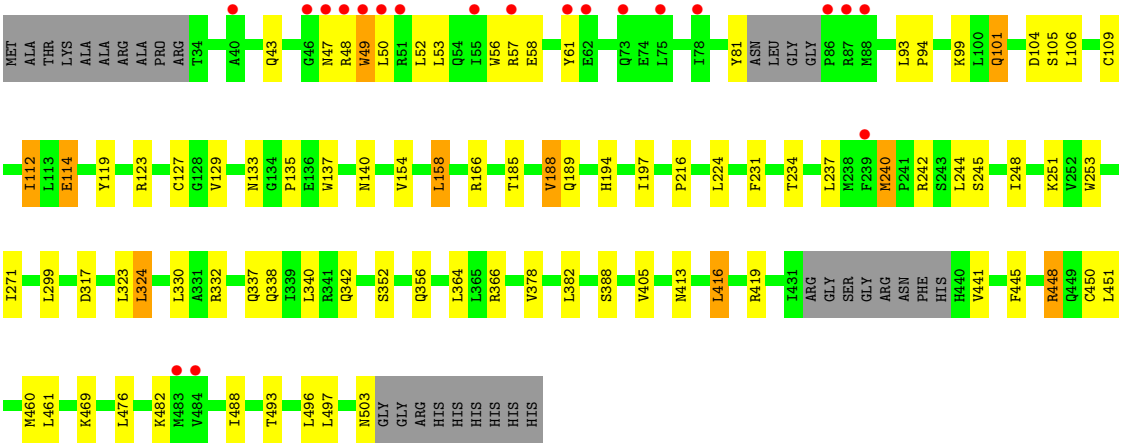
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain H:



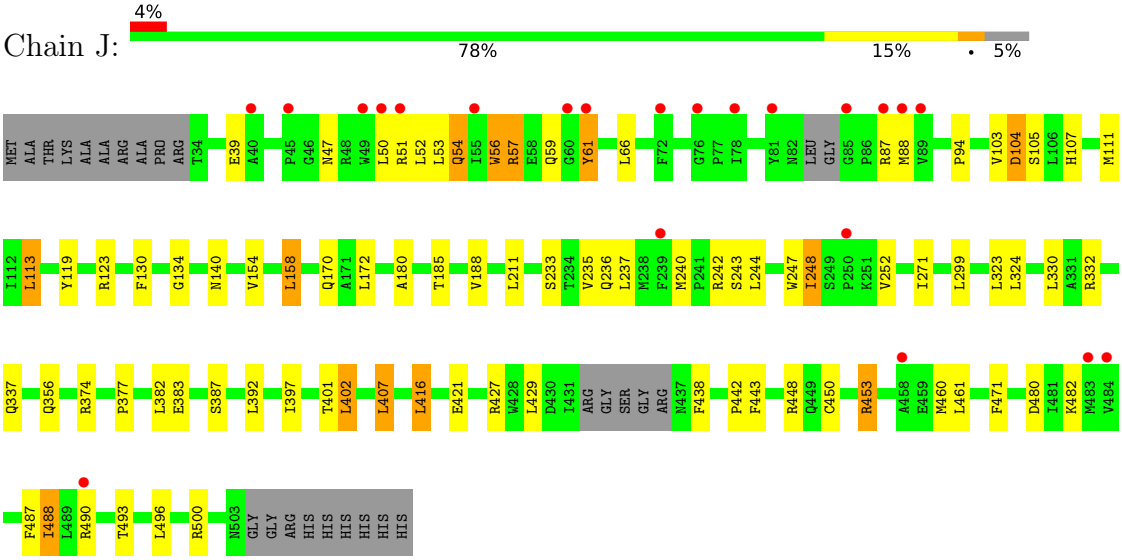
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain I:



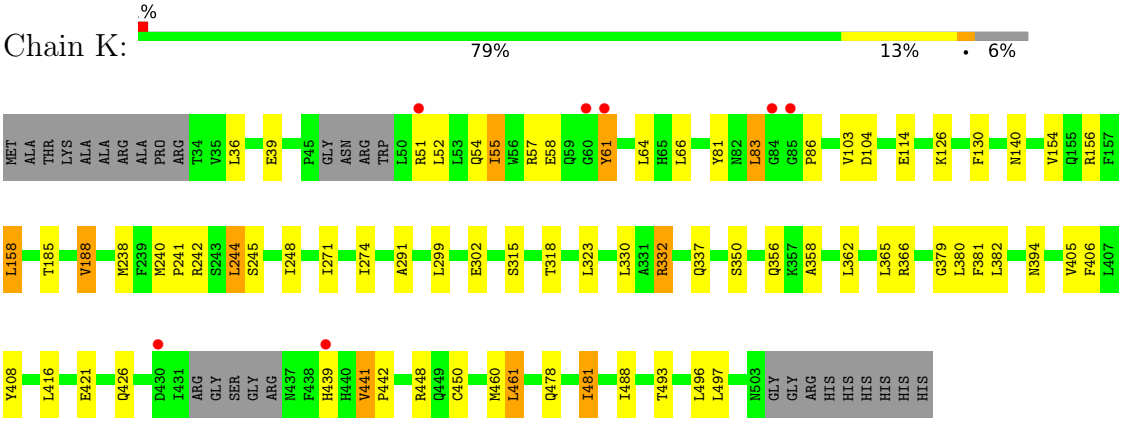
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain J:



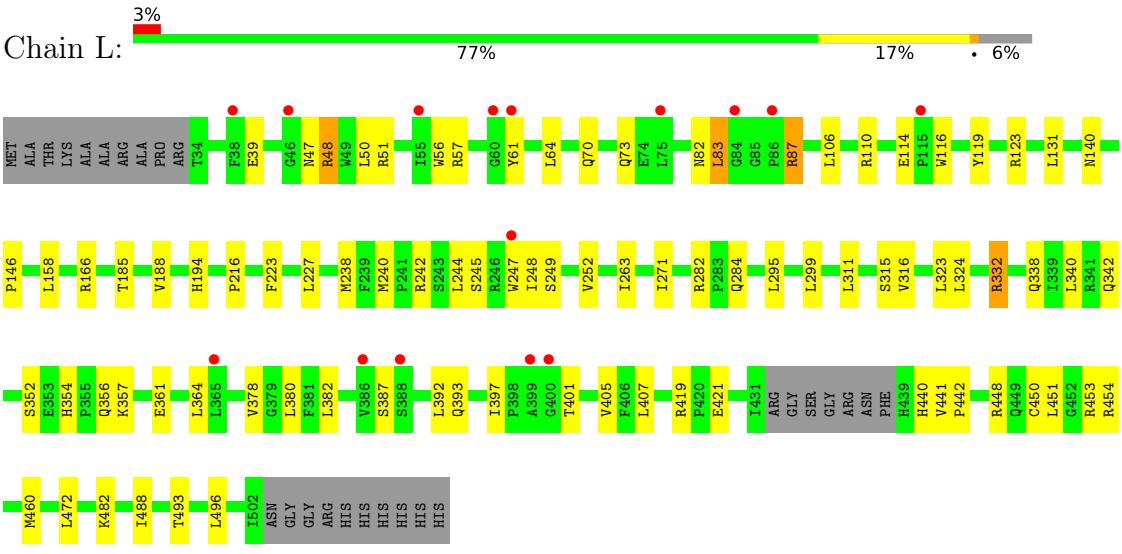
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain K:



• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	104.70Å 125.96Å 155.23Å 70.25° 85.87° 73.84°	Depositor
Resolution (Å)	88.20 – 3.20 88.20 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (88.20-3.20) 97.2 (88.20-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.212 , 0.255 0.234 , 0.279	Depositor DCC
R_{free} test set	5764 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 74.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	46675	wwPDB-VP
Average B, all atoms (Å^2)	72.0	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 21.13 % 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 7.4821e-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 (i)

5.1 Standard geometry (i)

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

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	0.46	0/3874	0.64	0/5257
1	B	0.44	0/3874	0.62	0/5257
1	C	0.44	0/3874	0.62	0/5257
1	D	0.45	0/3874	0.62	0/5257
1	E	0.45	0/3829	0.63	0/5194
1	F	0.44	0/3869	0.63	0/5249
1	G	0.44	0/3874	0.62	0/5257
1	H	0.43	0/3874	0.63	0/5257
1	I	0.44	0/3818	0.62	0/5179
1	J	0.43	0/3861	0.63	0/5238
1	K	0.43	0/3834	0.62	0/5201
1	L	0.44	0/3846	0.64	0/5219
All	All	0.44	0/46301	0.63	0/62822

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3774	0	3808	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3774	0	3808	23	0
1	C	3774	0	3808	33	0
1	D	3774	0	3808	39	0
1	E	3731	0	3770	28	0
1	F	3770	0	3804	36	0
1	G	3774	0	3809	30	0
1	H	3774	0	3809	40	0
1	I	3721	0	3763	37	0
1	J	3762	0	3793	29	0
1	K	3737	0	3775	37	0
1	L	3747	0	3787	40	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	2	0
2	E	43	0	30	4	0
2	F	43	0	30	8	0
2	G	43	0	30	1	0
2	H	43	0	30	7	0
2	I	43	0	30	3	0
2	J	43	0	30	1	0
2	K	43	0	30	4	0
2	L	43	0	30	4	0
3	A	23	0	18	7	0
3	B	23	0	18	5	0
3	C	23	0	18	5	0
3	D	23	0	18	0	0
3	E	23	0	18	2	0
3	F	23	0	18	5	0
3	I	23	0	18	4	0
3	J	23	0	18	4	0
3	K	23	0	18	5	0
3	L	23	0	18	3	0
4	A	108	0	0	0	0
4	B	81	0	0	0	0
4	C	64	0	0	1	0
4	D	100	0	0	0	0
4	E	54	0	0	1	0
4	F	73	0	0	1	0
4	G	45	0	0	0	0
4	H	68	0	0	0	0
4	I	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	50	0	0	0	0
4	K	53	0	0	1	0
4	L	67	0	0	2	0
All	All	46675	0	46082	412	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 4.

All (412) 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:K:52:LEU:HD11	1:K:240:MET:HB3	1.33	1.08
1:K:323:LEU:HG	1:K:460:MET:HG2	1.46	0.97
1:C:323:LEU:HD21	1:C:463:LEU:HD22	1.54	0.89
2:K:601:HEM:HMA3	3:K:602:QHC:H14	1.60	0.84
1:A:242:ARG:HD3	1:A:246:ARG:HD2	1.60	0.83
2:I:601:HEM:HMA2	3:I:602:QHC:H14	1.66	0.78
1:C:412:ARG:HH11	1:C:412:ARG:HB2	1.49	0.77
1:D:488:ILE:HD12	1:D:490:ARG:HG2	1.65	0.77
1:E:62:GLU:HG2	1:E:484:VAL:HG13	1.66	0.76
1:I:189:GLN:HA	1:I:324:LEU:HD21	1.65	0.76
1:K:441:VAL:H	1:K:442:PRO:HD3	1.51	0.76
1:A:315:SER:HA	2:A:601:HEM:HMC2	1.68	0.75
3:A:602:QHC:H12	3:A:602:QHC:H2	1.70	0.74
1:B:378:VAL:HG21	2:B:601:HEM:HAB	1.70	0.72
3:A:602:QHC:H12	3:A:602:QHC:C4	2.20	0.71
1:E:382:LEU:HG	1:E:407:LEU:HD11	1.71	0.71
1:E:281:ASN:HB3	1:F:500:ARG:HH12	1.55	0.71
2:A:601:HEM:HMA2	3:A:602:QHC:H14	1.74	0.70
1:G:235:VAL:HG21	1:G:486:SER:HA	1.74	0.70
1:H:383:GLU:HG2	1:H:402:LEU:HD11	1.74	0.70
1:G:61:TYR:HB3	1:G:64:LEU:HB2	1.74	0.69
1:C:380:LEU:HD23	1:C:489:LEU:HD13	1.76	0.68
1:L:382:LEU:HG	1:L:407:LEU:HD11	1.76	0.68
1:D:421:GLU:OE1	1:I:388:SER:HB3	1.94	0.67
2:C:601:HEM:HMA2	3:C:602:QHC:H14	1.78	0.66
1:D:242:ARG:HD2	1:D:246:ARG:HH21	1.60	0.66
1:D:485:TYR:HD1	1:D:489:LEU:HD12	1.61	0.66
1:I:47:ASN:HB3	1:I:49:TRP:HD1	1.61	0.65
1:D:478:GLN:HG3	1:I:135:PRO:HG2	1.78	0.65
1:D:315:SER:HA	2:D:601:HEM:HMC2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:HIS:HB3	1:C:380:LEU:HD21	1.77	0.64
1:E:281:ASN:CB	1:F:500:ARG:HH12	2.11	0.64
2:F:601:HEM:HBB2	2:F:601:HEM:HHC	1.79	0.64
1:E:241:PRO:HD2	1:E:244:LEU:HD12	1.80	0.63
1:J:88:MET:HG3	1:J:402:LEU:HD23	1.79	0.63
1:D:225:HIS:O	1:D:229:VAL:HG23	1.99	0.63
1:B:83:LEU:HD23	1:B:86:PRO:HB2	1.82	0.61
2:C:601:HEM:CMA	3:C:602:QHC:H14	2.30	0.61
1:L:382:LEU:HB2	1:L:405:VAL:HB	1.81	0.61
1:J:111:MET:HG3	1:J:402:LEU:HD13	1.82	0.60
1:D:166:ARG:HH22	1:D:352:SER:HA	1.64	0.60
1:I:245:SER:HA	1:I:248:ILE:HG22	1.84	0.60
1:B:107:HIS:CE1	1:K:36:LEU:HD11	2.36	0.60
1:H:456:ALA:HB2	2:H:601:HEM:HMC3	1.84	0.60
1:L:110:ARG:HD3	2:L:601:HEM:O1A	2.00	0.60
1:C:412:ARG:HB2	1:C:412:ARG:NH1	2.15	0.60
1:H:452:GLY:HA3	2:H:601:HEM:HBC2	1.83	0.60
1:L:64:LEU:HG	1:L:380:LEU:HD21	1.83	0.59
1:K:61:TYR:HD1	1:K:64:LEU:HD22	1.67	0.59
1:E:378:VAL:HG21	2:E:601:HEM:HAB	1.83	0.59
1:K:416:LEU:HB3	1:K:439:HIS:NE2	2.17	0.59
1:A:378:VAL:HG21	2:A:601:HEM:HAB	1.84	0.58
1:K:441:VAL:N	1:K:442:PRO:HD3	2.19	0.58
1:K:52:LEU:CD1	1:K:240:MET:HB3	2.22	0.58
1:K:83:LEU:HD23	1:K:86:PRO:HB2	1.86	0.58
1:L:378:VAL:HG13	1:L:488:ILE:HG23	1.85	0.58
1:J:233:SER:HA	1:J:236:GLN:HE21	1.69	0.58
1:A:354:HIS:HB2	1:A:357:LYS:HD2	1.86	0.58
1:F:52:LEU:HD21	1:F:240:MET:HB3	1.86	0.58
1:G:392:LEU:HD12	1:G:397:ILE:HG13	1.86	0.57
1:B:370:LYS:HA	1:B:440:HIS:CE1	2.39	0.57
1:L:244:LEU:HG	1:L:248:ILE:HD12	1.87	0.57
1:D:490:ARG:HB2	1:D:490:ARG:NH2	2.20	0.57
1:F:196:THR:CG2	1:F:319:THR:HB	2.35	0.57
1:I:101:GLN:HG2	1:I:445:PHE:CD1	2.39	0.57
1:F:158:LEU:HD22	1:F:356:GLN:HA	1.87	0.56
1:C:488:ILE:HG23	3:C:602:QHC:H9	1.87	0.56
1:D:421:GLU:CD	1:I:388:SER:HB3	2.25	0.56
1:E:456:ALA:O	1:E:460:MET:HG3	2.05	0.56
1:I:101:GLN:O	1:I:104:ASP:HB2	2.05	0.56
1:J:374:ARG:NE	1:J:427:ARG:HH12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:240:MET:HG3	1:L:245:SER:HB3	1.86	0.56
1:H:65:HIS:HB3	1:H:380:LEU:HD11	1.88	0.56
1:C:192:ILE:HD12	1:C:323:LEU:HD22	1.87	0.56
1:H:389:ASP:OD1	1:H:398:PRO:HA	2.05	0.56
1:E:61:TYR:CD1	1:E:64:LEU:HG	2.41	0.56
1:B:488:ILE:HD12	1:B:490:ARG:HD3	1.88	0.56
1:D:166:ARG:NH2	1:D:352:SER:HA	2.21	0.56
1:H:406:PHE:CE2	1:H:408:TYR:HB3	2.41	0.56
1:C:315:SER:HA	2:C:601:HEM:HMC2	1.87	0.55
1:J:56:TRP:HE1	1:J:248:ILE:HG12	1.71	0.55
1:K:441:VAL:N	1:K:442:PRO:CD	2.69	0.55
1:D:188:VAL:HG21	1:D:497:LEU:HD12	1.89	0.55
1:H:406:PHE:HE2	1:H:408:TYR:HB3	1.72	0.54
1:J:87:ARG:HB3	1:J:401:THR:HG23	1.88	0.54
1:L:392:LEU:HD12	1:L:397:ILE:HG13	1.88	0.54
1:A:382:LEU:HB2	1:A:405:VAL:HB	1.89	0.54
1:G:188:VAL:HG21	1:G:497:LEU:HD12	1.89	0.54
1:D:323:LEU:HG	1:D:460:MET:HG2	1.88	0.54
1:C:378:VAL:HG21	2:C:601:HEM:HAB	1.90	0.54
1:G:413:ASN:HD22	1:G:416:LEU:HG	1.72	0.54
1:G:323:LEU:HG	1:G:460:MET:HG2	1.90	0.54
1:L:227:LEU:HD22	1:L:263:ILE:HG12	1.90	0.54
3:A:602:QHC:C4	3:A:602:QHC:C17	2.83	0.54
1:I:330:LEU:HB3	1:I:337:GLN:HG3	1.88	0.54
1:I:57:ARG:HH11	1:I:58:GLU:HG3	1.73	0.54
2:E:601:HEM:CMA	3:E:602:QHC:H14	2.38	0.53
1:J:392:LEU:HD12	1:J:397:ILE:HG13	1.89	0.53
1:I:323:LEU:HG	1:I:460:MET:HG2	1.91	0.53
1:I:378:VAL:HG21	2:I:601:HEM:HAB	1.90	0.53
1:K:52:LEU:HD11	1:K:240:MET:CB	2.24	0.53
1:L:146:PRO:HD2	4:L:701:HOH:O	2.09	0.53
1:D:241:PRO:HD2	1:D:244:LEU:HD12	1.90	0.53
1:J:47:ASN:H	1:J:50:LEU:HD12	1.74	0.53
1:A:323:LEU:HG	1:A:460:MET:HG2	1.91	0.53
1:C:107:HIS:HE1	1:E:36:LEU:HD11	1.73	0.53
1:D:428:TRP:CZ3	1:D:440:HIS:HB2	2.43	0.53
2:F:601:HEM:HMA3	3:F:602:QHC:H14	1.90	0.53
1:J:130:PHE:CD1	3:J:602:QHC:H2	2.45	0.52
1:G:419:ARG:HD3	1:G:422:ARG:HD3	1.89	0.52
1:J:323:LEU:HG	1:J:460:MET:HG2	1.90	0.52
1:A:488:ILE:HG23	3:A:602:QHC:H9	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HB3	1:C:299:LEU:HD11	1.91	0.52
1:G:113:LEU:HB3	1:G:131:LEU:HD11	1.91	0.52
2:I:601:HEM:CMA	3:I:602:QHC:H14	2.36	0.52
1:F:332:ARG:HA	1:F:478:GLN:HE22	1.73	0.52
1:L:488:ILE:HG12	3:L:602:QHC:H9	1.89	0.52
2:E:601:HEM:HMA2	3:E:602:QHC:H14	1.92	0.52
1:H:441:VAL:N	1:H:442:PRO:HD3	2.25	0.52
1:A:47:ASN:HD21	1:A:50:LEU:HD12	1.74	0.52
1:H:378:VAL:HG21	2:H:601:HEM:HBB2	1.91	0.52
1:H:382:LEU:HG	1:H:407:LEU:HD11	1.91	0.52
1:L:282:ARG:HG3	1:L:295:LEU:HD22	1.92	0.52
1:H:188:VAL:HG21	1:H:497:LEU:HD12	1.92	0.52
1:K:330:LEU:HB3	1:K:337:GLN:HG3	1.92	0.52
1:B:452:GLY:HA3	2:B:601:HEM:HBC2	1.92	0.51
1:A:188:VAL:HG21	1:A:497:LEU:HD12	1.91	0.51
1:F:378:VAL:HG21	2:F:601:HEM:HAB	1.92	0.51
1:B:323:LEU:HG	1:B:460:MET:HG2	1.93	0.51
1:G:417:PHE:HZ	1:G:439:HIS:HB3	1.75	0.51
1:D:194:HIS:NE2	1:D:216:PRO:HB3	2.25	0.51
1:B:143:ARG:HB3	1:B:299:LEU:HD11	1.93	0.51
1:C:107:HIS:CE1	1:E:36:LEU:HD11	2.46	0.51
1:C:330:LEU:HB3	1:C:337:GLN:HG3	1.93	0.51
1:L:315:SER:HA	2:L:601:HEM:HMC2	1.92	0.51
1:B:188:VAL:HG21	1:B:497:LEU:HD12	1.93	0.51
1:L:323:LEU:HG	1:L:460:MET:HG2	1.93	0.51
1:A:194:HIS:NE2	1:A:216:PRO:HB3	2.26	0.51
1:L:223:PHE:HE2	1:L:316:VAL:HG21	1.75	0.51
1:C:488:ILE:HD12	1:C:490:ARG:HD3	1.93	0.51
2:G:601:HEM:HMB2	2:G:601:HEM:HBB2	1.93	0.50
1:I:317:ASP:HB3	1:I:488:ILE:HD13	1.92	0.50
1:J:94:PRO:HG3	1:J:416:LEU:HD11	1.93	0.50
1:L:441:VAL:N	1:L:442:PRO:HD3	2.27	0.50
1:I:194:HIS:NE2	1:I:216:PRO:HB3	2.26	0.50
1:E:330:LEU:HB3	1:E:337:GLN:HG3	1.93	0.50
1:F:406:PHE:HD2	1:F:409:SER:HB2	1.77	0.50
1:L:223:PHE:CE2	1:L:316:VAL:HG21	2.46	0.50
1:E:194:HIS:NE2	1:E:216:PRO:HB3	2.27	0.50
1:K:315:SER:HA	2:K:601:HEM:HMC2	1.94	0.50
1:G:113:LEU:H	1:G:131:LEU:HD21	1.75	0.50
1:C:382:LEU:HB2	1:C:405:VAL:HB	1.93	0.50
1:D:421:GLU:OE1	1:I:388:SER:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:323:LEU:HG	1:H:460:MET:HG2	1.93	0.50
1:I:137:TRP:NE1	1:I:448:ARG:HD3	2.27	0.50
1:B:382:LEU:HB2	1:B:405:VAL:HB	1.94	0.49
1:G:194:HIS:NE2	1:G:216:PRO:HB3	2.27	0.49
1:B:107:HIS:HE1	1:K:36:LEU:CD1	2.26	0.49
1:B:241:PRO:HD2	1:B:244:LEU:HD12	1.94	0.49
1:F:488:ILE:HG23	3:F:602:QHC:H9	1.95	0.49
1:J:330:LEU:HB3	1:J:337:GLN:HG3	1.95	0.49
1:B:488:ILE:HG23	3:B:602:QHC:H9	1.94	0.49
1:G:330:LEU:HB3	1:G:337:GLN:HG3	1.94	0.49
1:B:330:LEU:HB3	1:B:337:GLN:HG3	1.95	0.49
1:L:453:ARG:HH12	1:L:454:ARG:HH21	1.59	0.49
1:A:380:LEU:HG	1:A:406:PHE:CE1	2.47	0.49
1:E:281:ASN:CB	1:F:500:ARG:NH1	2.75	0.49
1:K:188:VAL:HG21	1:K:497:LEU:HD12	1.93	0.49
1:A:126:LYS:HG2	1:H:418:PRO:HG2	1.94	0.49
1:K:382:LEU:HB2	1:K:405:VAL:HB	1.94	0.49
1:I:366:ARG:HG3	1:I:461:LEU:HD21	1.95	0.49
1:A:315:SER:CA	2:A:601:HEM:HMC2	2.40	0.48
1:E:51:ARG:HG3	1:E:61:TYR:CE1	2.48	0.48
1:K:441:VAL:H	1:K:442:PRO:CD	2.22	0.48
1:L:87:ARG:HB2	1:L:401:THR:HG23	1.94	0.48
1:F:194:HIS:NE2	1:F:216:PRO:HB3	2.27	0.48
1:F:323:LEU:HG	1:F:460:MET:HG2	1.95	0.48
1:H:428:TRP:HE3	1:H:431:ILE:HG12	1.79	0.48
1:I:112:ILE:HD11	1:I:114:GLU:HG2	1.94	0.48
1:L:378:VAL:CG1	1:L:488:ILE:HG23	2.44	0.48
1:E:140:ASN:HA	1:E:299:LEU:HD21	1.95	0.48
1:H:140:ASN:HA	1:H:299:LEU:HD21	1.96	0.48
1:L:357:LYS:O	1:L:361:GLU:HB2	2.13	0.48
1:B:379:GLY:HA3	3:B:602:QHC:C18	2.44	0.48
1:E:382:LEU:HB2	1:E:405:VAL:HB	1.95	0.48
1:H:382:LEU:HB2	1:H:405:VAL:HB	1.96	0.48
1:C:194:HIS:NE2	1:C:216:PRO:HB3	2.28	0.48
1:E:315:SER:HA	2:E:601:HEM:HMC2	1.95	0.48
1:A:63:HIS:CD2	1:A:63:HIS:H	2.30	0.48
1:G:50:LEU:HG	1:G:53:LEU:HD21	1.94	0.48
1:L:440:HIS:CG	1:L:441:VAL:H	2.29	0.48
1:F:381:PHE:HA	1:F:405:VAL:O	2.14	0.47
1:E:98:GLU:HA	1:E:101:GLN:OE1	2.14	0.47
1:H:194:HIS:NE2	1:H:216:PRO:HB3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:ASN:HA	1:I:299:LEU:HD21	1.96	0.47
1:J:488:ILE:HD12	1:J:490:ARG:HD3	1.95	0.47
1:L:194:HIS:NE2	1:L:216:PRO:HB3	2.29	0.47
1:D:140:ASN:HA	1:D:299:LEU:HD21	1.96	0.47
1:D:192:ILE:HG13	1:D:324:LEU:HD23	1.95	0.47
1:D:340:LEU:CD2	1:D:364:LEU:HB3	2.44	0.47
1:L:140:ASN:HA	1:L:299:LEU:HD21	1.96	0.47
1:F:245:SER:HA	1:F:248:ILE:HG22	1.96	0.47
1:G:119:TYR:CZ	1:G:123:ARG:HG3	2.49	0.47
1:L:48:ARG:HD3	1:L:83:LEU:HA	1.95	0.47
1:A:424:ASN:O	1:A:427:ARG:HG2	2.14	0.47
1:G:276:GLN:HG3	1:I:476:LEU:HG	1.97	0.47
1:H:330:LEU:HB3	1:H:337:GLN:HG3	1.95	0.47
1:L:116:TRP:HE3	1:L:131:LEU:HD21	1.79	0.47
1:E:188:VAL:HG21	1:E:497:LEU:HD12	1.96	0.47
1:H:65:HIS:HB3	1:H:380:LEU:CD1	2.44	0.47
1:H:242:ARG:HG2	1:H:253:TRP:CZ2	2.49	0.47
1:K:380:LEU:HD23	1:K:381:PHE:CE1	2.49	0.47
1:E:281:ASN:HB3	1:F:500:ARG:NH1	2.26	0.47
1:F:382:LEU:HD12	1:F:405:VAL:HB	1.97	0.47
1:H:452:GLY:HA3	2:H:601:HEM:CBC	2.44	0.47
1:I:237:LEU:HD22	1:I:253:TRP:NE1	2.30	0.47
1:G:185:THR:HG22	1:G:496:LEU:HG	1.97	0.47
1:A:241:PRO:HD2	1:A:244:LEU:HD12	1.96	0.47
1:F:315:SER:HA	2:F:601:HEM:HMC2	1.96	0.47
1:F:452:GLY:HA3	2:F:601:HEM:HBC2	1.95	0.47
2:K:601:HEM:CMA	3:K:602:QHC:H14	2.37	0.47
1:A:413:ASN:HB3	1:A:416:LEU:HD12	1.96	0.46
1:A:140:ASN:HA	1:A:299:LEU:HD21	1.97	0.46
1:G:264:PHE:O	1:G:268:ASP:HB3	2.16	0.46
1:K:245:SER:HA	1:K:248:ILE:HG22	1.97	0.46
1:J:407:LEU:HD11	1:J:442:PRO:HA	1.96	0.46
1:A:488:ILE:HD12	1:A:490:ARG:HD3	1.97	0.46
1:G:357:LYS:O	1:G:361:GLU:HB2	2.16	0.46
1:I:197:ILE:HD11	1:I:224:LEU:HD21	1.96	0.46
1:K:381:PHE:HB2	4:K:722:HOH:O	2.15	0.46
1:F:119:TYR:CZ	1:F:123:ARG:HG3	2.50	0.46
1:I:382:LEU:HB2	1:I:405:VAL:HB	1.97	0.46
1:B:315:SER:HA	2:B:601:HEM:HMC2	1.98	0.46
1:F:166:ARG:HH22	1:F:352:SER:HA	1.80	0.46
1:L:378:VAL:HG12	3:L:602:QHC:H6	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:QHC:H12	3:B:602:QHC:C4	2.45	0.46
1:G:382:LEU:HB2	1:G:405:VAL:HB	1.97	0.46
1:H:185:THR:HG22	1:H:496:LEU:HG	1.97	0.46
3:I:602:QHC:C4	3:I:602:QHC:H12	2.46	0.46
1:B:242:ARG:NH2	1:B:246:ARG:HH21	2.14	0.46
1:C:487:PHE:CD2	3:C:602:QHC:H10	2.51	0.46
2:F:601:HEM:CMA	3:F:602:QHC:H14	2.45	0.46
1:G:424:ASN:O	1:G:427:ARG:HG2	2.16	0.46
1:H:48:ARG:HD3	1:H:83:LEU:HG	1.98	0.46
1:H:378:VAL:HG21	2:H:601:HEM:CBB	2.46	0.46
1:K:240:MET:HE1	1:K:248:ILE:HG21	1.98	0.46
1:I:93:LEU:HD23	1:I:413:ASN:HD21	1.80	0.45
1:I:188:VAL:HG21	1:I:497:LEU:HD12	1.97	0.45
1:J:107:HIS:HB3	1:J:134:GLY:HA2	1.99	0.45
1:E:166:ARG:HH22	1:E:352:SER:HA	1.82	0.45
1:K:140:ASN:HA	1:K:299:LEU:HD21	1.99	0.45
1:K:185:THR:HG22	1:K:496:LEU:HG	1.98	0.45
2:L:601:HEM:HMA3	3:L:602:QHC:H14	1.99	0.45
1:E:185:THR:HG22	1:E:496:LEU:HG	1.99	0.45
1:L:354:HIS:O	1:L:357:LYS:HB2	2.17	0.45
1:H:456:ALA:HB2	2:H:601:HEM:CMC	2.47	0.45
1:A:175:LYS:HA	1:A:178:GLN:HG3	1.98	0.45
1:D:321:PHE:CZ	1:D:490:ARG:HB3	2.51	0.45
1:E:154:VAL:O	1:E:158:LEU:HB2	2.16	0.45
1:G:417:PHE:CZ	1:G:439:HIS:HB3	2.52	0.45
1:C:389:ASP:OD2	1:C:398:PRO:HA	2.17	0.45
1:D:119:TYR:CZ	1:D:123:ARG:HG3	2.52	0.45
1:D:381:PHE:HA	1:D:405:VAL:O	2.17	0.45
1:F:330:LEU:HD21	1:F:340:LEU:HD12	1.99	0.45
1:H:452:GLY:CA	2:H:601:HEM:HBC2	2.46	0.45
1:J:54:GLN:HG3	1:J:61:TYR:CZ	2.52	0.45
1:L:185:THR:HG22	1:L:496:LEU:HG	1.98	0.45
1:G:158:LEU:HD22	1:G:356:GLN:HA	1.99	0.45
1:A:166:ARG:HH22	1:A:352:SER:HA	1.81	0.44
1:D:185:THR:HG22	1:D:496:LEU:HG	1.98	0.44
1:D:490:ARG:HB2	1:D:490:ARG:HH21	1.82	0.44
1:L:440:HIS:C	1:L:442:PRO:HD3	2.37	0.44
1:F:407:LEU:CD1	3:F:602:QHC:H15	2.47	0.44
1:H:224:LEU:HA	1:H:227:LEU:HD12	2.00	0.44
1:A:154:VAL:O	1:A:158:LEU:HB2	2.17	0.44
1:C:158:LEU:HD22	1:C:356:GLN:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:HG22	1:B:496:LEU:HG	2.00	0.44
1:F:483:MET:HE3	1:F:489:LEU:HB3	2.00	0.44
1:I:166:ARG:HH22	1:I:352:SER:HA	1.82	0.44
3:I:602:QHC:H12	3:I:602:QHC:H2	1.99	0.44
1:D:107:HIS:HB3	1:D:134:GLY:HA2	2.00	0.44
1:K:274:ILE:HD11	1:K:291:ALA:HB2	2.00	0.44
1:L:166:ARG:HH22	1:L:352:SER:HA	1.83	0.44
1:C:185:THR:HG22	1:C:496:LEU:HG	1.99	0.44
1:A:119:TYR:CZ	1:A:123:ARG:HG3	2.53	0.44
1:E:107:HIS:HB3	1:E:134:GLY:HA2	2.00	0.44
1:H:61:TYR:O	1:H:485:TYR:HB3	2.18	0.44
1:D:330:LEU:HB3	1:D:337:GLN:HG3	2.00	0.44
1:K:379:GLY:HA3	3:K:602:QHC:H17	1.99	0.44
1:G:107:HIS:HB3	1:G:134:GLY:HA2	2.00	0.43
1:J:488:ILE:HG23	3:J:602:QHC:H9	1.99	0.43
1:A:185:THR:HG22	1:A:496:LEU:HG	2.00	0.43
1:C:323:LEU:CD2	1:C:463:LEU:HD22	2.36	0.43
1:L:83:LEU:HD11	4:L:709:HOH:O	2.17	0.43
1:F:330:LEU:HD21	1:F:340:LEU:CD1	2.48	0.43
1:G:140:ASN:HA	1:G:299:LEU:HD21	2.00	0.43
1:L:119:TYR:CZ	1:L:123:ARG:HG3	2.53	0.43
2:B:601:HEM:CMA	3:B:602:QHC:H13	2.48	0.43
1:K:481:ILE:HD12	1:K:481:ILE:H	1.82	0.43
1:C:370:LYS:HA	1:C:440:HIS:CE1	2.54	0.43
1:D:154:VAL:O	1:D:158:LEU:HB2	2.18	0.43
1:D:324:LEU:HD22	1:D:324:LEU:HA	1.86	0.43
1:K:366:ARG:HG2	1:K:461:LEU:HD11	1.99	0.43
1:A:378:VAL:HG12	3:A:602:QHC:H6	2.00	0.43
1:H:332:ARG:HD3	1:H:478:GLN:HA	2.01	0.43
1:I:185:THR:HG22	1:I:496:LEU:HG	2.01	0.43
1:B:154:VAL:O	1:B:158:LEU:HB2	2.18	0.43
1:C:154:VAL:O	1:C:158:LEU:HB2	2.18	0.43
1:D:315:SER:HB3	2:D:601:HEM:CBC	2.48	0.43
1:F:456:ALA:HB2	2:F:601:HEM:HMC3	2.01	0.43
1:D:227:LEU:HA	1:D:263:ILE:HD11	2.01	0.43
1:D:382:LEU:HB2	1:D:405:VAL:HB	1.99	0.43
1:F:365:LEU:HD23	1:F:461:LEU:HD13	2.00	0.43
1:I:338:GLN:HG3	1:I:342:GLN:HE21	1.84	0.43
1:J:113:LEU:HD21	1:J:487:PHE:HZ	1.84	0.43
1:J:154:VAL:O	1:J:158:LEU:HB2	2.18	0.43
1:J:407:LEU:HD12	3:J:602:QHC:H15	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:51:ARG:HB2	1:K:61:TYR:OH	2.19	0.43
1:F:330:LEU:HB3	1:F:337:GLN:HG3	2.01	0.42
1:J:377:PRO:HB3	1:J:407:LEU:HD13	2.00	0.42
2:A:601:HEM:CMA	3:A:602:QHC:H14	2.46	0.42
1:B:240:MET:HG3	1:B:245:SER:HB3	2.01	0.42
1:C:379:GLY:HA3	3:C:602:QHC:C18	2.48	0.42
1:D:419:ARG:HD2	1:I:388:SER:OG	2.19	0.42
1:H:61:TYR:HB3	1:H:64:LEU:HB2	2.02	0.42
1:D:380:LEU:HD11	1:D:406:PHE:CE1	2.54	0.42
1:J:185:THR:HG22	1:J:496:LEU:HG	2.00	0.42
1:K:416:LEU:HB3	1:K:439:HIS:CE1	2.54	0.42
1:A:107:HIS:HB3	1:A:134:GLY:HA2	2.01	0.42
1:C:61:TYR:CD1	1:C:64:LEU:HD13	2.54	0.42
1:C:438:PHE:HE2	4:C:728:HOH:O	2.02	0.42
1:C:455:LEU:HD23	2:C:601:HEM:CBC	2.50	0.42
1:B:116:TRP:O	1:B:120:ARG:HG2	2.19	0.42
1:C:107:HIS:HB3	1:C:134:GLY:HA2	2.01	0.42
1:E:47:ASN:HB3	1:E:82:ASN:HD22	1.84	0.42
1:I:129:VAL:HG11	1:I:451:LEU:HD22	2.02	0.42
1:I:231:PHE:O	1:I:234:THR:HB	2.19	0.42
1:C:202:LEU:HD22	1:C:208:ARG:HD3	2.01	0.42
1:F:149:LEU:HD23	4:F:747:HOH:O	2.20	0.42
1:G:290:VAL:HA	1:G:293:LEU:HD12	2.01	0.42
1:J:140:ASN:HA	1:J:299:LEU:HD21	2.02	0.42
1:D:334:PRO:HD2	1:I:106:LEU:HD21	2.01	0.42
1:E:52:LEU:HD11	1:E:240:MET:HB3	2.01	0.42
1:J:172:LEU:HD23	1:J:471:PHE:CE1	2.54	0.42
1:J:237:LEU:HD12	1:J:252:VAL:HG12	2.02	0.42
1:G:154:VAL:O	1:G:158:LEU:HB2	2.19	0.42
1:I:119:TYR:CZ	1:I:123:ARG:HG3	2.55	0.42
1:H:166:ARG:HH22	1:H:352:SER:HA	1.85	0.41
1:A:444:GLY:HA3	2:A:601:HEM:HBA1	2.02	0.41
1:E:187:ASP:HB3	4:E:711:HOH:O	2.18	0.41
1:F:88:MET:HG3	1:F:402:LEU:HD23	2.01	0.41
1:F:453:ARG:HH12	1:F:454:ARG:HH21	1.69	0.41
1:F:99:LYS:O	1:F:102:GLN:HB2	2.19	0.41
1:H:287:THR:HG22	1:J:180:ALA:HB1	2.01	0.41
1:H:380:LEU:HD13	1:H:489:LEU:HD11	2.02	0.41
1:K:154:VAL:O	1:K:158:LEU:HB2	2.20	0.41
1:E:366:ARG:HG2	1:E:461:LEU:HD11	2.03	0.41
1:I:94:PRO:HG3	1:I:416:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HH21	1:A:246:ARG:NH2	2.18	0.41
1:C:338:GLN:HG3	1:C:342:GLN:HE21	1.85	0.41
1:D:231:PHE:CD1	1:D:487:PHE:HD2	2.39	0.41
1:F:128:GLY:HA3	1:F:310:GLU:CD	2.40	0.41
2:F:601:HEM:HHC	2:F:601:HEM:CBB	2.47	0.41
1:K:55:ILE:HG12	1:K:61:TYR:CE2	2.56	0.41
1:L:249:SER:HB3	1:L:252:VAL:HB	2.01	0.41
1:D:89:VAL:CG1	1:D:403:VAL:HG22	2.50	0.41
1:F:185:THR:HG22	1:F:496:LEU:HG	2.02	0.41
1:G:332:ARG:HD3	1:G:478:GLN:HA	2.01	0.41
3:K:602:QHC:C6	3:K:602:QHC:H12	2.51	0.41
1:L:340:LEU:HD23	1:L:364:LEU:HB3	2.02	0.41
1:C:119:TYR:CZ	1:C:123:ARG:HG3	2.56	0.41
1:D:338:GLN:HG3	1:D:342:GLN:HE21	1.86	0.41
1:F:486:SER:C	1:F:488:ILE:H	2.23	0.41
1:H:107:HIS:HB3	1:H:134:GLY:HA2	2.02	0.41
1:I:109:CYS:HA	1:I:133:ASN:OD1	2.21	0.41
1:K:241:PRO:HD2	1:K:244:LEU:HD12	2.03	0.41
1:K:332:ARG:HD3	1:K:478:GLN:HA	2.02	0.41
1:K:358:ALA:O	1:K:362:LEU:HB2	2.21	0.41
1:K:406:PHE:CZ	1:K:408:TYR:HB3	2.56	0.41
1:L:442:PRO:O	2:L:601:HEM:HMB3	2.20	0.41
1:D:340:LEU:HD23	1:D:364:LEU:HB3	2.02	0.41
1:I:154:VAL:O	1:I:158:LEU:HB2	2.20	0.41
1:J:119:TYR:CZ	1:J:123:ARG:HG3	2.55	0.41
1:A:139:PHE:CZ	1:H:430:ASP:HA	2.56	0.41
1:A:338:GLN:HG3	1:A:342:GLN:HE21	1.86	0.41
1:A:380:LEU:HG	1:A:406:PHE:HE1	1.85	0.41
1:G:317:ASP:HB3	1:G:488:ILE:HD13	2.02	0.41
1:L:311:LEU:HD21	1:L:451:LEU:HD23	2.02	0.41
1:B:338:GLN:HG3	1:B:342:GLN:HE21	1.86	0.41
1:C:39:GLU:H	1:C:39:GLU:HG2	1.73	0.41
1:F:107:HIS:HB3	1:F:134:GLY:HA2	2.03	0.41
1:H:158:LEU:HD22	1:H:356:GLN:HA	2.01	0.41
1:H:261:ASP:O	1:H:265:GLN:HB2	2.21	0.41
2:J:601:HEM:C1B	3:J:602:QHC:H5	2.56	0.41
1:L:338:GLN:HG3	1:L:342:GLN:HE21	1.86	0.41
1:H:280:PHE:HB2	1:J:500:ARG:HH21	1.86	0.40
3:B:602:QHC:H12	3:B:602:QHC:H2	2.03	0.40
1:C:340:LEU:HD23	1:C:364:LEU:HB3	2.02	0.40
1:H:154:VAL:O	1:H:158:LEU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:340:LEU:HD23	1:I:364:LEU:HB3	2.03	0.40
1:L:116:TRP:CE3	1:L:131:LEU:HD21	2.55	0.40
1:A:340:LEU:HD23	1:A:364:LEU:HB3	2.02	0.40
1:A:428:TRP:CZ3	1:A:440:HIS:HB2	2.56	0.40
1:J:443:PHE:CG	1:J:453:ARG:HG3	2.57	0.40
1:K:318:THR:O	2:K:601:HEM:HAB	2.22	0.40
1:B:101:GLN:O	1:B:104:ASP:HB2	2.22	0.40
1:G:338:GLN:HG3	1:G:342:GLN:HE21	1.87	0.40
1:H:119:TYR:CZ	1:H:123:ARG:HG3	2.57	0.40
1:K:130:PHE:CD1	3:K:602:QHC:H2	2.56	0.40
1:L:332:ARG:HH21	1:L:332:ARG:HB3	1.87	0.40
1:F:407:LEU:HD13	3:F:602:QHC:H15	2.02	0.40
1:G:166:ARG:HH22	1:G:352:SER:HA	1.86	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	461/489 (94%)	447 (97%)	13 (3%)	1 (0%)	47	79
1	B	461/489 (94%)	446 (97%)	14 (3%)	1 (0%)	47	79
1	C	461/489 (94%)	448 (97%)	11 (2%)	2 (0%)	34	69
1	D	461/489 (94%)	441 (96%)	18 (4%)	2 (0%)	34	69
1	E	453/489 (93%)	440 (97%)	12 (3%)	1 (0%)	47	79
1	F	458/489 (94%)	441 (96%)	15 (3%)	2 (0%)	34	69
1	G	461/489 (94%)	440 (95%)	16 (4%)	5 (1%)	14	51
1	H	461/489 (94%)	440 (95%)	17 (4%)	4 (1%)	17	56
1	I	452/489 (92%)	433 (96%)	16 (4%)	3 (1%)	22	61
1	J	457/489 (94%)	433 (95%)	17 (4%)	7 (2%)	10	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	455/489 (93%)	437 (96%)	15 (3%)	3 (1%)	22	61
1	L	458/489 (94%)	436 (95%)	18 (4%)	4 (1%)	17	56
All	All	5499/5868 (94%)	5282 (96%)	182 (3%)	35 (1%)	25	64

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	59	GLN
1	G	242	ARG
1	J	105	SER
1	L	57	ARG
1	F	489	LEU
1	G	57	ARG
1	J	103	VAL
1	J	104	ASP
1	L	48	ARG
1	A	450	CYS
1	B	450	CYS
1	E	450	CYS
1	H	57	ARG
1	H	450	CYS
1	I	450	CYS
1	J	450	CYS
1	L	82	ASN
1	C	450	CYS
1	D	450	CYS
1	G	450	CYS
1	G	489	LEU
1	H	489	LEU
1	J	243	SER
1	K	450	CYS
1	L	450	CYS
1	F	450	CYS
1	H	243	SER
1	J	242	ARG
1	K	441	VAL
1	C	316	VAL
1	G	85	GLY
1	I	105	SER
1	J	57	ARG
1	K	103	VAL

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Mol	Chain	Res	Type
1	I	240	MET

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	410/426 (96%)	379 (92%)	31 (8%)	13	45
1	B	410/426 (96%)	382 (93%)	28 (7%)	16	49
1	C	410/426 (96%)	379 (92%)	31 (8%)	13	45
1	D	410/426 (96%)	379 (92%)	31 (8%)	13	45
1	E	406/426 (95%)	381 (94%)	25 (6%)	18	53
1	F	410/426 (96%)	374 (91%)	36 (9%)	10	36
1	G	410/426 (96%)	382 (93%)	28 (7%)	16	49
1	H	410/426 (96%)	377 (92%)	33 (8%)	12	42
1	I	405/426 (95%)	373 (92%)	32 (8%)	12	43
1	J	409/426 (96%)	368 (90%)	41 (10%)	7	30
1	K	407/426 (96%)	375 (92%)	32 (8%)	12	43
1	L	407/426 (96%)	377 (93%)	30 (7%)	13	46
All	All	4904/5112 (96%)	4526 (92%)	378 (8%)	13	44

All (378) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	47	ASN
1	A	51	ARG
1	A	61	TYR
1	A	81	TYR
1	A	101	GLN
1	A	104	ASP
1	A	106	LEU
1	A	114	GLU

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Mol	Chain	Res	Type
1	A	158	LEU
1	A	178	GLN
1	A	181	ARG
1	A	183	SER
1	A	188	VAL
1	A	242	ARG
1	A	251	LYS
1	A	271	ILE
1	A	284	GLN
1	A	324	LEU
1	A	332	ARG
1	A	356	GLN
1	A	413	ASN
1	A	416	LEU
1	A	421	GLU
1	A	437	ASN
1	A	439	HIS
1	A	448	ARG
1	A	461	LEU
1	A	482	LYS
1	A	488	ILE
1	A	493	THR
1	B	39	GLU
1	B	48	ARG
1	B	58	GLU
1	B	61	TYR
1	B	101	GLN
1	B	104	ASP
1	B	106	LEU
1	B	139	PHE
1	B	155	GLN
1	B	156	ARG
1	B	158	LEU
1	B	188	VAL
1	B	238	MET
1	B	242	ARG
1	B	271	ILE
1	B	299	LEU
1	B	324	LEU
1	B	332	ARG
1	B	352	SER
1	B	356	GLN

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Mol	Chain	Res	Type
1	B	421	GLU
1	B	448	ARG
1	B	454	ARG
1	B	461	LEU
1	B	482	LYS
1	B	488	ILE
1	B	493	THR
1	B	503	ASN
1	C	39	GLU
1	C	57	ARG
1	C	61	TYR
1	C	101	GLN
1	C	104	ASP
1	C	114	GLU
1	C	126	LYS
1	C	139	PHE
1	C	143	ARG
1	C	145	ASN
1	C	158	LEU
1	C	188	VAL
1	C	191	SER
1	C	221	LEU
1	C	238	MET
1	C	242	ARG
1	C	271	ILE
1	C	323	LEU
1	C	324	LEU
1	C	356	GLN
1	C	380	LEU
1	C	394	ASN
1	C	412	ARG
1	C	419	ARG
1	C	421	GLU
1	C	427	ARG
1	C	438	PHE
1	C	448	ARG
1	C	482	LYS
1	C	488	ILE
1	C	493	THR
1	D	39	GLU
1	D	54	GLN
1	D	61	TYR

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Mol	Chain	Res	Type
1	D	100	LEU
1	D	101	GLN
1	D	104	ASP
1	D	111	MET
1	D	113	LEU
1	D	114	GLU
1	D	158	LEU
1	D	170	GLN
1	D	188	VAL
1	D	238	MET
1	D	242	ARG
1	D	271	ILE
1	D	302	GLU
1	D	324	LEU
1	D	332	ARG
1	D	352	SER
1	D	356	GLN
1	D	419	ARG
1	D	421	GLU
1	D	431	ILE
1	D	439	HIS
1	D	448	ARG
1	D	482	LYS
1	D	488	ILE
1	D	489	LEU
1	D	490	ARG
1	D	493	THR
1	D	503	ASN
1	E	39	GLU
1	E	47	ASN
1	E	61	TYR
1	E	64	LEU
1	E	101	GLN
1	E	104	ASP
1	E	114	GLU
1	E	156	ARG
1	E	158	LEU
1	E	188	VAL
1	E	238	MET
1	E	242	ARG
1	E	271	ILE
1	E	324	LEU

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Mol	Chain	Res	Type
1	E	332	ARG
1	E	356	GLN
1	E	416	LEU
1	E	419	ARG
1	E	421	GLU
1	E	422	ARG
1	E	449	GLN
1	E	461	LEU
1	E	482	LYS
1	E	489	LEU
1	E	493	THR
1	F	47	ASN
1	F	50	LEU
1	F	52	LEU
1	F	61	TYR
1	F	73	GLN
1	F	74	GLU
1	F	81	TYR
1	F	104	ASP
1	F	114	GLU
1	F	125	HIS
1	F	158	LEU
1	F	188	VAL
1	F	196	THR
1	F	238	MET
1	F	242	ARG
1	F	244	LEU
1	F	248	ILE
1	F	271	ILE
1	F	282	ARG
1	F	284	GLN
1	F	302	GLU
1	F	310	GLU
1	F	324	LEU
1	F	332	ARG
1	F	356	GLN
1	F	387	SER
1	F	419	ARG
1	F	421	GLU
1	F	422	ARG
1	F	448	ARG
1	F	461	LEU

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Mol	Chain	Res	Type
1	F	473	VAL
1	F	477	THR
1	F	479	GLU
1	F	489	LEU
1	F	493	THR
1	G	39	GLU
1	G	50	LEU
1	G	53	LEU
1	G	56	TRP
1	G	57	ARG
1	G	61	TYR
1	G	104	ASP
1	G	106	LEU
1	G	158	LEU
1	G	188	VAL
1	G	207	GLU
1	G	244	LEU
1	G	268	ASP
1	G	271	ILE
1	G	324	LEU
1	G	332	ARG
1	G	356	GLN
1	G	359	THR
1	G	392	LEU
1	G	409	SER
1	G	416	LEU
1	G	421	GLU
1	G	422	ARG
1	G	438	PHE
1	G	448	ARG
1	G	461	LEU
1	G	486	SER
1	G	488	ILE
1	H	39	GLU
1	H	47	ASN
1	H	50	LEU
1	H	58	GLU
1	H	61	TYR
1	H	83	LEU
1	H	92	MET
1	H	104	ASP
1	H	106	LEU

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Mol	Chain	Res	Type
1	H	114	GLU
1	H	158	LEU
1	H	188	VAL
1	H	193	PHE
1	H	242	ARG
1	H	243	SER
1	H	244	LEU
1	H	246	ARG
1	H	251	LYS
1	H	271	ILE
1	H	302	GLU
1	H	324	LEU
1	H	332	ARG
1	H	381	PHE
1	H	383	GLU
1	H	421	GLU
1	H	427	ARG
1	H	431	ILE
1	H	437	ASN
1	H	448	ARG
1	H	461	LEU
1	H	482	LYS
1	H	488	ILE
1	H	493	THR
1	I	43	GLN
1	I	48	ARG
1	I	49	TRP
1	I	50	LEU
1	I	52	LEU
1	I	53	LEU
1	I	56	TRP
1	I	61	TYR
1	I	81	TYR
1	I	99	LYS
1	I	101	GLN
1	I	112	ILE
1	I	114	GLU
1	I	127	CYS
1	I	158	LEU
1	I	188	VAL
1	I	240	MET
1	I	242	ARG

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Mol	Chain	Res	Type
1	I	244	LEU
1	I	251	LYS
1	I	271	ILE
1	I	324	LEU
1	I	332	ARG
1	I	356	GLN
1	I	416	LEU
1	I	419	ARG
1	I	441	VAL
1	I	448	ARG
1	I	469	LYS
1	I	482	LYS
1	I	493	THR
1	I	503	ASN
1	J	39	GLU
1	J	51	ARG
1	J	52	LEU
1	J	53	LEU
1	J	54	GLN
1	J	56	TRP
1	J	57	ARG
1	J	59	GLN
1	J	61	TYR
1	J	66	LEU
1	J	104	ASP
1	J	113	LEU
1	J	158	LEU
1	J	170	GLN
1	J	188	VAL
1	J	211	LEU
1	J	235	VAL
1	J	240	MET
1	J	244	LEU
1	J	247	TRP
1	J	248	ILE
1	J	271	ILE
1	J	324	LEU
1	J	332	ARG
1	J	356	GLN
1	J	382	LEU
1	J	383	GLU
1	J	387	SER

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Mol	Chain	Res	Type
1	J	402	LEU
1	J	407	LEU
1	J	416	LEU
1	J	421	GLU
1	J	429	LEU
1	J	438	PHE
1	J	448	ARG
1	J	453	ARG
1	J	461	LEU
1	J	480	ASP
1	J	482	LYS
1	J	488	ILE
1	J	493	THR
1	K	39	GLU
1	K	54	GLN
1	K	55	ILE
1	K	57	ARG
1	K	58	GLU
1	K	61	TYR
1	K	66	LEU
1	K	81	TYR
1	K	83	LEU
1	K	104	ASP
1	K	114	GLU
1	K	126	LYS
1	K	156	ARG
1	K	158	LEU
1	K	188	VAL
1	K	238	MET
1	K	242	ARG
1	K	244	LEU
1	K	271	ILE
1	K	302	GLU
1	K	332	ARG
1	K	350	SER
1	K	356	GLN
1	K	365	LEU
1	K	394	ASN
1	K	421	GLU
1	K	426	GLN
1	K	448	ARG
1	K	461	LEU

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Mol	Chain	Res	Type
1	K	481	ILE
1	K	488	ILE
1	K	493	THR
1	L	39	GLU
1	L	47	ASN
1	L	50	LEU
1	L	51	ARG
1	L	56	TRP
1	L	61	TYR
1	L	70	GLN
1	L	73	GLN
1	L	83	LEU
1	L	87	ARG
1	L	106	LEU
1	L	114	GLU
1	L	158	LEU
1	L	188	VAL
1	L	238	MET
1	L	242	ARG
1	L	247	TRP
1	L	271	ILE
1	L	284	GLN
1	L	324	LEU
1	L	332	ARG
1	L	356	GLN
1	L	387	SER
1	L	393	GLN
1	L	419	ARG
1	L	421	GLU
1	L	448	ARG
1	L	472	LEU
1	L	482	LYS
1	L	493	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	63	HIS
1	A	155	GLN
1	A	236	GLN
1	A	338	GLN

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Mol	Chain	Res	Type
1	A	342	GLN
1	A	393	GLN
1	A	396	HIS
1	A	404	GLN
1	B	82	ASN
1	B	107	HIS
1	B	338	GLN
1	B	342	GLN
1	B	393	GLN
1	B	439	HIS
1	B	440	HIS
1	C	107	HIS
1	C	284	GLN
1	C	338	GLN
1	C	342	GLN
1	C	393	GLN
1	C	404	GLN
1	C	440	HIS
1	D	101	GLN
1	D	338	GLN
1	D	342	GLN
1	D	393	GLN
1	D	404	GLN
1	D	440	HIS
1	E	82	ASN
1	E	121	GLN
1	E	338	GLN
1	E	393	GLN
1	E	404	GLN
1	E	440	HIS
1	F	155	GLN
1	F	236	GLN
1	F	338	GLN
1	F	393	GLN
1	F	478	GLN
1	G	59	GLN
1	G	125	HIS
1	G	236	GLN
1	G	269	ASN
1	G	338	GLN
1	G	342	GLN
1	G	393	GLN

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Mol	Chain	Res	Type
1	G	413	ASN
1	G	439	HIS
1	G	440	HIS
1	H	338	GLN
1	H	342	GLN
1	H	393	GLN
1	H	439	HIS
1	H	478	GLN
1	I	338	GLN
1	I	342	GLN
1	I	393	GLN
1	I	413	ASN
1	J	155	GLN
1	J	236	GLN
1	J	338	GLN
1	J	342	GLN
1	J	393	GLN
1	J	426	GLN
1	J	440	HIS
1	K	155	GLN
1	K	236	GLN
1	K	338	GLN
1	K	393	GLN
1	K	404	GLN
1	K	437	ASN
1	L	155	GLN
1	L	225	HIS
1	L	236	GLN
1	L	338	GLN
1	L	342	GLN
1	L	393	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	$\#\|Z\| > 2$
2	HEM	E	601	3,1	41,50,50	1.76	9 (21%)	45,82,82	1.62	10 (22%)
2	HEM	F	601	3,1	41,50,50	1.55	11 (26%)	45,82,82	1.18	4 (8%)
2	HEM	J	601	3	41,50,50	1.53	8 (19%)	45,82,82	1.67	11 (24%)
2	HEM	I	601	3,1	41,50,50	1.53	6 (14%)	45,82,82	1.68	11 (24%)
3	QHC	D	602	2	25,25,25	0.84	1 (4%)	31,35,35	1.88	7 (22%)
2	HEM	A	601	3,1	41,50,50	1.56	9 (21%)	45,82,82	1.37	5 (11%)
3	QHC	F	602	2	25,25,25	0.79	0	31,35,35	1.86	8 (25%)
2	HEM	B	601	3,1	41,50,50	1.51	6 (14%)	45,82,82	1.39	6 (13%)
3	QHC	I	602	2	25,25,25	0.90	1 (4%)	31,35,35	1.57	5 (16%)
3	QHC	L	602	2	25,25,25	0.72	0	31,35,35	1.49	6 (19%)
3	QHC	B	602	2	25,25,25	0.98	1 (4%)	31,35,35	1.60	6 (19%)
2	HEM	H	601	-	41,50,50	1.42	5 (12%)	45,82,82	1.69	11 (24%)
2	HEM	K	601	3,1	41,50,50	1.42	6 (14%)	45,82,82	1.58	8 (17%)
2	HEM	L	601	3,1	41,50,50	1.39	5 (12%)	45,82,82	1.88	11 (24%)
3	QHC	A	602	2	25,25,25	0.71	0	31,35,35	1.76	10 (32%)
3	QHC	E	602	2	25,25,25	0.77	0	31,35,35	1.89	11 (35%)
3	QHC	K	602	2	25,25,25	0.75	0	31,35,35	1.42	6 (19%)
3	QHC	J	602	2	25,25,25	0.81	1 (4%)	31,35,35	1.79	5 (16%)
2	HEM	D	601	3,1	41,50,50	1.53	9 (21%)	45,82,82	1.52	9 (20%)
2	HEM	C	601	3,1	41,50,50	1.55	9 (21%)	45,82,82	1.70	9 (20%)
2	HEM	G	601	-	41,50,50	1.51	8 (19%)	45,82,82	1.62	10 (22%)
3	QHC	C	602	2	25,25,25	0.75	0	31,35,35	1.44	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	E	601	3,1	-	4/12/54/54	-
2	HEM	F	601	3,1	-	3/12/54/54	-
2	HEM	J	601	3	-	3/12/54/54	-
2	HEM	I	601	3,1	-	4/12/54/54	-
3	QHC	D	602	2	-	1/10/20/20	0/3/3/3
2	HEM	A	601	3,1	-	5/12/54/54	-
3	QHC	F	602	2	-	1/10/20/20	0/3/3/3
2	HEM	B	601	3,1	-	5/12/54/54	-
3	QHC	I	602	2	-	1/10/20/20	0/3/3/3
3	QHC	L	602	2	-	1/10/20/20	0/3/3/3
3	QHC	B	602	2	-	3/10/20/20	0/3/3/3
2	HEM	H	601	-	-	2/12/54/54	-
2	HEM	K	601	3,1	-	3/12/54/54	-
2	HEM	L	601	3,1	-	7/12/54/54	-
3	QHC	A	602	2	-	1/10/20/20	0/3/3/3
3	QHC	E	602	2	-	1/10/20/20	0/3/3/3
3	QHC	K	602	2	-	2/10/20/20	0/3/3/3
3	QHC	J	602	2	-	1/10/20/20	0/3/3/3
2	HEM	D	601	3,1	-	2/12/54/54	-
2	HEM	C	601	3,1	-	3/12/54/54	-
2	HEM	G	601	-	-	0/12/54/54	-
3	QHC	C	602	2	-	1/10/20/20	0/3/3/3

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	HEM	C4D-ND	-5.38	1.31	1.40
2	H	601	HEM	C3C-C2C	-4.87	1.33	1.40
2	D	601	HEM	C1D-C2D	4.46	1.53	1.44
2	E	601	HEM	C1B-NB	-4.36	1.32	1.40
2	F	601	HEM	C3C-C2C	-4.31	1.34	1.40
2	I	601	HEM	C3B-C4B	4.24	1.53	1.44
2	A	601	HEM	C1D-C2D	4.17	1.52	1.44
2	C	601	HEM	C3B-C4B	3.90	1.52	1.44
2	J	601	HEM	C1D-C2D	3.88	1.52	1.44
2	B	601	HEM	C1D-C2D	3.73	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C1B-NB	-3.50	1.34	1.40
2	A	601	HEM	C3C-C2C	-3.48	1.35	1.40
2	L	601	HEM	C3C-C2C	-3.47	1.35	1.40
2	L	601	HEM	C4D-ND	-3.38	1.34	1.40
2	C	601	HEM	C4D-ND	-3.23	1.34	1.40
2	J	601	HEM	C1B-NB	-3.21	1.34	1.40
2	K	601	HEM	C1B-NB	-3.20	1.34	1.40
2	B	601	HEM	C4D-C3D	3.20	1.50	1.45
2	C	601	HEM	C1D-C2D	3.18	1.50	1.44
2	K	601	HEM	C1D-ND	-3.13	1.32	1.38
2	A	601	HEM	C3B-C4B	3.10	1.51	1.44
2	K	601	HEM	C4D-ND	-3.10	1.35	1.40
2	E	601	HEM	C3B-C4B	3.09	1.51	1.44
2	B	601	HEM	C1A-NA	3.03	1.42	1.36
2	G	601	HEM	C1B-NB	-3.02	1.35	1.40
2	B	601	HEM	C1B-NB	-2.98	1.35	1.40
2	G	601	HEM	C1D-C2D	2.97	1.50	1.44
2	I	601	HEM	C1D-C2D	2.95	1.50	1.44
2	D	601	HEM	C1B-NB	-2.92	1.35	1.40
2	B	601	HEM	C4A-NA	2.85	1.42	1.36
2	G	601	HEM	C4D-ND	-2.83	1.35	1.40
2	B	601	HEM	C3B-C4B	2.80	1.50	1.44
2	A	601	HEM	C4A-NA	2.78	1.41	1.36
2	H	601	HEM	C3B-C4B	2.76	1.50	1.44
2	I	601	HEM	C4A-NA	2.76	1.41	1.36
2	A	601	HEM	C4D-ND	-2.75	1.35	1.40
2	E	601	HEM	C1D-C2D	2.74	1.49	1.44
2	E	601	HEM	C4B-NB	-2.74	1.33	1.38
2	K	601	HEM	C1D-C2D	2.66	1.49	1.44
2	E	601	HEM	C1A-CHA	-2.62	1.33	1.41
2	J	601	HEM	C4D-ND	-2.61	1.35	1.40
2	D	601	HEM	C4B-NB	-2.60	1.33	1.38
2	G	601	HEM	CHB-C1B	2.60	1.41	1.35
2	G	601	HEM	CMB-C2B	2.59	1.56	1.50
2	H	601	HEM	C1D-ND	-2.57	1.33	1.38
3	B	602	QHC	C14-N23	2.57	1.50	1.46
2	F	601	HEM	C4D-ND	-2.55	1.35	1.40
2	I	601	HEM	C3B-C2B	-2.55	1.32	1.37
2	H	601	HEM	C1D-C2D	2.54	1.49	1.44
2	C	601	HEM	C1D-ND	-2.54	1.33	1.38
2	C	601	HEM	O2A-CGA	2.51	1.39	1.30
2	K	601	HEM	C3B-C2B	-2.50	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	HEM	C1D-ND	-2.49	1.33	1.38
2	A	601	HEM	CMC-C2C	-2.48	1.45	1.51
2	D	601	HEM	C1A-CHA	-2.47	1.34	1.41
2	D	601	HEM	C4D-C3D	2.43	1.49	1.45
2	F	601	HEM	C1A-CHA	-2.43	1.34	1.41
2	C	601	HEM	CBD-CGD	2.42	1.56	1.50
2	E	601	HEM	CAA-C2A	2.41	1.55	1.52
2	L	601	HEM	C1B-NB	-2.41	1.36	1.40
2	A	601	HEM	C1B-C2B	-2.38	1.40	1.44
2	E	601	HEM	C4D-C3D	2.38	1.49	1.45
2	K	601	HEM	C1A-CHA	-2.37	1.34	1.41
3	J	602	QHC	C14-N23	2.37	1.49	1.46
2	J	601	HEM	CHB-C1B	2.34	1.41	1.35
2	E	601	HEM	O2A-CGA	2.33	1.38	1.30
2	G	601	HEM	C1A-CHA	-2.33	1.34	1.41
2	J	601	HEM	C1A-NA	2.30	1.40	1.36
2	D	601	HEM	C3B-C2B	-2.29	1.32	1.37
2	F	601	HEM	C1A-NA	2.28	1.40	1.36
2	F	601	HEM	C3B-C4B	2.26	1.49	1.44
2	G	601	HEM	CBA-CGA	2.26	1.55	1.50
2	J	601	HEM	C3D-C2D	-2.25	1.31	1.36
2	D	601	HEM	C3B-C4B	2.24	1.49	1.44
2	C	601	HEM	C4A-CHB	-2.24	1.34	1.41
2	F	601	HEM	CAA-C2A	-2.23	1.48	1.52
2	D	601	HEM	CHB-C1B	2.22	1.40	1.35
2	I	601	HEM	C4B-NB	-2.19	1.34	1.38
2	A	601	HEM	C3B-C2B	-2.17	1.32	1.37
2	F	601	HEM	C1D-C2D	2.16	1.48	1.44
2	D	601	HEM	C4A-NA	2.15	1.40	1.36
2	A	601	HEM	C1A-CHA	-2.15	1.35	1.41
2	G	601	HEM	C3B-C4B	2.14	1.49	1.44
2	H	601	HEM	C4D-ND	-2.13	1.36	1.40
2	I	601	HEM	C3C-C2C	-2.12	1.37	1.40
2	F	601	HEM	C1B-NB	-2.11	1.36	1.40
2	L	601	HEM	CHB-C1B	2.09	1.40	1.35
2	L	601	HEM	C4A-NA	2.09	1.40	1.36
3	D	602	QHC	C8-C12	2.08	1.44	1.41
2	C	601	HEM	CAA-C2A	2.06	1.55	1.52
2	F	601	HEM	C2A-C3A	-2.05	1.31	1.37
2	F	601	HEM	C2C-C1C	-2.05	1.37	1.42
3	I	602	QHC	C14-N23	2.02	1.49	1.46
2	J	601	HEM	CBA-CGA	2.02	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	601	HEM	O2D-CGD	2.00	1.37	1.30

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	QHC	C14-N23-C18	5.88	132.69	123.33
2	L	601	HEM	CBA-CAA-C2A	5.74	122.42	112.62
3	I	602	QHC	C14-N23-C18	5.41	131.94	123.33
3	B	602	QHC	C14-N23-C18	5.11	131.47	123.33
2	C	601	HEM	C2B-C1B-NB	5.07	115.85	109.84
3	J	602	QHC	C14-N23-C18	4.85	131.06	123.33
3	D	602	QHC	C13-C14-N23	4.72	117.71	110.80
2	K	601	HEM	CBA-CAA-C2A	4.62	120.50	112.62
3	J	602	QHC	C13-C14-N23	4.27	117.06	110.80
3	C	602	QHC	C11-N10-C9	4.24	123.26	117.48
3	B	602	QHC	C11-N10-C9	4.15	123.14	117.48
3	E	602	QHC	C14-N23-C18	4.13	129.90	123.33
3	D	602	QHC	C11-N10-C9	4.09	123.06	117.48
2	H	601	HEM	C2B-C1B-NB	4.09	114.68	109.84
2	J	601	HEM	CMD-C2D-C1D	4.04	131.19	125.04
3	L	602	QHC	C11-N10-C9	3.87	122.77	117.48
2	E	601	HEM	C4B-C3B-C2B	-3.84	104.07	107.11
3	E	602	QHC	C1-C2-CL7	-3.82	115.16	119.78
2	D	601	HEM	CAD-CBD-CGD	-3.79	105.44	113.60
2	E	601	HEM	C3D-C4D-ND	3.71	114.30	110.17
3	A	602	QHC	C11-N10-C9	3.70	122.53	117.48
3	D	602	QHC	C11-C13-C14	-3.70	114.93	124.08
3	C	602	QHC	C14-N23-C18	3.69	129.21	123.33
3	F	602	QHC	C11-N10-C9	3.62	122.42	117.48
3	A	602	QHC	C3-C2-C1	3.59	121.82	118.94
2	E	601	HEM	C2B-C1B-NB	3.59	114.10	109.84
3	I	602	QHC	C11-N10-C9	3.54	122.32	117.48
3	E	602	QHC	C3-C2-CL7	3.54	125.52	118.41
3	J	602	QHC	C11-N10-C9	3.52	122.29	117.48
2	K	601	HEM	CHA-C4D-C3D	-3.51	118.75	125.33
2	L	601	HEM	CHC-C4B-NB	3.46	128.19	124.43
2	A	601	HEM	C3D-C4D-ND	3.44	114.00	110.17
2	I	601	HEM	C3B-C2B-C1B	-3.44	103.94	106.49
3	D	602	QHC	C19-C18-N23	3.43	120.19	115.77
2	A	601	HEM	CHA-C4D-C3D	-3.43	118.89	125.33
3	K	602	QHC	C11-N10-C9	3.42	122.14	117.48
2	B	601	HEM	C4B-C3B-C2B	-3.42	104.40	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	602	QHC	C11-N10-C9	3.36	122.07	117.48
2	G	601	HEM	CHA-C4D-C3D	-3.35	119.05	125.33
2	L	601	HEM	CHD-C1D-ND	3.34	128.06	124.43
2	J	601	HEM	CHC-C4B-NB	3.32	128.04	124.43
2	H	601	HEM	C4A-C3A-C2A	-3.29	104.71	107.00
2	B	601	HEM	C2C-C3C-C4C	3.25	109.17	106.90
2	L	601	HEM	CHD-C1D-C2D	-3.20	119.99	124.98
2	J	601	HEM	C1D-C2D-C3D	-3.19	103.61	106.96
2	I	601	HEM	C2B-C1B-NB	3.17	113.60	109.84
3	J	602	QHC	C19-C18-N23	3.17	119.84	115.77
2	G	601	HEM	C2B-C1B-NB	3.15	113.58	109.84
2	J	601	HEM	CHD-C1D-C2D	-3.14	120.08	124.98
2	K	601	HEM	C2B-C1B-NB	3.11	113.52	109.84
2	D	601	HEM	CHA-C4D-C3D	-3.11	119.50	125.33
2	I	601	HEM	CHA-C4D-C3D	-3.10	119.51	125.33
2	B	601	HEM	C2B-C1B-NB	3.10	113.51	109.84
2	G	601	HEM	C3B-C2B-C1B	-3.09	104.19	106.49
3	K	602	QHC	C14-N23-C18	3.09	128.25	123.33
2	C	601	HEM	CMB-C2B-C1B	3.08	129.72	125.04
2	K	601	HEM	C3D-C4D-ND	3.06	113.57	110.17
2	C	601	HEM	O2D-CGD-O1D	-3.04	115.73	123.30
3	F	602	QHC	C11-C13-C12	3.03	120.43	117.83
2	E	601	HEM	CMD-C2D-C1D	2.95	129.54	125.04
2	I	601	HEM	C4B-C3B-C2B	2.95	109.46	107.11
2	F	601	HEM	CHA-C4D-C3D	-2.94	119.81	125.33
3	B	602	QHC	C19-C18-N23	2.87	119.46	115.77
3	E	602	QHC	C15-C14-C13	2.87	115.20	111.34
2	H	601	HEM	CHC-C4B-NB	2.84	127.52	124.43
2	G	601	HEM	C4B-C3B-C2B	-2.84	104.86	107.11
2	G	601	HEM	O2D-CGD-CBD	2.83	123.11	114.03
2	I	601	HEM	C3D-C4D-ND	2.82	113.30	110.17
2	L	601	HEM	C4B-C3B-C2B	-2.80	104.89	107.11
3	D	602	QHC	C14-N23-C18	2.78	127.75	123.33
3	E	602	QHC	F22-C1-C2	-2.78	116.42	118.98
2	D	601	HEM	C3D-C4D-ND	2.73	113.21	110.17
2	D	601	HEM	C2B-C1B-NB	2.72	113.06	109.84
2	J	601	HEM	CHA-C4D-C3D	-2.70	120.26	125.33
2	G	601	HEM	C3D-C4D-ND	2.69	113.16	110.17
3	B	602	QHC	C8-C9-N10	-2.68	120.11	124.16
2	D	601	HEM	CHD-C1D-ND	2.68	127.34	124.43
3	K	602	QHC	C11-C13-C12	2.67	120.12	117.83
2	C	601	HEM	C1B-NB-C4B	-2.66	102.32	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	601	HEM	CHA-C4D-C3D	-2.66	120.34	125.33
3	I	602	QHC	C13-C14-N23	2.65	114.68	110.80
2	I	601	HEM	CBB-CAB-C3B	-2.64	114.50	127.62
2	H	601	HEM	C2D-C1D-ND	2.62	113.02	109.88
2	B	601	HEM	C3D-C4D-ND	2.58	113.04	110.17
2	K	601	HEM	CHC-C4B-NB	2.58	127.23	124.43
2	H	601	HEM	C3D-C4D-ND	2.58	113.03	110.17
3	E	602	QHC	C11-C13-C14	-2.56	117.74	124.08
2	I	601	HEM	CHB-C1B-C2B	-2.55	119.66	126.72
2	D	601	HEM	C4B-CHC-C1C	2.55	125.92	122.56
2	H	601	HEM	C3B-C2B-C1B	-2.54	104.60	106.49
3	L	602	QHC	C14-N23-C18	2.52	127.35	123.33
2	I	601	HEM	CMB-C2B-C1B	2.51	128.86	125.04
3	A	602	QHC	C5-C6-C1	-2.51	117.46	119.59
2	G	601	HEM	CHC-C4B-C3B	-2.50	120.74	124.57
3	F	602	QHC	C3-C2-C1	2.49	120.94	118.94
3	C	602	QHC	C11-C13-C14	-2.49	117.91	124.08
2	E	601	HEM	O2A-CGA-CBA	2.49	122.04	114.03
3	A	602	QHC	F22-C1-C2	-2.49	116.68	118.98
2	L	601	HEM	C3D-C4D-ND	2.48	112.92	110.17
2	C	601	HEM	C4B-C3B-C2B	-2.47	105.15	107.11
2	J	601	HEM	O2D-CGD-CBD	2.47	121.96	114.03
2	J	601	HEM	C2D-C1D-ND	2.46	112.83	109.88
3	F	602	QHC	C11-C13-C14	-2.45	118.01	124.08
2	K	601	HEM	CHA-C4D-ND	2.45	127.40	124.38
2	L	601	HEM	CAD-C3D-C2D	2.42	132.38	127.88
3	K	602	QHC	F22-C1-C2	2.41	121.20	118.98
3	L	602	QHC	C3-C2-C1	2.40	120.87	118.94
2	D	601	HEM	CMA-C3A-C2A	-2.40	120.42	124.94
3	E	602	QHC	C16-C17-C12	-2.39	107.94	112.84
3	B	602	QHC	C11-C13-C14	-2.38	118.19	124.08
3	D	602	QHC	C3-C2-C1	2.37	120.84	118.94
2	H	601	HEM	CHC-C4B-C3B	-2.37	120.94	124.57
3	L	602	QHC	C11-C13-C14	-2.36	118.23	124.08
2	E	601	HEM	CHA-C4D-C3D	-2.36	120.90	125.33
2	L	601	HEM	CAD-CBD-CGD	-2.36	108.53	113.60
2	J	601	HEM	C2B-C1B-NB	2.35	112.62	109.84
2	G	601	HEM	CHA-C4D-ND	2.34	127.28	124.38
3	A	602	QHC	C1-C2-CL7	-2.34	116.94	119.78
2	L	601	HEM	O2A-CGA-CBA	2.34	121.55	114.03
2	D	601	HEM	CHA-C4D-ND	2.34	127.27	124.38
2	F	601	HEM	C3D-C4D-ND	2.34	112.77	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	HEM	CMA-C3A-C4A	2.32	132.02	128.46
2	I	601	HEM	CHD-C1D-ND	2.31	126.94	124.43
2	E	601	HEM	C2D-C1D-ND	2.28	112.62	109.88
2	F	601	HEM	CHA-C4D-ND	2.28	127.20	124.38
2	H	601	HEM	CHD-C1D-C2D	-2.28	121.42	124.98
2	B	601	HEM	C2D-C1D-ND	2.27	112.61	109.88
3	E	602	QHC	C17-C12-C13	-2.27	118.07	121.58
2	E	601	HEM	O2D-CGD-O1D	-2.26	117.68	123.30
2	H	601	HEM	O2D-CGD-O1D	-2.25	117.68	123.30
3	A	602	QHC	C4-C3-C2	-2.25	116.74	120.00
2	G	601	HEM	CHC-C4B-NB	2.25	126.87	124.43
3	D	602	QHC	C8-C9-N10	-2.23	120.78	124.16
2	I	601	HEM	CHA-C4D-ND	2.21	127.11	124.38
2	A	601	HEM	C2B-C1B-NB	2.21	112.45	109.84
3	F	602	QHC	C13-C14-N23	-2.20	107.58	110.80
3	C	602	QHC	C8-C9-N10	-2.20	120.83	124.16
2	A	601	HEM	CHA-C4D-ND	2.20	127.10	124.38
2	I	601	HEM	CHD-C1D-C2D	-2.18	121.57	124.98
2	F	601	HEM	O2D-CGD-O1D	-2.18	117.87	123.30
2	L	601	HEM	CMD-C2D-C3D	2.17	132.01	126.12
2	C	601	HEM	C3D-C4D-ND	2.17	112.58	110.17
2	J	601	HEM	CAA-CBA-CGA	2.17	119.83	113.76
3	A	602	QHC	C4-C5-C8	-2.17	117.40	120.91
2	H	601	HEM	CHB-C1B-C2B	-2.16	120.75	126.72
3	L	602	QHC	C8-C9-N10	-2.15	120.91	124.16
3	K	602	QHC	C11-C13-C14	-2.14	118.77	124.08
3	A	602	QHC	C5-C8-C12	-2.14	119.84	122.93
2	J	601	HEM	CHA-C4D-ND	2.14	127.03	124.38
2	C	601	HEM	C1D-C2D-C3D	-2.14	104.71	106.96
3	J	602	QHC	C15-C14-C13	-2.13	108.47	111.34
2	E	601	HEM	C1D-C2D-C3D	-2.13	104.72	106.96
3	A	602	QHC	C13-C11-N10	-2.13	120.25	124.14
2	A	601	HEM	CHB-C1B-C2B	-2.12	120.87	126.72
3	I	602	QHC	C11-C13-C14	-2.11	118.85	124.08
2	J	601	HEM	CHD-C1D-ND	2.11	126.72	124.43
3	F	602	QHC	C15-C16-C17	2.10	116.65	110.64
3	E	602	QHC	C5-C8-C12	2.08	125.93	122.93
3	B	602	QHC	O20-C18-C19	-2.08	116.28	122.08
2	E	601	HEM	C4B-CHC-C1C	2.07	125.29	122.56
2	H	601	HEM	CAB-C3B-C2B	2.07	135.42	128.60
2	K	601	HEM	CMC-C2C-C3C	2.06	128.53	124.68
3	L	602	QHC	C19-C18-N23	2.06	118.42	115.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	601	HEM	CMC-C2C-C3C	2.05	128.52	124.68
2	C	601	HEM	CHB-C1B-C2B	-2.05	121.04	126.72
3	C	602	QHC	C13-C11-N10	-2.05	120.38	124.14
2	K	601	HEM	CAD-C3D-C2D	2.05	131.69	127.88
2	C	601	HEM	O2A-CGA-CBA	2.04	120.59	114.03
3	K	602	QHC	C13-C11-N10	-2.03	120.43	124.14
2	B	601	HEM	C4D-ND-C1D	-2.02	102.99	105.07
3	A	602	QHC	C8-C9-N10	-2.02	121.11	124.16
3	I	602	QHC	F22-C1-C2	2.02	120.84	118.98
3	F	602	QHC	C13-C11-N10	-2.01	120.46	124.14
3	E	602	QHC	C13-C11-N10	-2.00	120.47	124.14

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	HEM	C2B-C3B-CAB-CBB
2	E	601	HEM	C4B-C3B-CAB-CBB
2	I	601	HEM	C4B-C3B-CAB-CBB
2	L	601	HEM	C1A-C2A-CAA-CBA
2	L	601	HEM	C3A-C2A-CAA-CBA
3	A	602	QHC	C15-C14-N23-C18
3	B	602	QHC	C15-C14-N23-C18
3	C	602	QHC	C15-C14-N23-C18
3	D	602	QHC	C13-C14-N23-C18
3	F	602	QHC	C15-C14-N23-C18
3	I	602	QHC	C15-C14-N23-C18
3	J	602	QHC	C13-C14-N23-C18
3	K	602	QHC	C15-C14-N23-C18
3	L	602	QHC	C15-C14-N23-C18
3	B	602	QHC	O20-C18-C19-C21
2	A	601	HEM	C2B-C3B-CAB-CBB
2	B	601	HEM	C2B-C3B-CAB-CBB
2	C	601	HEM	C2B-C3B-CAB-CBB
2	I	601	HEM	C2B-C3B-CAB-CBB
2	A	601	HEM	C4B-C3B-CAB-CBB
2	B	601	HEM	C4B-C3B-CAB-CBB
2	C	601	HEM	C4B-C3B-CAB-CBB
3	B	602	QHC	N23-C18-C19-C21
2	C	601	HEM	C2A-CAA-CBA-CGA
2	K	601	HEM	C2B-C3B-CAB-CBB
2	L	601	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	F	601	HEM	C2A-CAA-CBA-CGA
2	A	601	HEM	C1A-C2A-CAA-CBA
2	L	601	HEM	CAD-CBD-CGD-O1D
2	H	601	HEM	CAD-CBD-CGD-O1D
2	D	601	HEM	CAD-CBD-CGD-O1D
2	H	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	C3D-CAD-CBD-CGD
2	D	601	HEM	CAD-CBD-CGD-O2D
2	L	601	HEM	CAD-CBD-CGD-O2D
3	K	602	QHC	C13-C14-N23-C18
3	E	602	QHC	C15-C14-N23-C18
2	L	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAD-CBD-CGD-O1D
2	E	601	HEM	CAD-CBD-CGD-O1D
2	J	601	HEM	CAD-CBD-CGD-O1D
2	F	601	HEM	CAD-CBD-CGD-O1D
2	K	601	HEM	C4B-C3B-CAB-CBB
2	E	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	J	601	HEM	CAD-CBD-CGD-O2D
2	F	601	HEM	CAD-CBD-CGD-O2D
2	L	601	HEM	CAA-CBA-CGA-O2A
2	J	601	HEM	C2A-CAA-CBA-CGA
2	I	601	HEM	C3D-CAD-CBD-CGD
2	A	601	HEM	CAD-CBD-CGD-O2D
2	K	601	HEM	CAD-CBD-CGD-O1D
2	I	601	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

21 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	HEM	4	0
2	F	601	HEM	8	0
2	J	601	HEM	1	0
2	I	601	HEM	3	0
2	A	601	HEM	6	0
3	F	602	QHC	5	0
2	B	601	HEM	4	0
3	I	602	QHC	4	0
3	L	602	QHC	3	0

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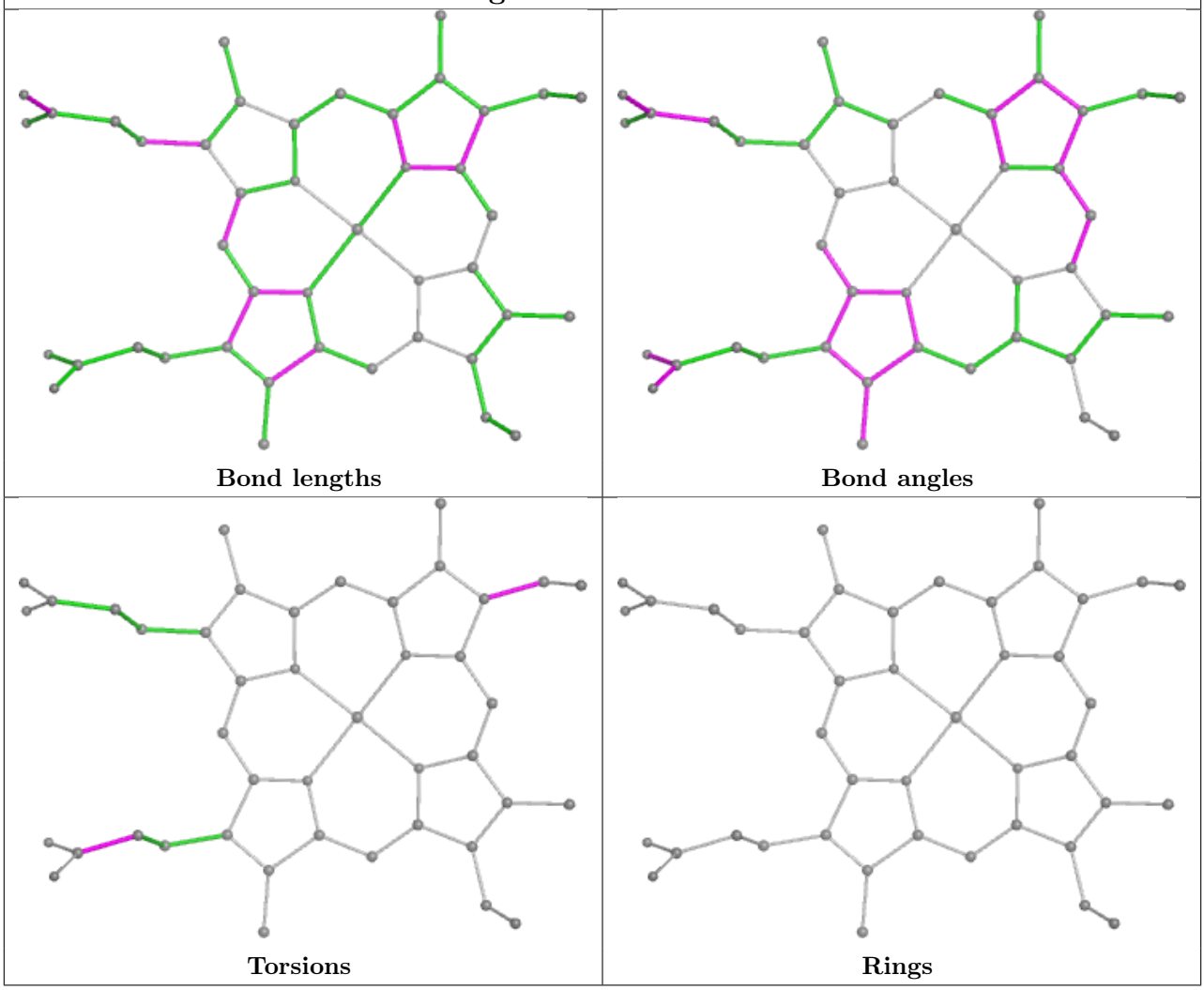
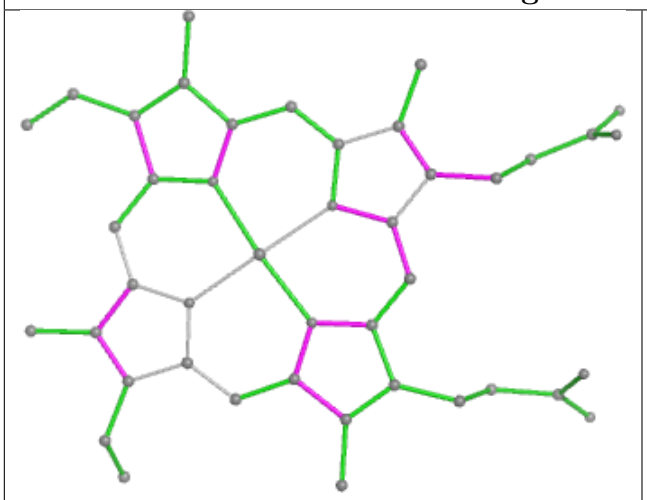
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	QHC	5	0
2	H	601	HEM	7	0
2	K	601	HEM	4	0
2	L	601	HEM	4	0
3	A	602	QHC	7	0
3	E	602	QHC	2	0
3	K	602	QHC	5	0
3	J	602	QHC	4	0
2	D	601	HEM	2	0
2	C	601	HEM	5	0
2	G	601	HEM	1	0
3	C	602	QHC	5	0

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

Ligand HEM E 601



Ligand HEM F 601



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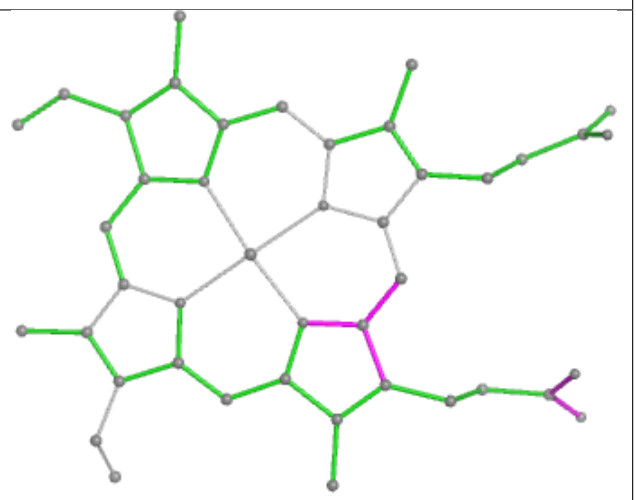
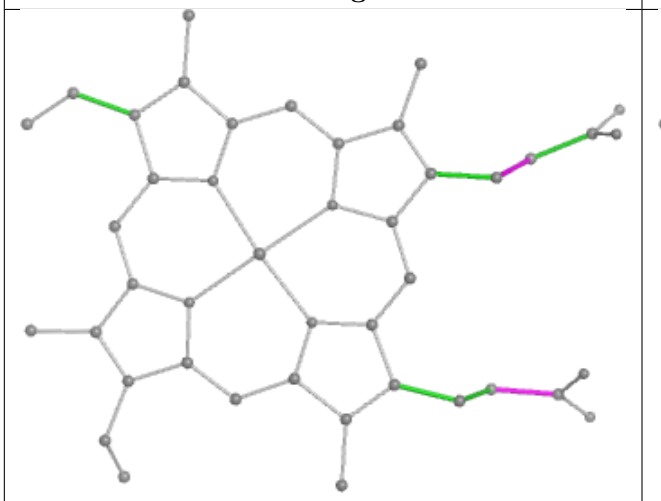
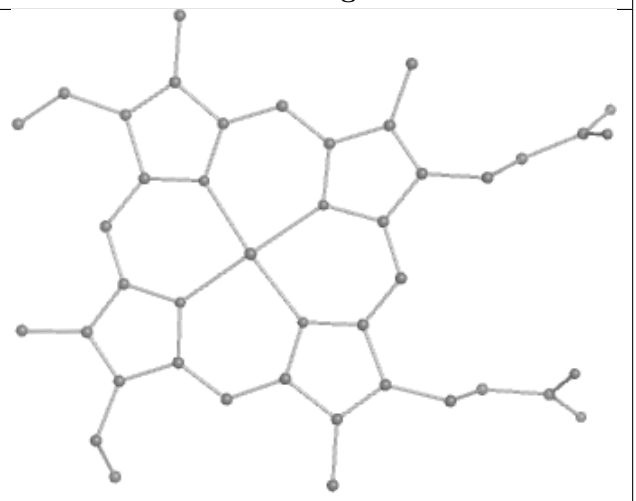


Bond angles



Torsions



Rings

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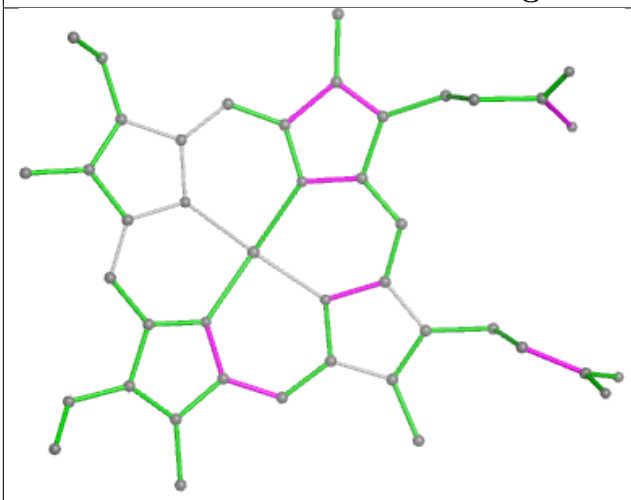

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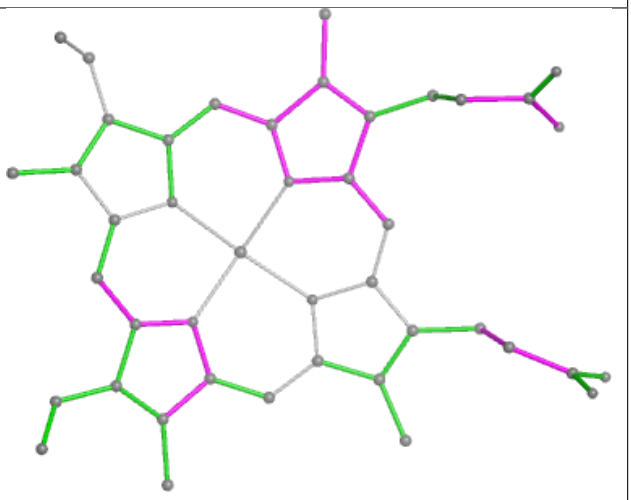

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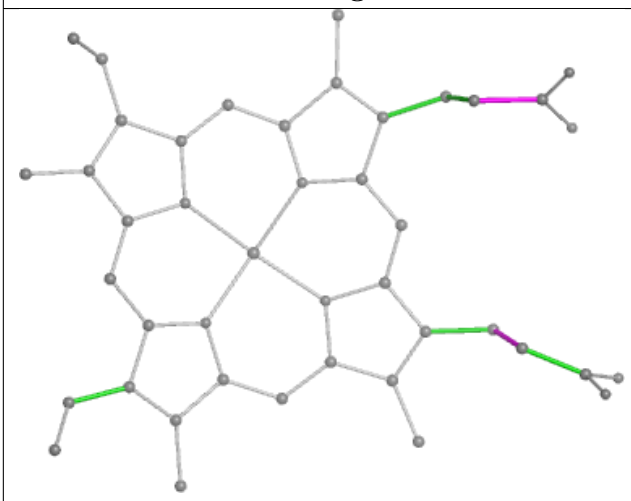

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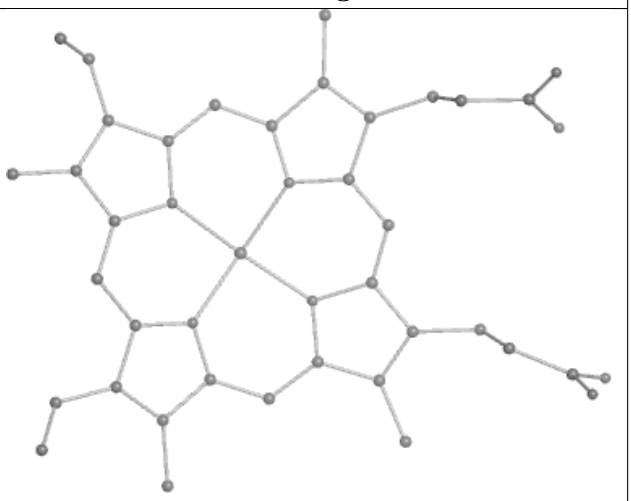

Rings

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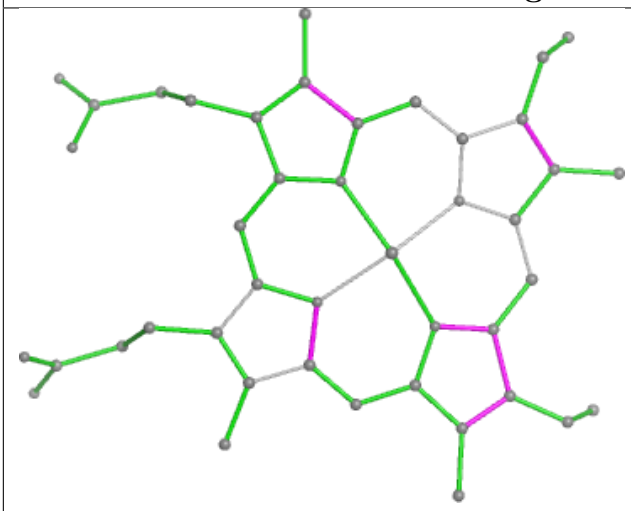

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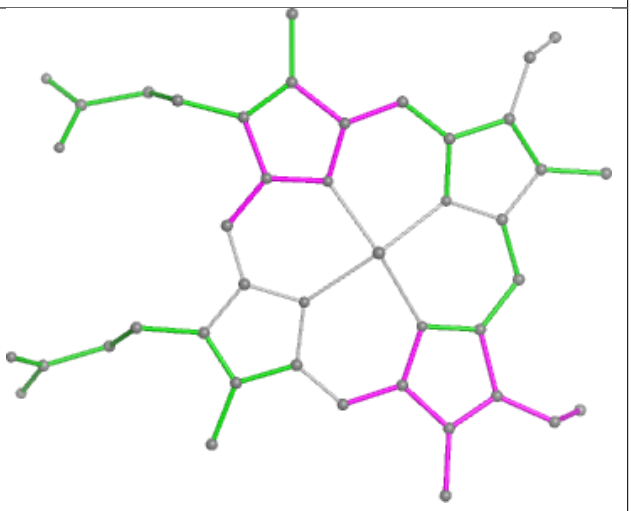

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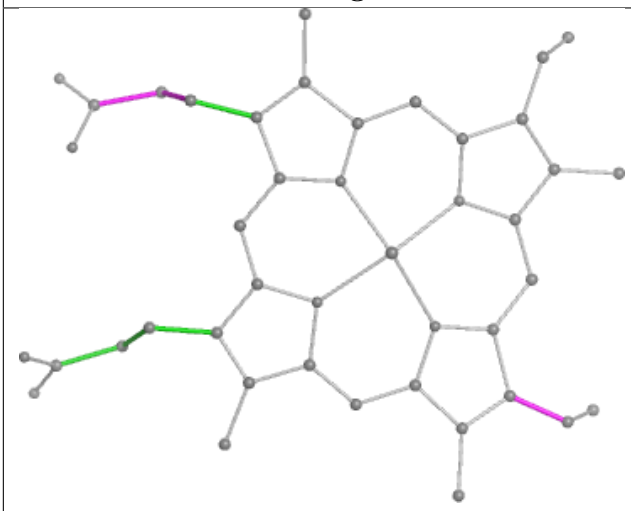

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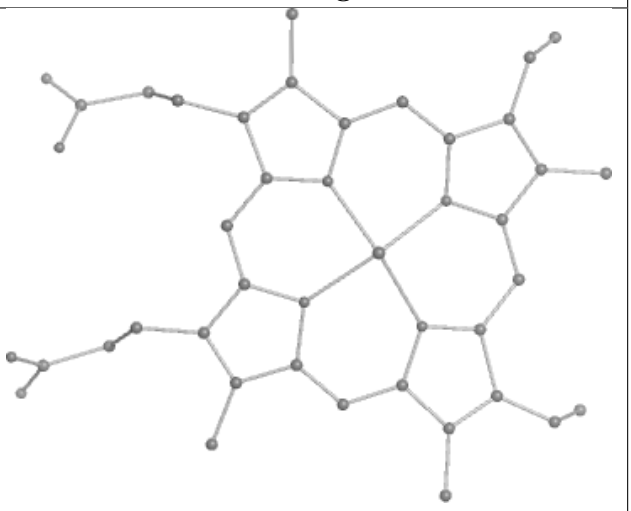

Rings

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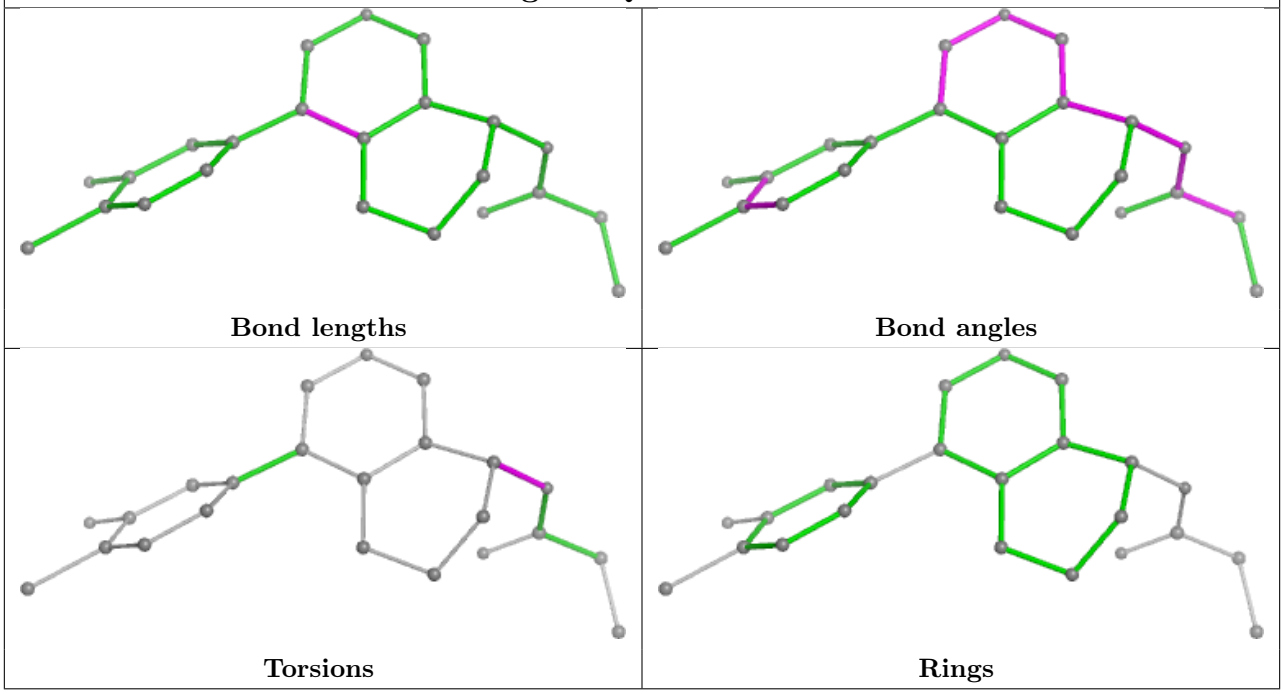
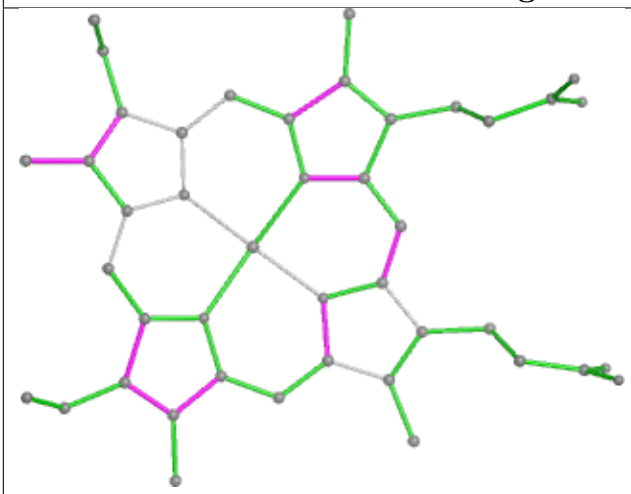


Ligand HEM A 601



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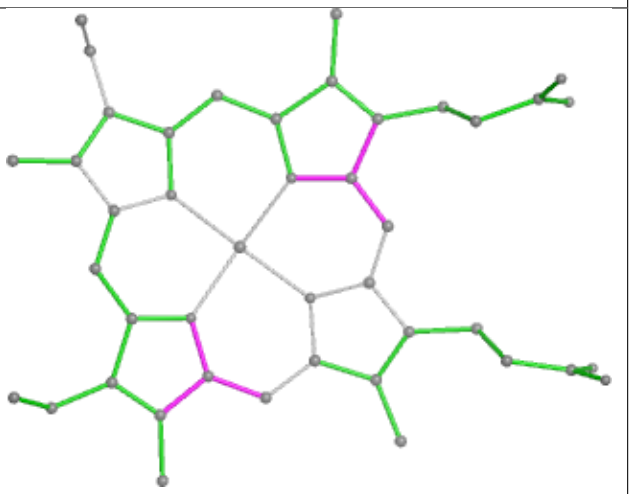

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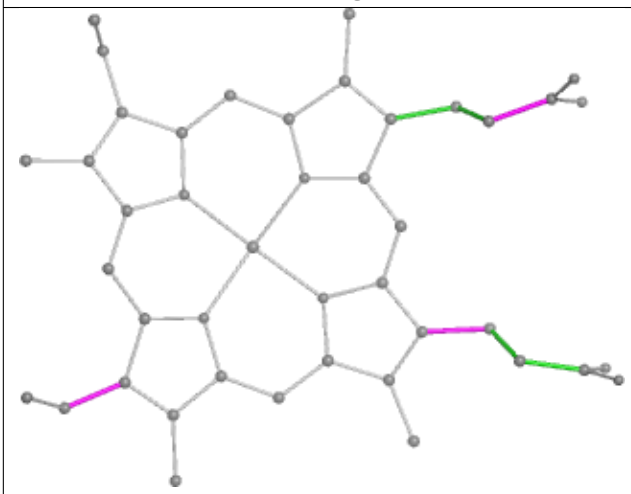

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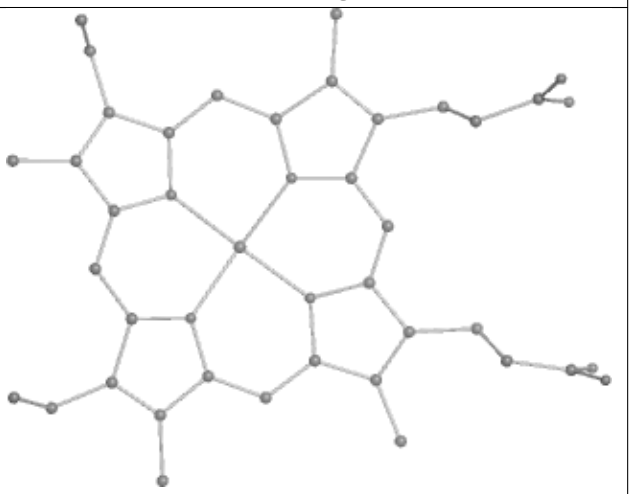

Rings

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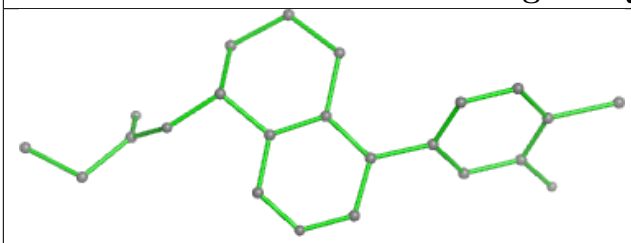

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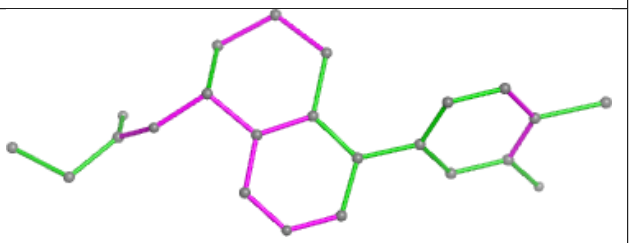

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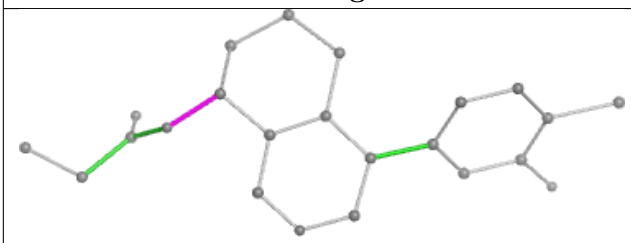

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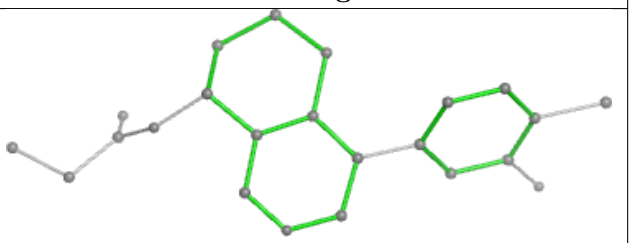

Rings

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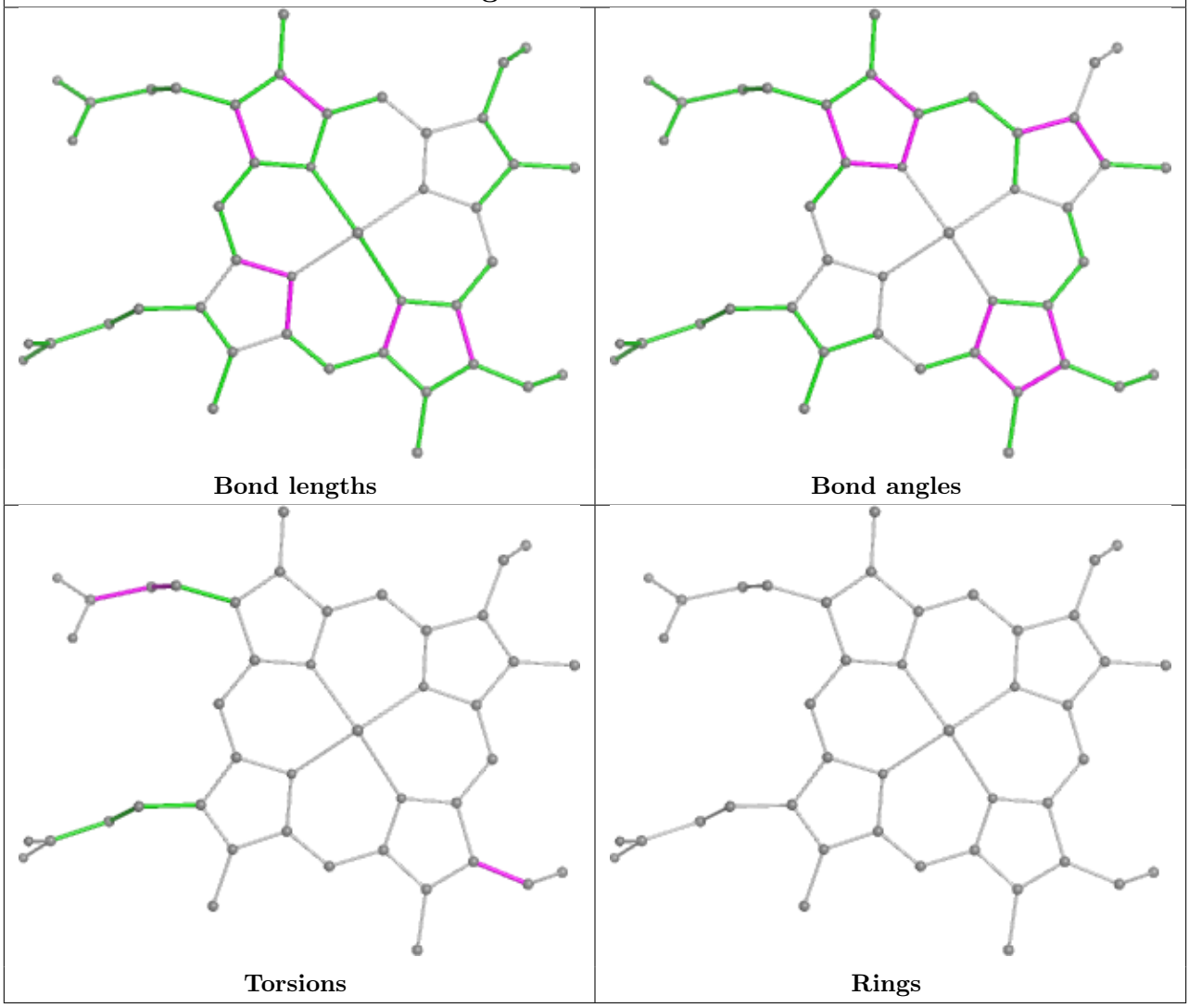

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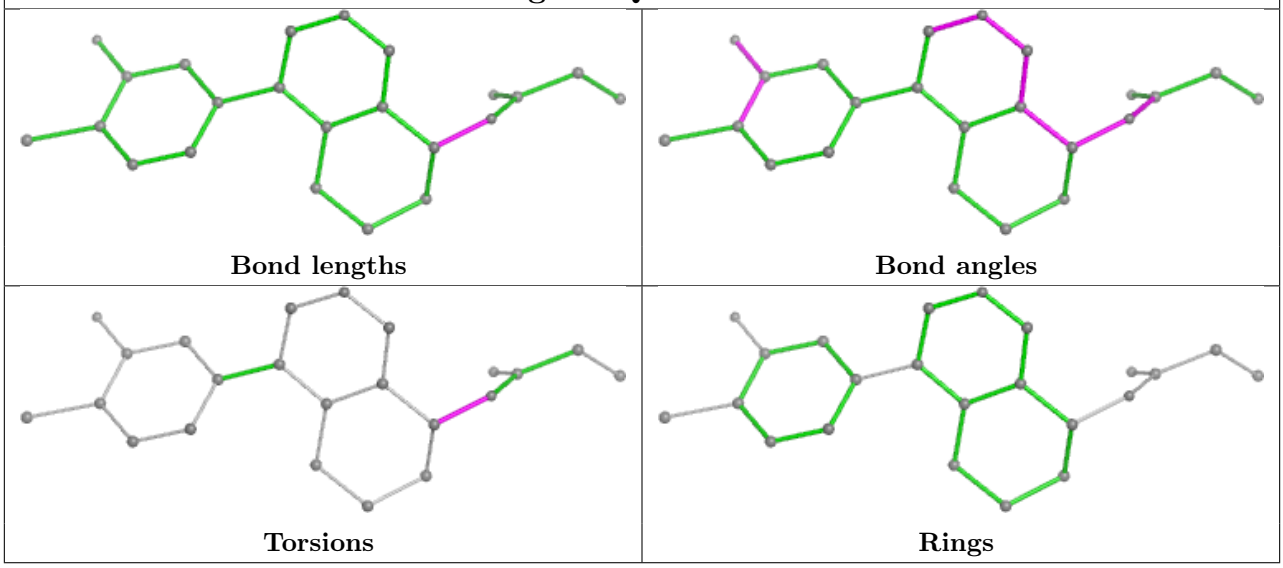

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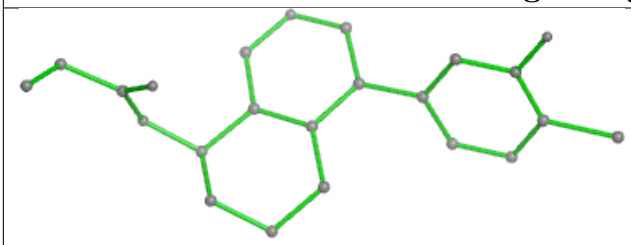
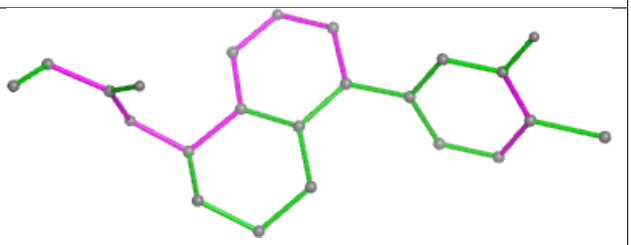
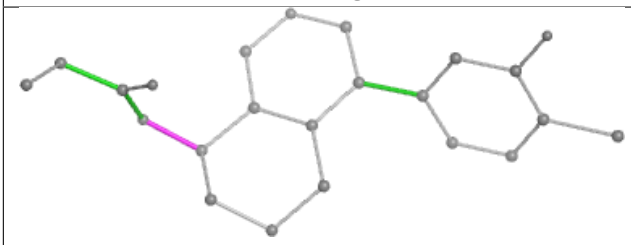
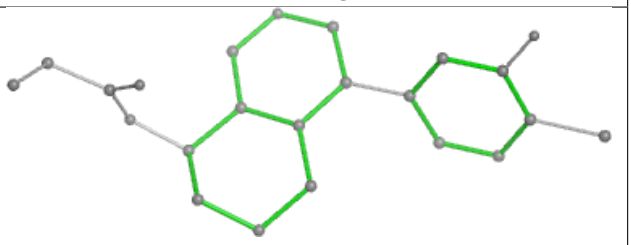
 Bond lengths	 Bond angles
 Torsions	 Rings

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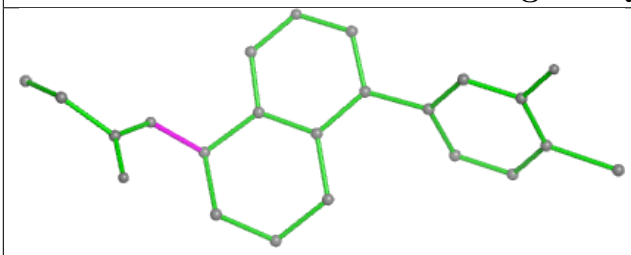
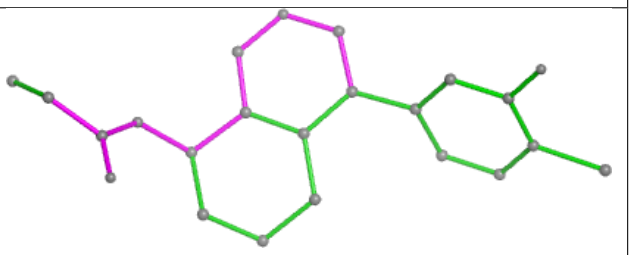
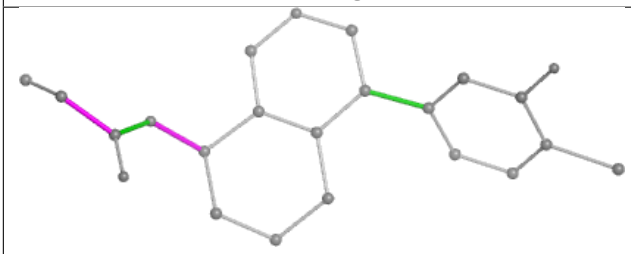
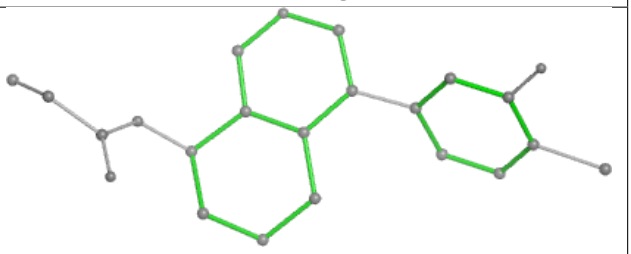
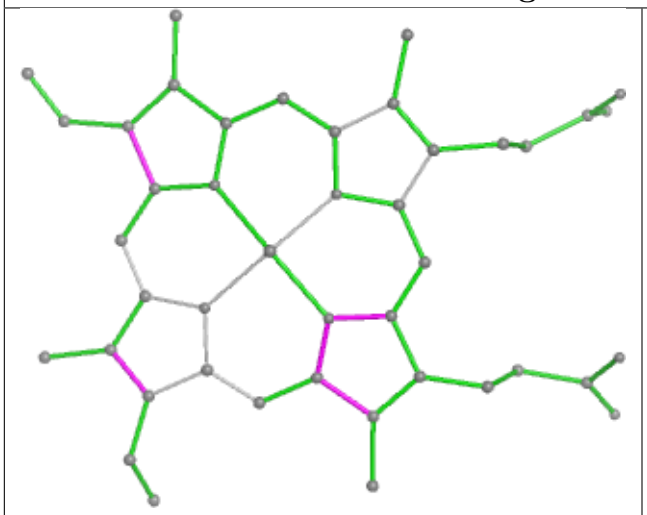
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM H 601



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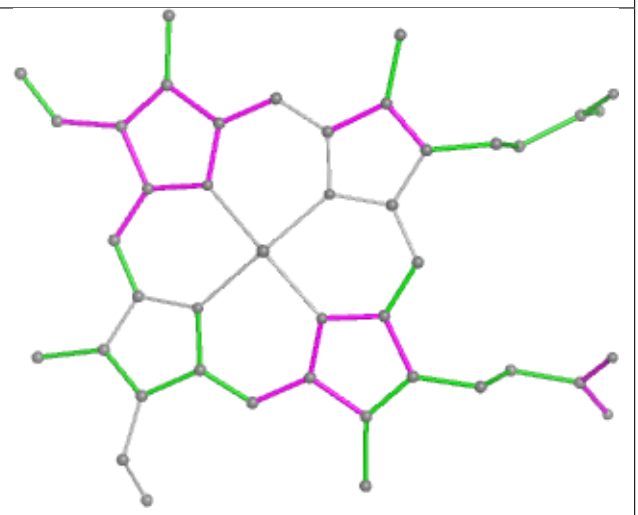
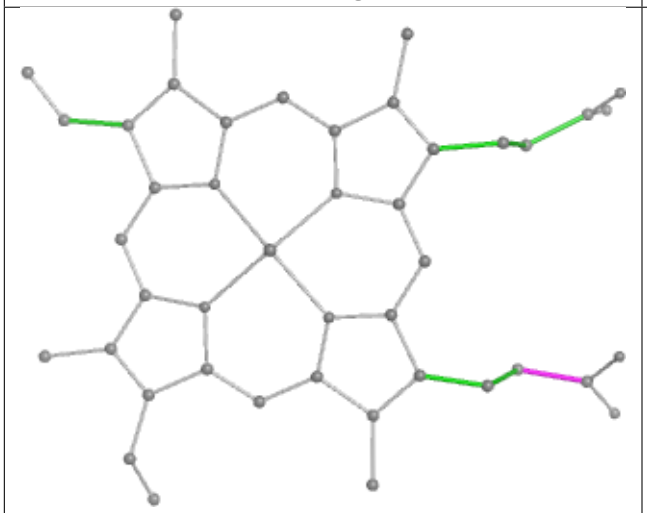
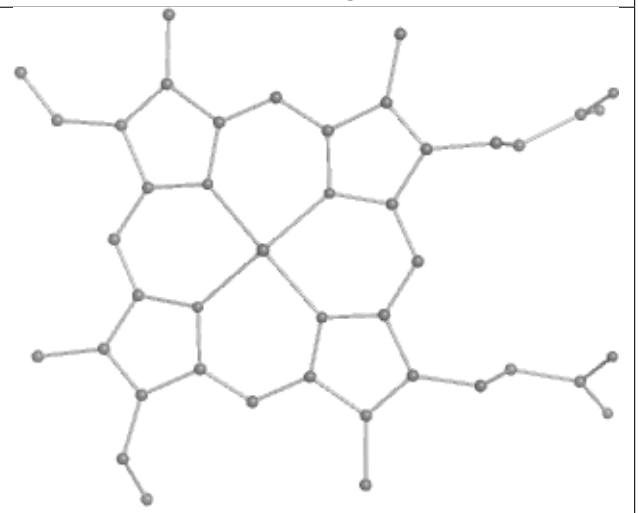


Bond angles



Torsions



Rings

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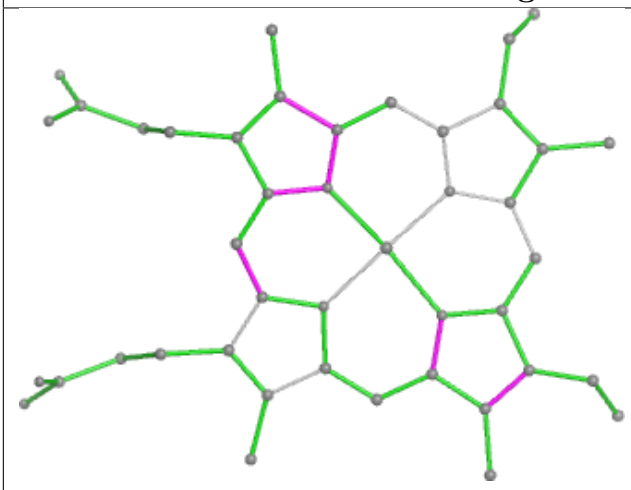

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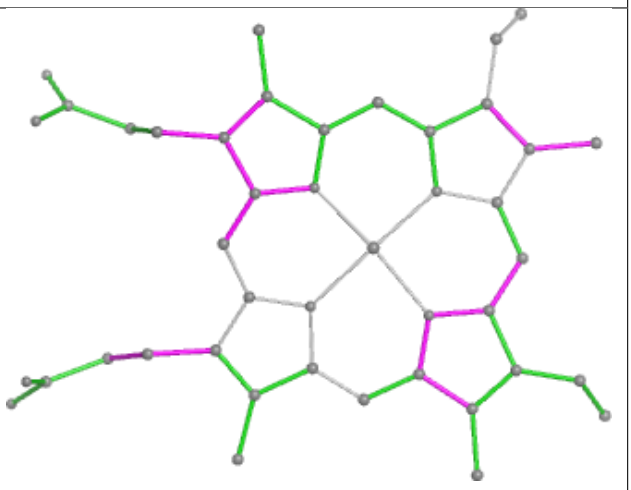
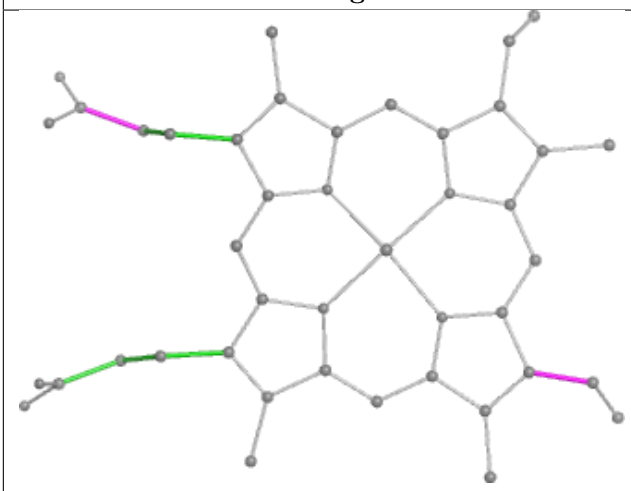
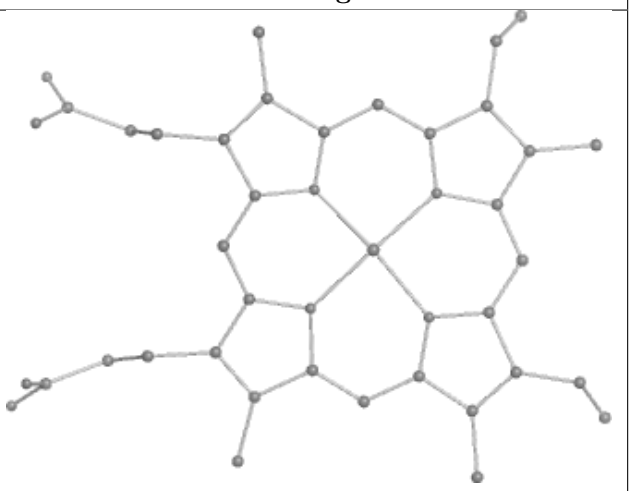


Bond angles

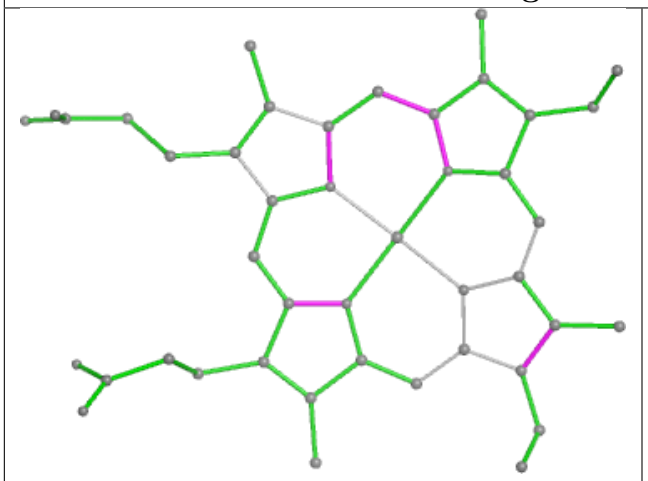


Torsions

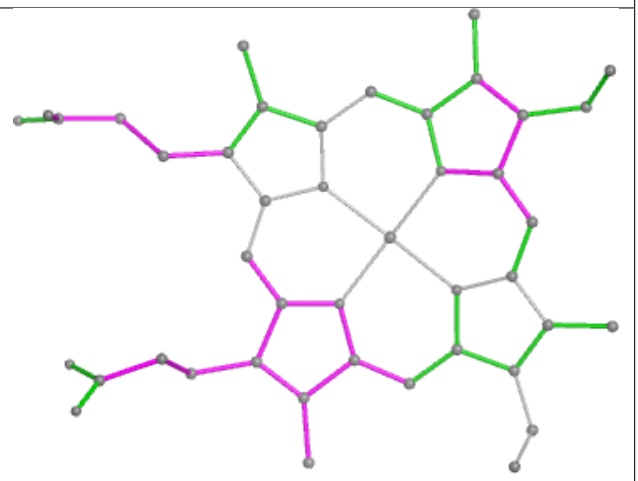


Rings

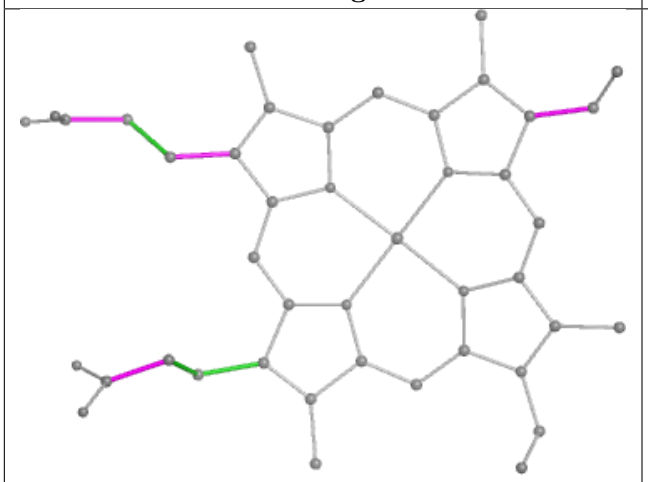
Ligand HEM L 601



Bond lengths



Bond angles



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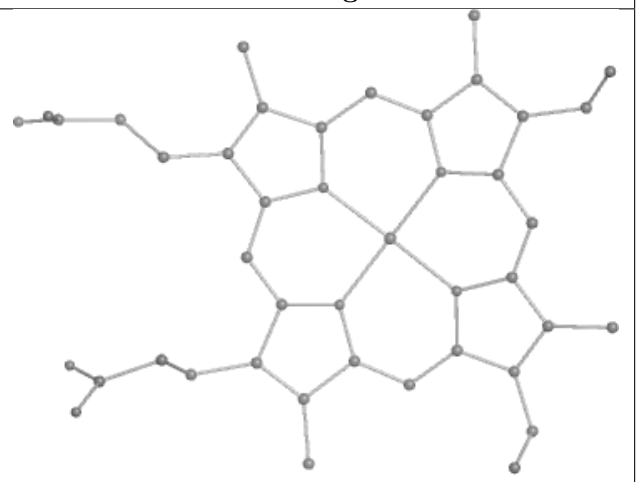
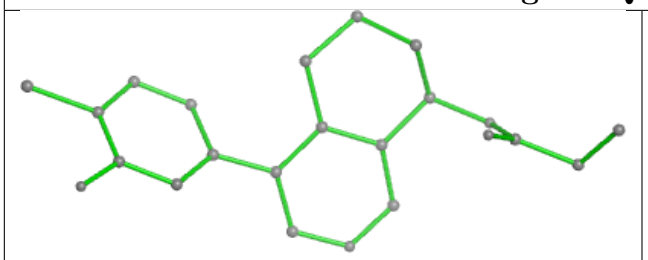
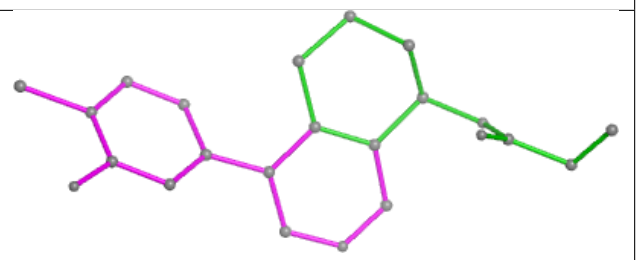


Rings

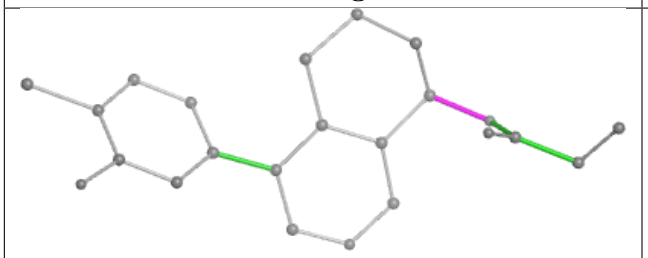
Ligand QHC A 602



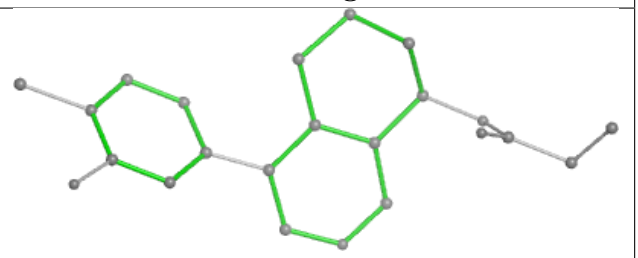
Bond lengths



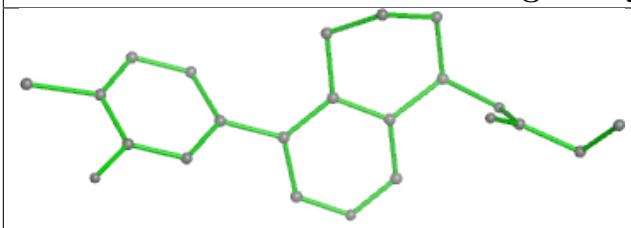
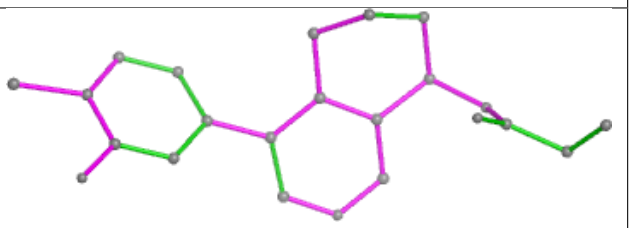
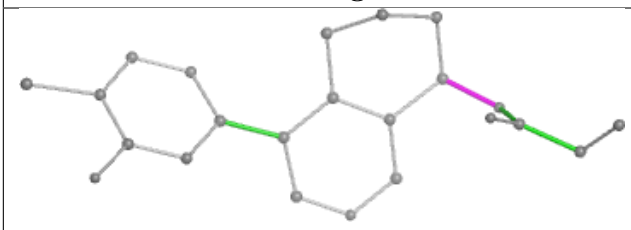
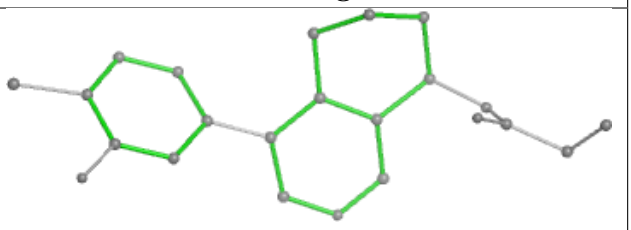
Bond angles

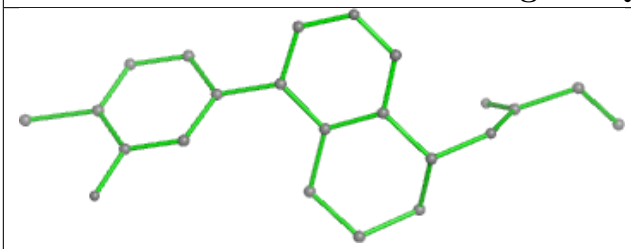
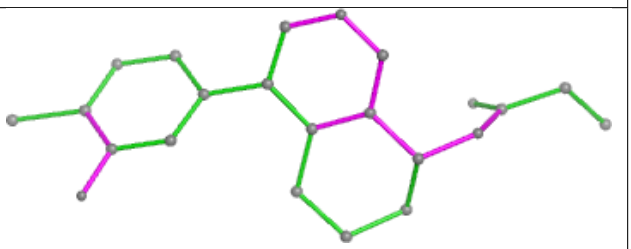
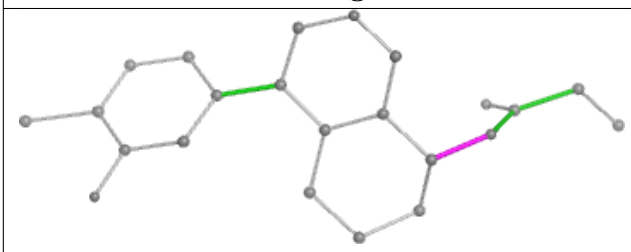
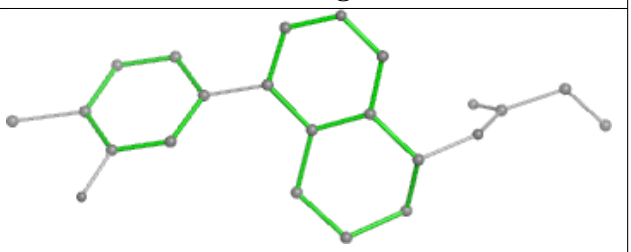


Torsions

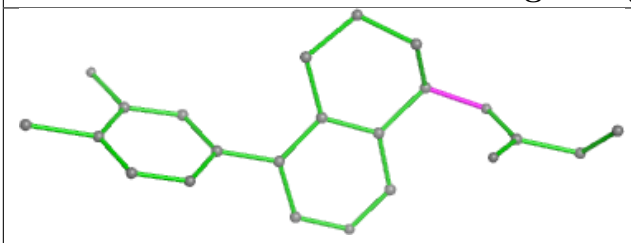


Rings

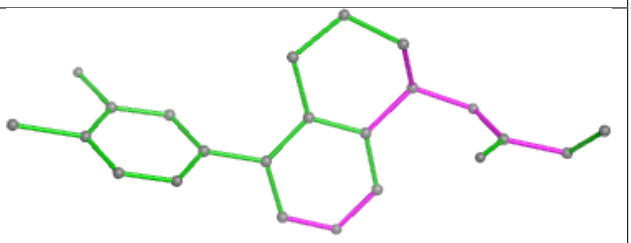
Ligand QHC E 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand QHC K 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

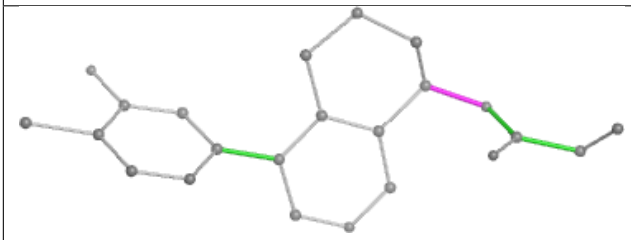
Ligand QHC J 602



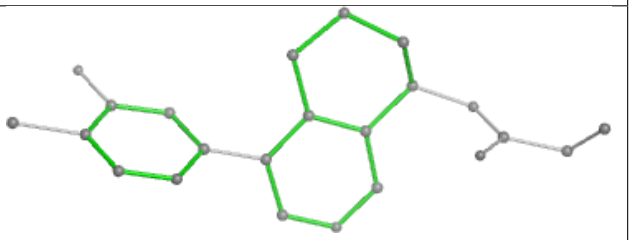
Bond lengths



Bond angles

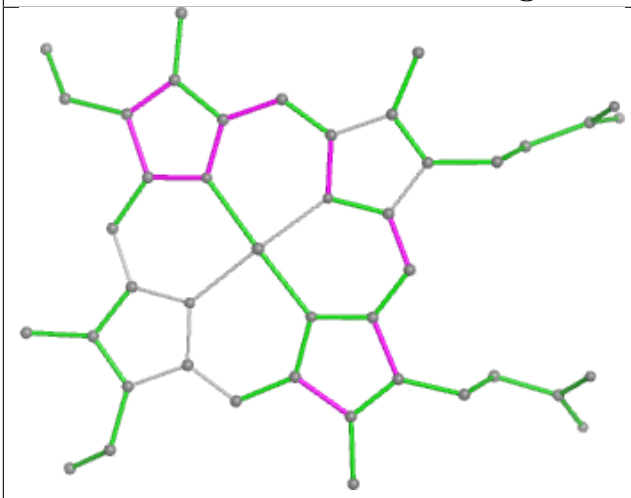


Torsions

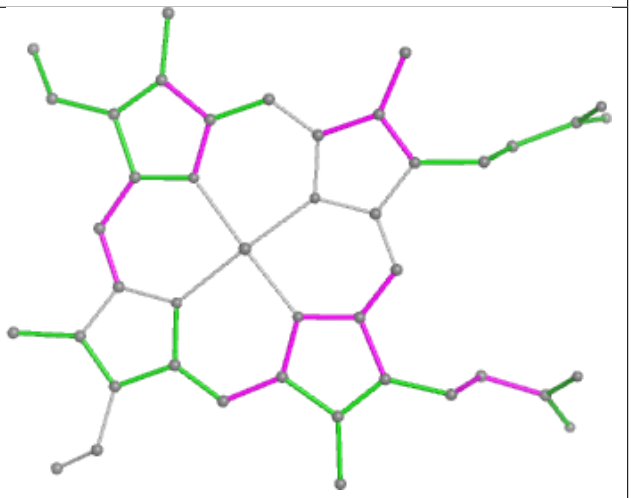


Rings

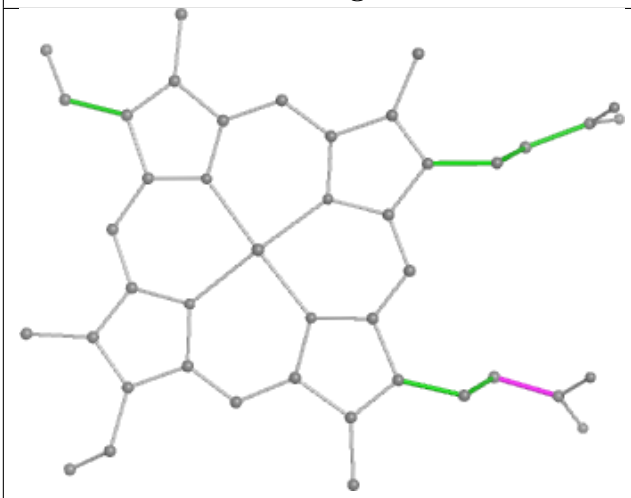
Ligand HEM D 601



Bond lengths



Bond angles



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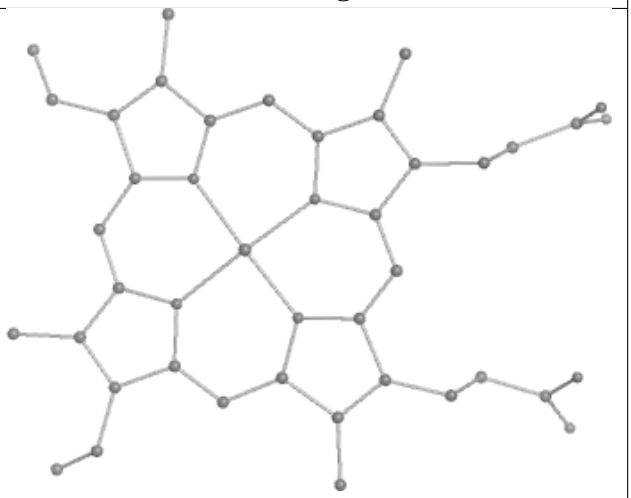

Rings

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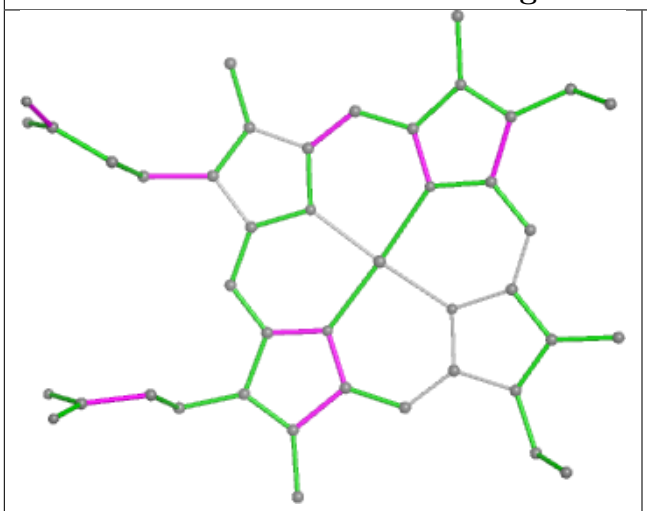

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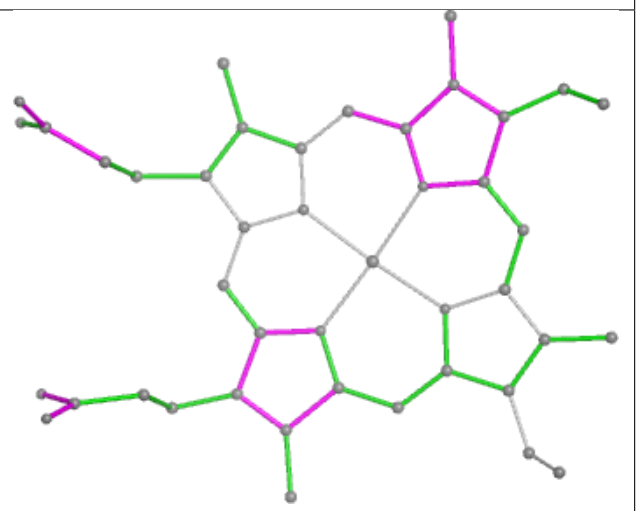
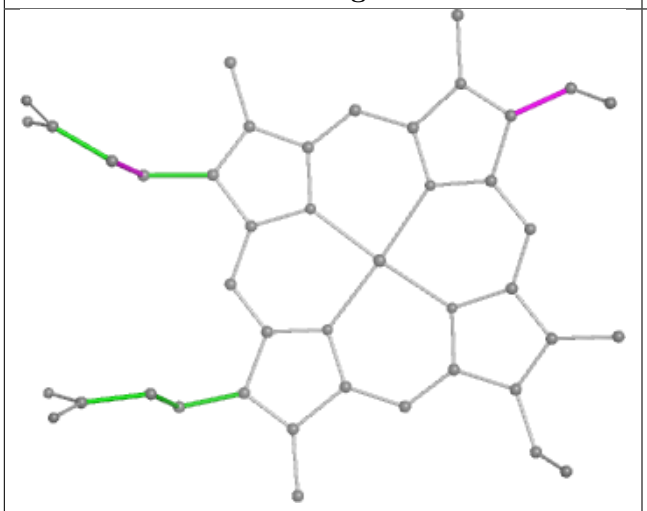
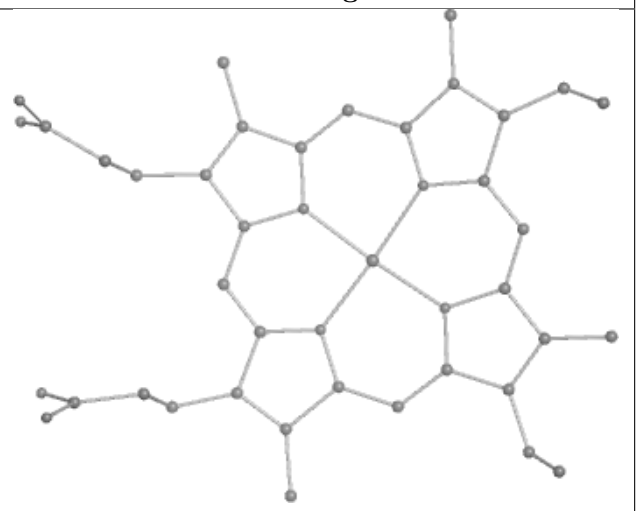


Bond angles

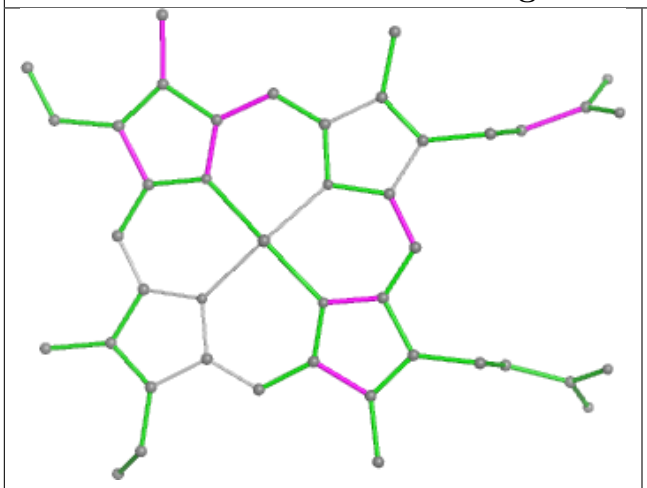


Torsions

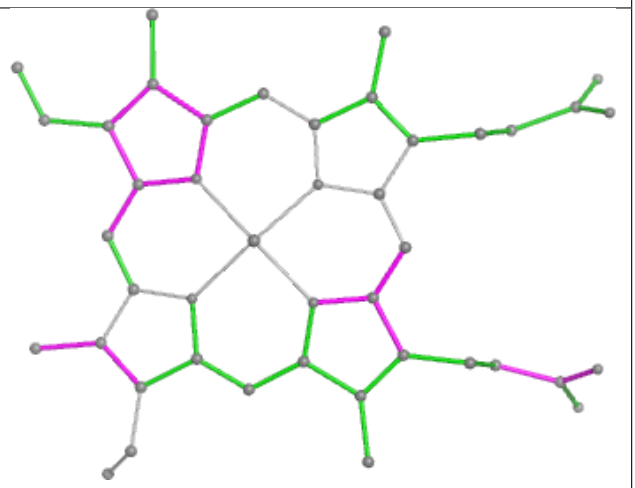


Rings

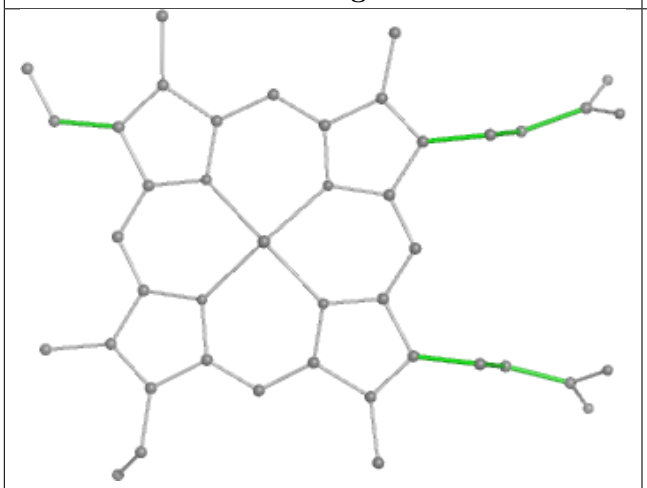
Ligand HEM G 601



Bond lengths



Bond angles



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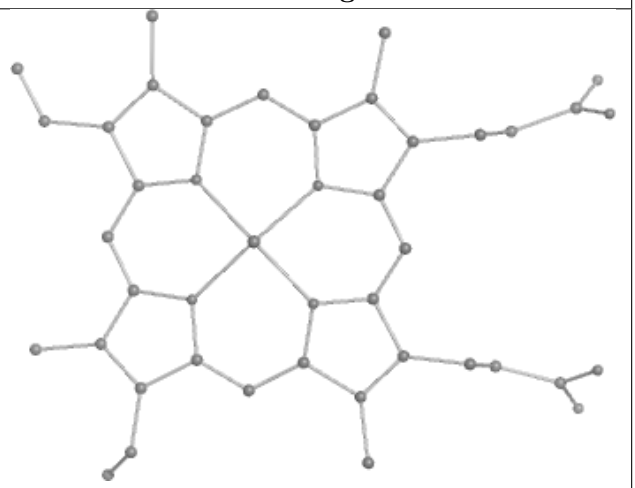
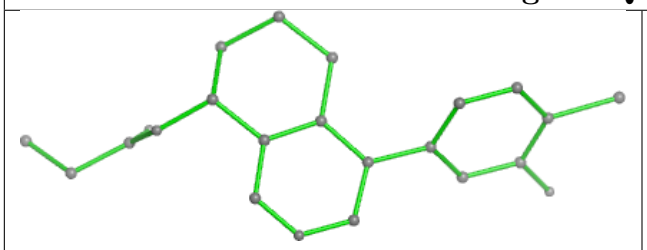
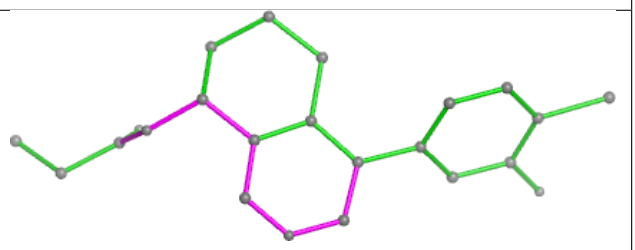


Rings

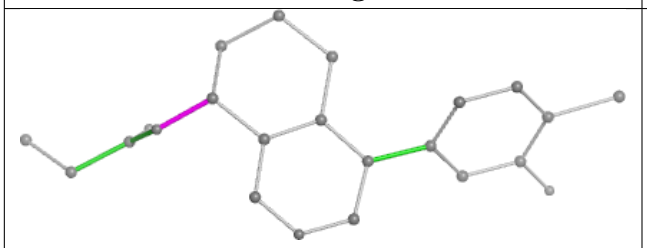
Ligand QHC C 602



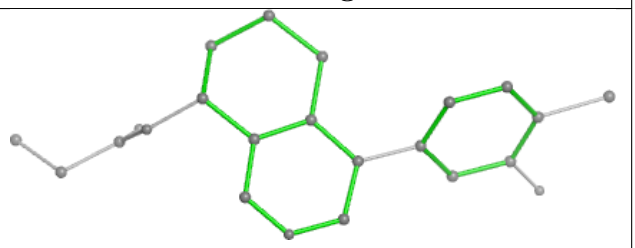
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	465/489 (95%)	-0.20	0	100	100	25, 50, 78, 112	0
1	B	465/489 (95%)	0.01	4 (0%)	84	75	27, 64, 99, 126	0
1	C	465/489 (95%)	0.19	5 (1%)	80	69	34, 70, 106, 138	0
1	D	465/489 (95%)	0.06	4 (0%)	84	75	27, 58, 99, 136	0
1	E	459/489 (93%)	0.06	12 (2%)	56	40	31, 58, 105, 140	0
1	F	464/489 (94%)	0.15	9 (1%)	66	53	35, 68, 106, 125	0
1	G	465/489 (95%)	0.30	20 (4%)	35	22	44, 76, 124, 145	0
1	H	465/489 (95%)	0.30	18 (3%)	39	25	43, 78, 122, 173	0
1	I	458/489 (93%)	0.18	20 (4%)	34	21	33, 74, 143, 216	0
1	J	463/489 (94%)	0.19	22 (4%)	30	18	44, 82, 145, 230	0
1	K	461/489 (94%)	0.02	7 (1%)	73	61	35, 68, 107, 127	0
1	L	462/489 (94%)	0.34	15 (3%)	47	31	44, 82, 149, 239	0
All	All	5557/5868 (94%)	0.13	136 (2%)	59	44	25, 69, 118, 239	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	GLY	6.4
1	G	86	PRO	6.0
1	L	55	ILE	6.0
1	I	55	ILE	5.4
1	E	55	ILE	5.3
1	I	88	MET	4.6
1	L	247	TRP	4.4
1	E	51	ARG	4.3
1	I	49	TRP	4.2
1	I	61	TYR	4.0
1	E	115	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	47	ASN	3.9
1	G	109	CYS	3.9
1	L	115	PRO	3.8
1	G	85	GLY	3.8
1	J	85	GLY	3.8
1	I	75	LEU	3.8
1	F	386	VAL	3.8
1	I	87	ARG	3.7
1	E	247	TRP	3.6
1	G	383	GLU	3.6
1	L	399	ALA	3.5
1	J	61	TYR	3.4
1	L	400	GLY	3.4
1	F	402	LEU	3.3
1	K	60	GLY	3.3
1	I	47	ASN	3.2
1	G	396	HIS	3.2
1	G	429	LEU	3.2
1	L	60	GLY	3.2
1	G	430	ASP	3.2
1	F	247	TRP	3.1
1	J	78	ILE	3.1
1	E	50	LEU	3.1
1	C	503	ASN	3.1
1	G	87	ARG	3.1
1	H	269	ASN	3.0
1	G	503	ASN	3.0
1	H	454	ARG	3.0
1	H	316	VAL	3.0
1	J	51	ARG	3.0
1	J	76	GLY	2.9
1	K	61	TYR	2.9
1	J	239	PHE	2.9
1	J	484	VAL	2.9
1	L	86	PRO	2.9
1	I	57	ARG	2.8
1	F	395	TYR	2.8
1	J	483	MET	2.8
1	L	61	TYR	2.8
1	L	38	PHE	2.8
1	D	35	VAL	2.8
1	C	368	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	84	GLY	2.8
1	I	50	LEU	2.7
1	F	73	GLN	2.7
1	J	60	GLY	2.7
1	L	386	VAL	2.7
1	J	40	ALA	2.7
1	J	49	TRP	2.7
1	J	55	ILE	2.7
1	J	72	PHE	2.7
1	I	73	GLN	2.6
1	H	201	ASN	2.6
1	B	162	ASP	2.6
1	J	88	MET	2.6
1	J	89	VAL	2.6
1	L	365	LEU	2.6
1	K	84	GLY	2.6
1	L	388	SER	2.5
1	G	398	PRO	2.5
1	G	60	GLY	2.5
1	K	439	HIS	2.5
1	H	317	ASP	2.5
1	G	42	PRO	2.5
1	H	286	TYR	2.5
1	L	75	LEU	2.5
1	L	84	GLY	2.5
1	J	87	ARG	2.5
1	D	75	LEU	2.5
1	F	403	VAL	2.4
1	E	430	ASP	2.4
1	G	385	VAL	2.4
1	G	252	VAL	2.4
1	E	61	TYR	2.4
1	J	81	TYR	2.4
1	G	49	TRP	2.4
1	F	60	GLY	2.4
1	I	239	PHE	2.4
1	K	51	ARG	2.3
1	H	65	HIS	2.3
1	H	274	ILE	2.3
1	I	86	PRO	2.3
1	D	34	THR	2.3
1	E	48	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	45	PRO	2.3
1	J	458	ALA	2.2
1	G	43	GLN	2.2
1	I	484	VAL	2.2
1	C	430	ASP	2.2
1	H	240	MET	2.2
1	F	81	TYR	2.2
1	H	203	ALA	2.2
1	E	54	GLN	2.2
1	H	236	GLN	2.2
1	J	45	PRO	2.2
1	H	271	ILE	2.2
1	B	118	ALA	2.1
1	H	40	ALA	2.1
1	G	104	ASP	2.1
1	D	394	ASN	2.1
1	I	48	ARG	2.1
1	H	147	ASP	2.1
1	C	344	SER	2.1
1	E	269	ASN	2.1
1	I	46	GLY	2.1
1	I	51	ARG	2.1
1	C	317	ASP	2.1
1	K	430	ASP	2.1
1	H	150	SER	2.1
1	I	78	ILE	2.1
1	I	483	MET	2.1
1	G	38	PHE	2.1
1	I	40	ALA	2.1
1	H	315	SER	2.1
1	L	46	GLY	2.1
1	F	401	THR	2.1
1	H	247	TRP	2.0
1	G	72	PHE	2.0
1	J	50	LEU	2.0
1	J	250	PRO	2.0
1	B	409	SER	2.0
1	J	490	ARG	2.0
1	B	335	ASP	2.0
1	K	85	GLY	2.0
1	I	62	GLU	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)

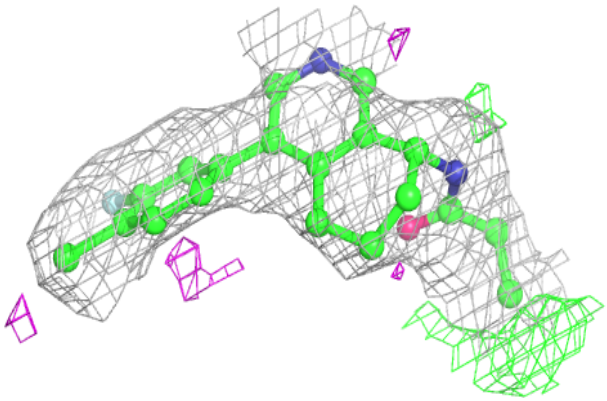
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

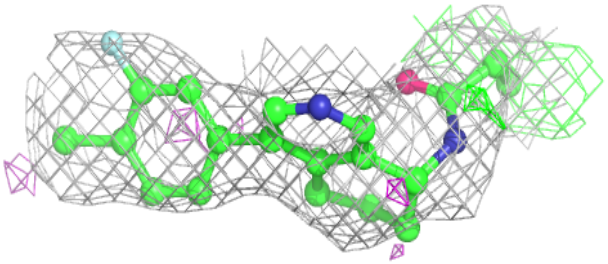
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QHC	D	602	23/23	0.86	0.29	54,60,61,61	0
3	QHC	C	602	23/23	0.88	0.32	84,85,89,91	0
3	QHC	I	602	23/23	0.91	0.30	56,66,73,75	0
2	HEM	H	601	43/43	0.92	0.25	62,64,67,68	0
3	QHC	L	602	23/23	0.92	0.28	65,74,84,86	0
3	QHC	J	602	23/23	0.93	0.27	50,54,68,74	0
3	QHC	F	602	23/23	0.93	0.25	51,61,68,68	0
3	QHC	B	602	23/23	0.94	0.29	56,62,69,72	0
2	HEM	B	601	43/43	0.94	0.21	54,56,60,61	0
2	HEM	L	601	43/43	0.94	0.21	59,60,64,64	0
3	QHC	E	602	23/23	0.94	0.33	44,49,53,54	0
2	HEM	K	601	43/43	0.95	0.25	55,56,60,64	0
3	QHC	K	602	23/23	0.95	0.30	51,60,72,72	0
2	HEM	G	601	43/43	0.95	0.25	51,52,56,58	0
2	HEM	A	601	43/43	0.96	0.25	39,39,44,51	0
2	HEM	D	601	43/43	0.96	0.23	32,33,38,43	0
2	HEM	I	601	43/43	0.96	0.26	53,54,58,65	0
2	HEM	J	601	43/43	0.96	0.25	51,52,56,58	0
2	HEM	F	601	43/43	0.96	0.23	46,48,52,52	0
2	HEM	C	601	43/43	0.97	0.21	39,41,46,48	0
2	HEM	E	601	43/43	0.97	0.20	43,44,48,49	0
3	QHC	A	602	23/23	0.98	0.20	3,13,32,37	0

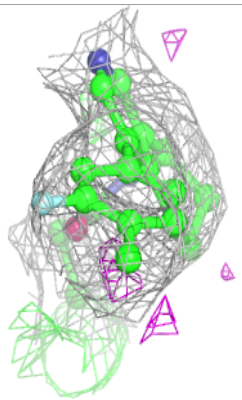
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QHC D 602:

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

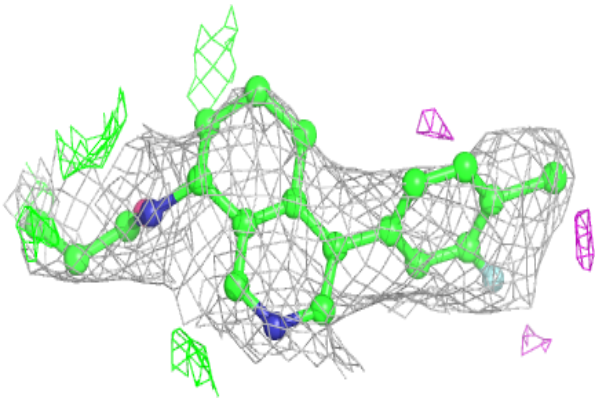


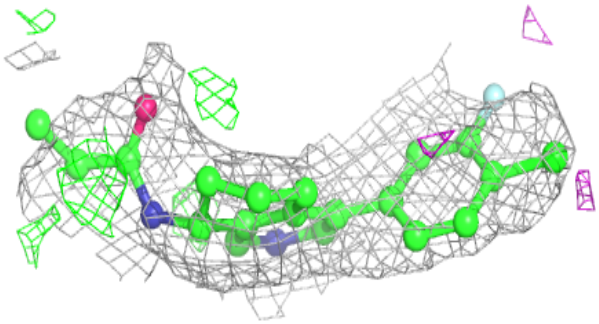


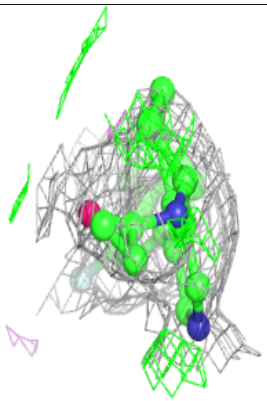


Electron density around QHC C 602:

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

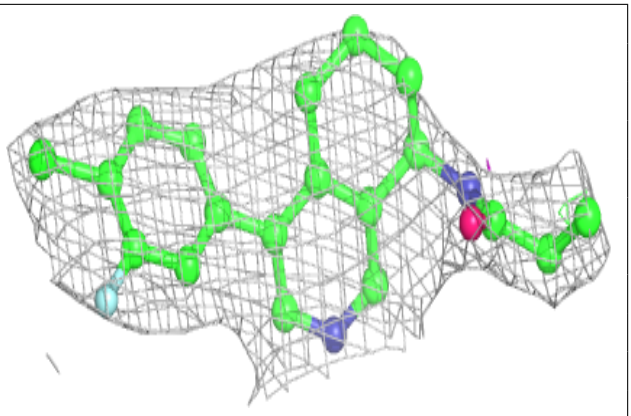


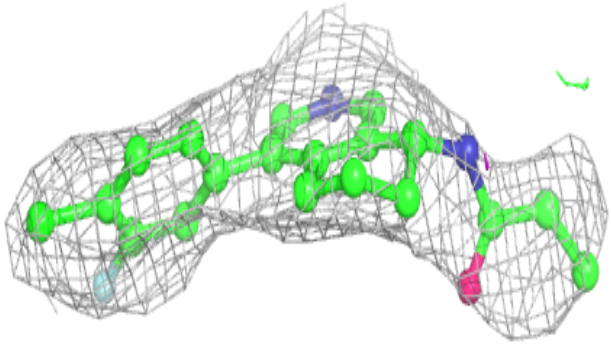


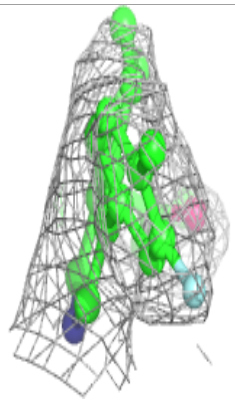


Electron density around QHC I 602:

$2mF_o$-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 601:

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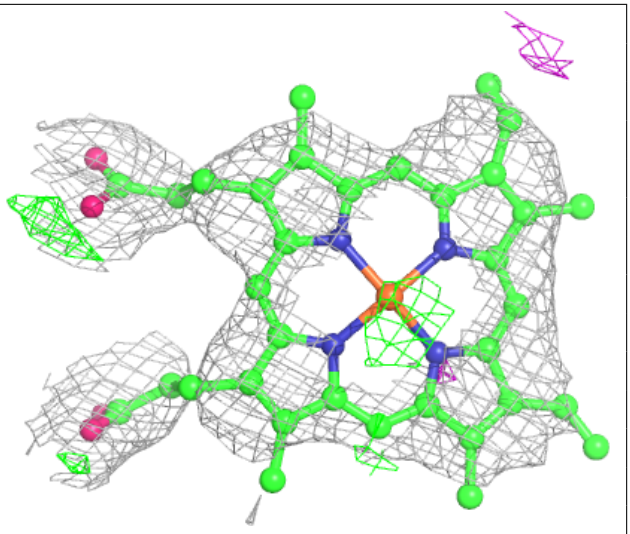
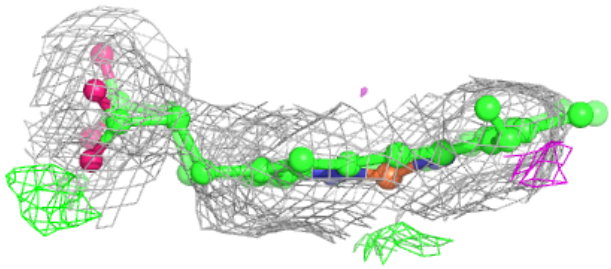
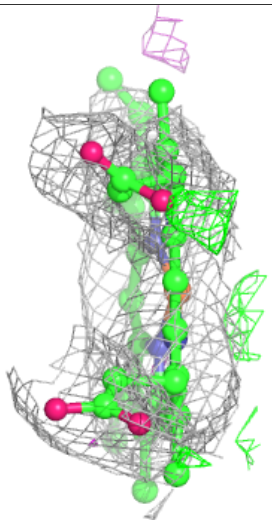
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

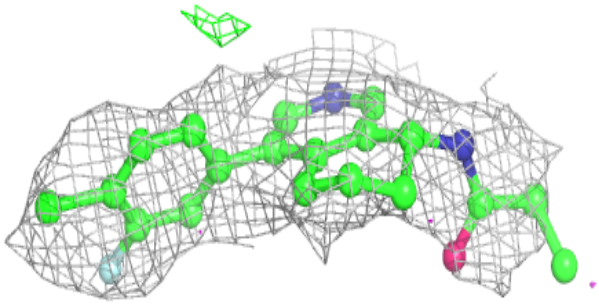


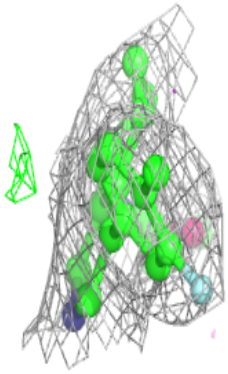




Electron density around QHC L 602:

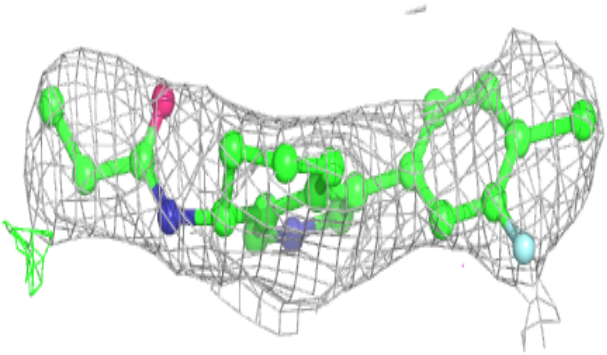
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

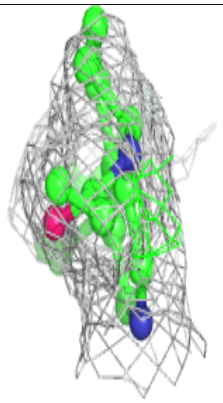




Electron density around QHC J 602:

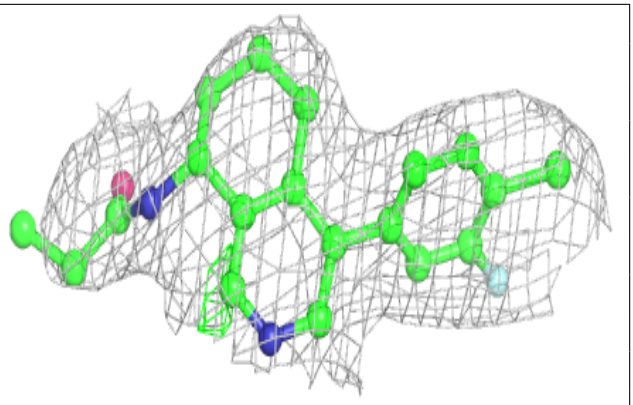
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

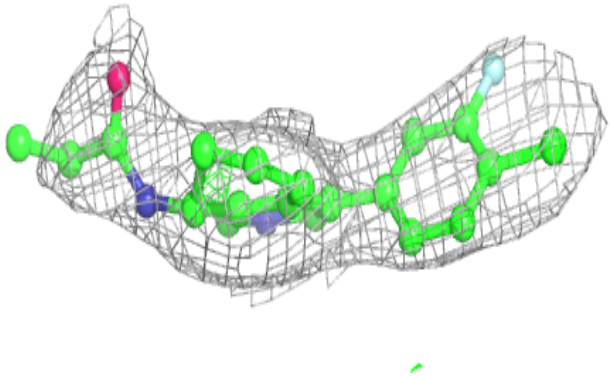


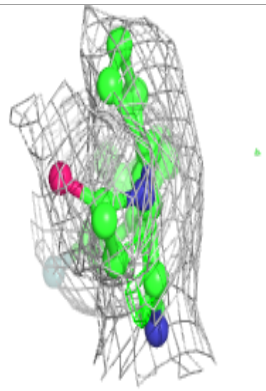


Electron density around QHC F 602:

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







Electron density around QHC B 602:

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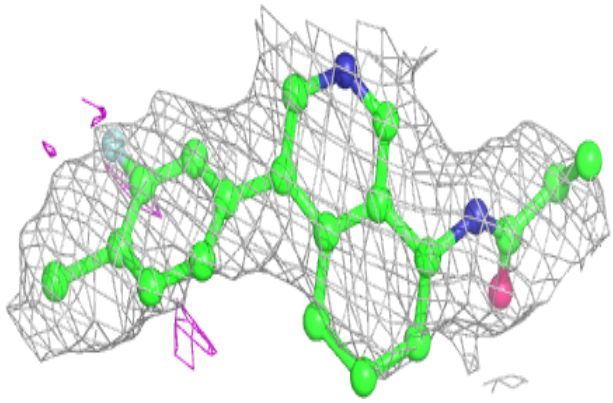
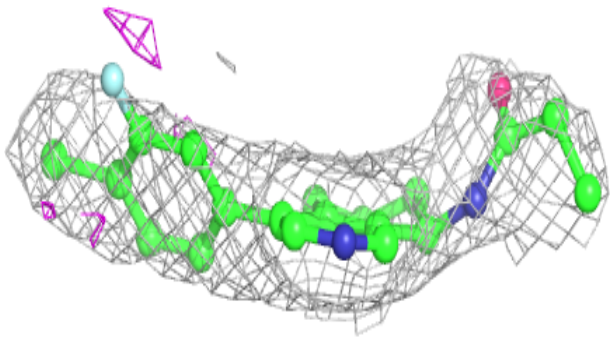
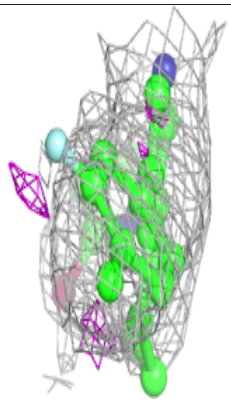
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM B 601:

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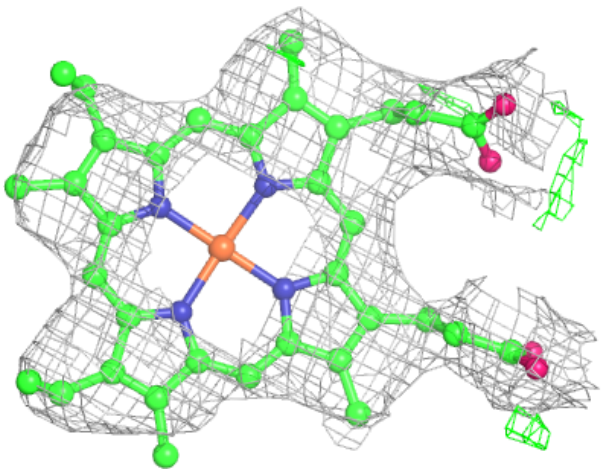
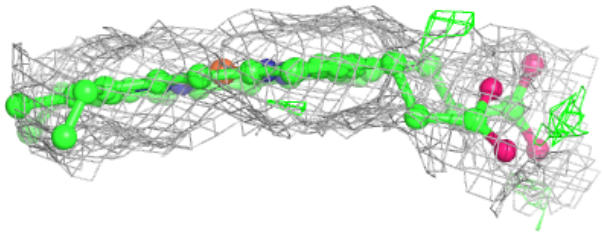
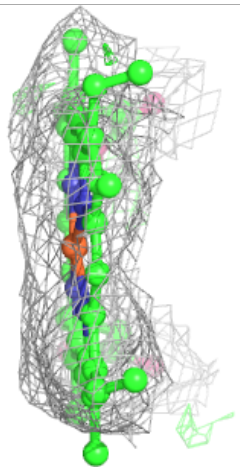
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM L 601:

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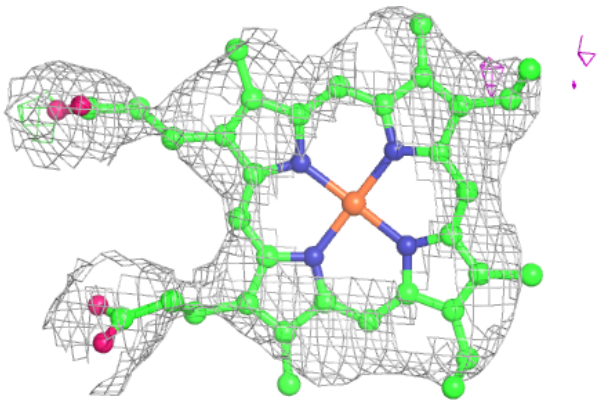
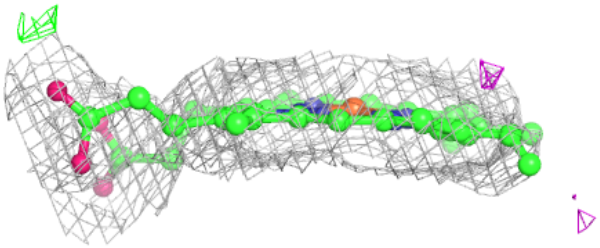
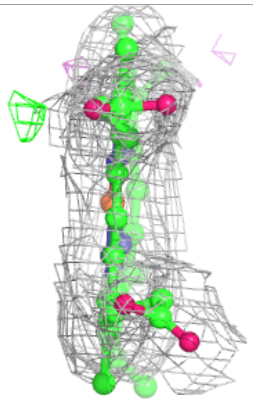
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around QHC E 602:

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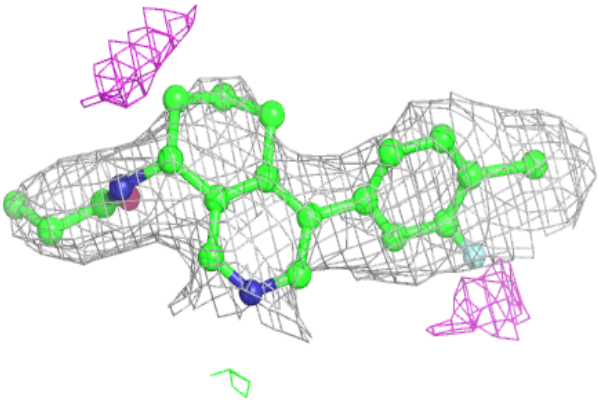
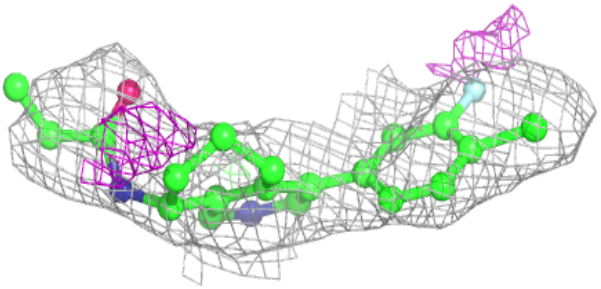
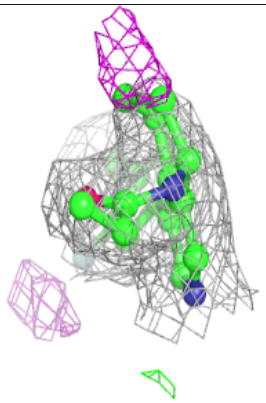
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

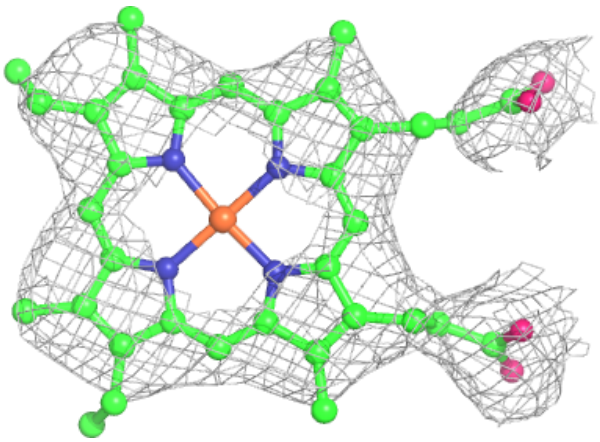


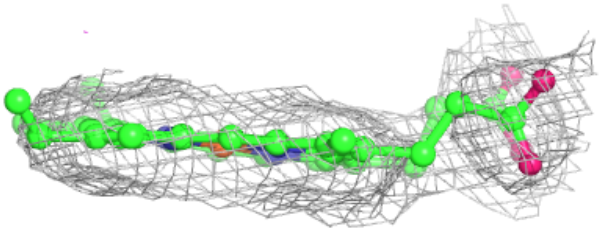


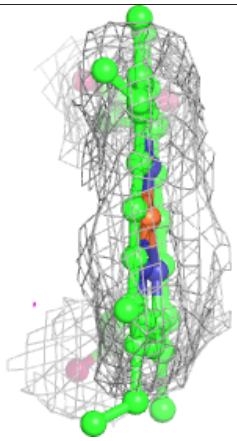


Electron density around HEM K 601:

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

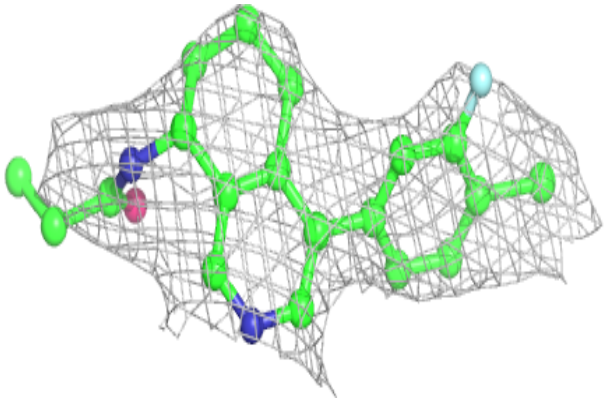


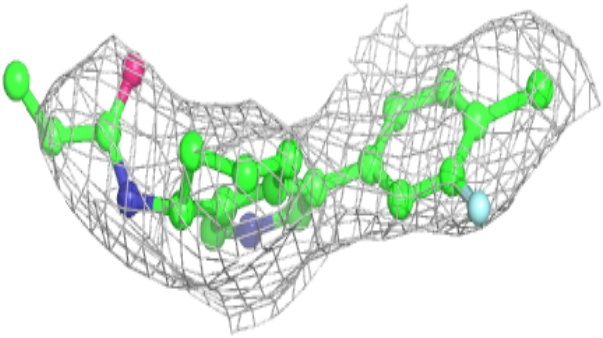


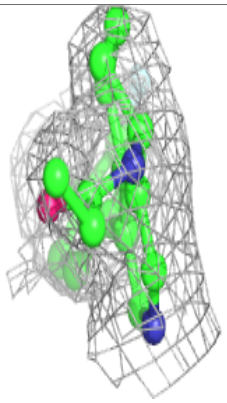


Electron density around QHC K 602:

$2mF_o$-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 601:

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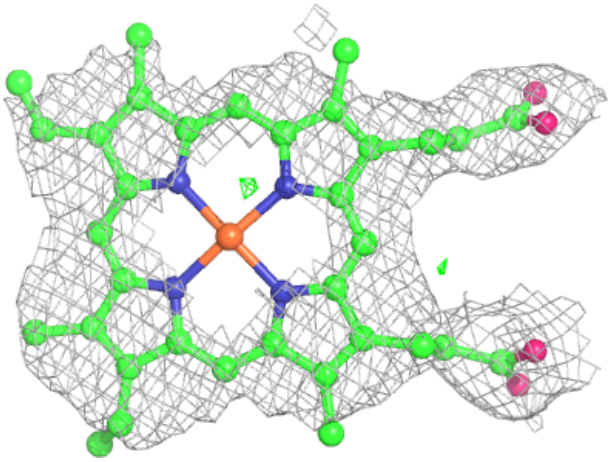
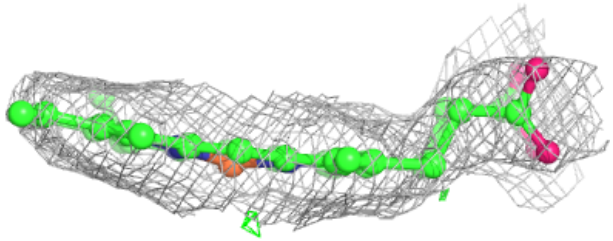
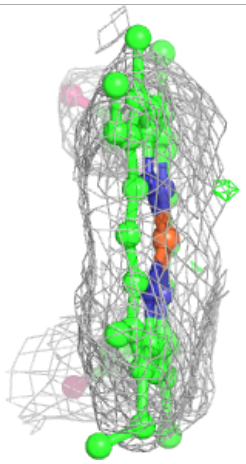
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM A 601:

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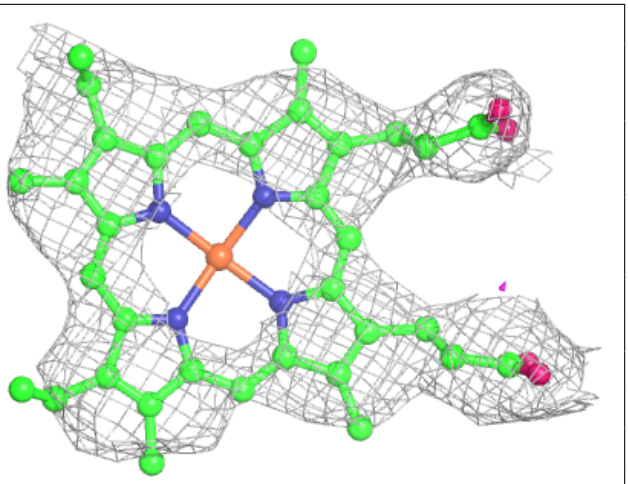
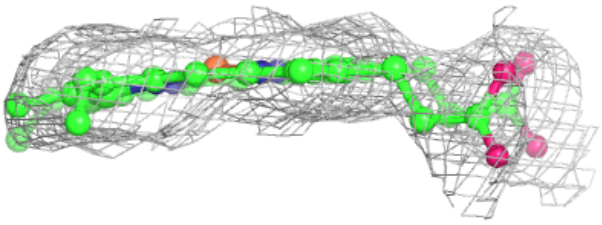
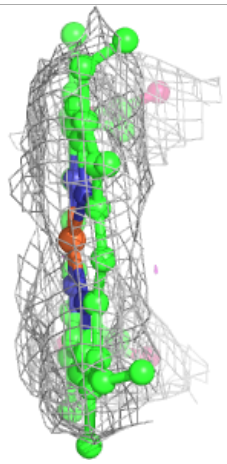
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

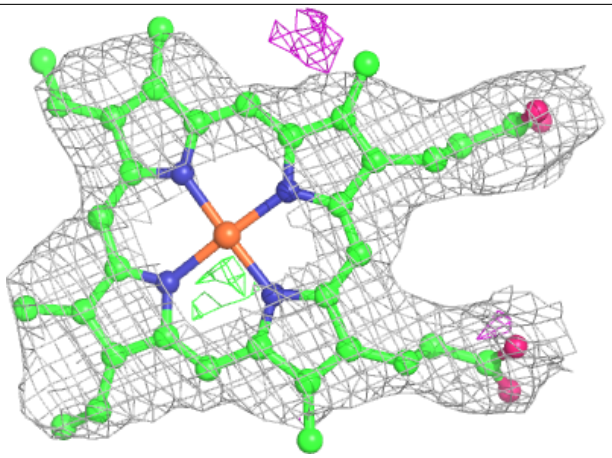


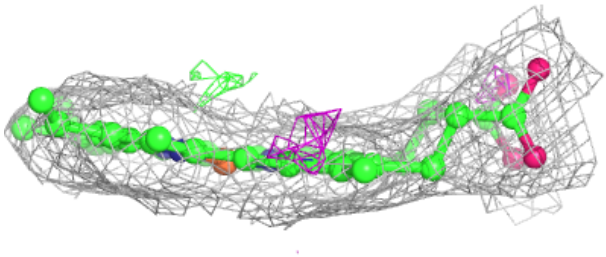


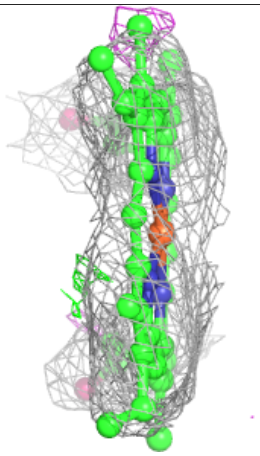


Electron density around HEM D 601:

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

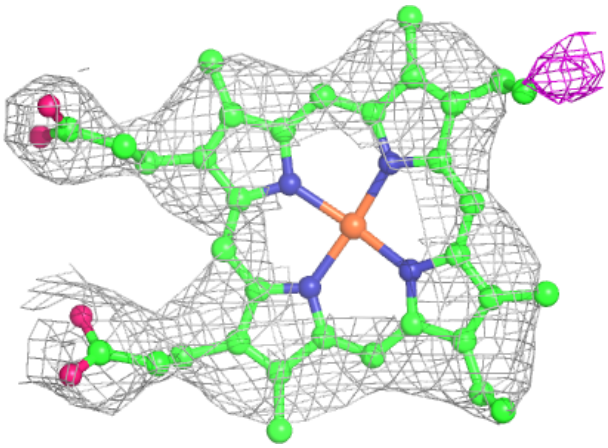


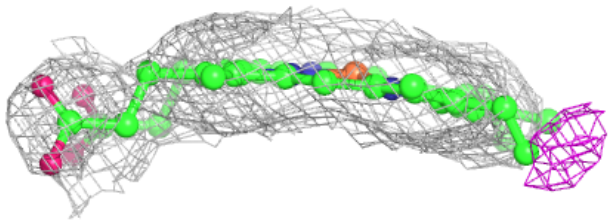


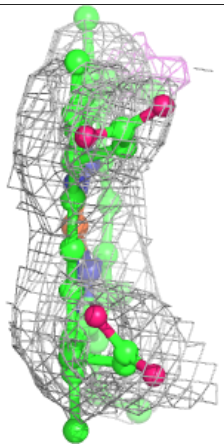


Electron density around HEM I 601:

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

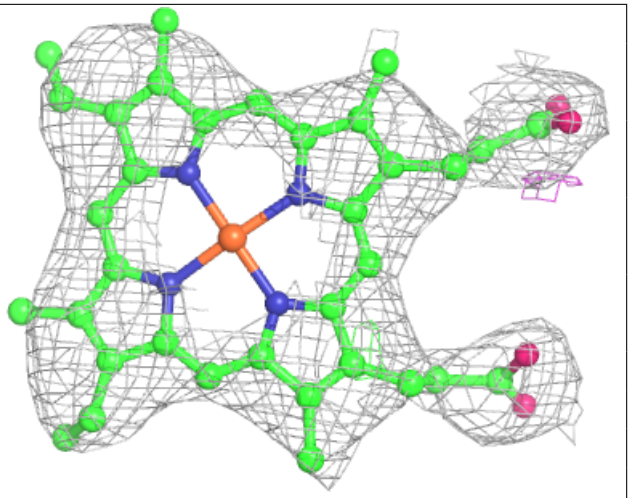


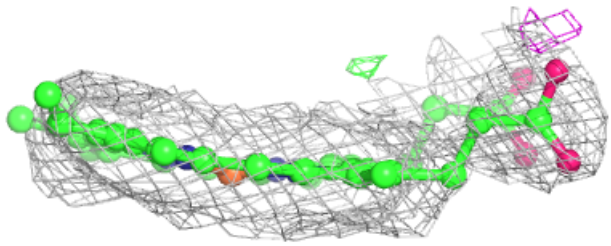


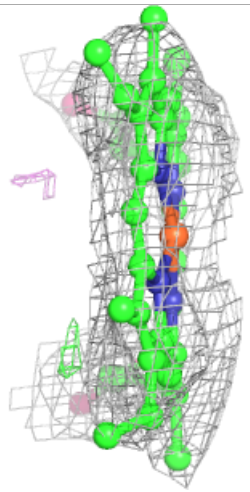


Electron density around HEM J 601:

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

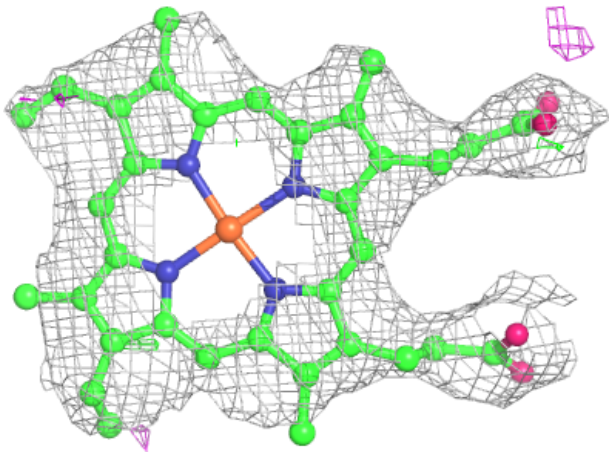


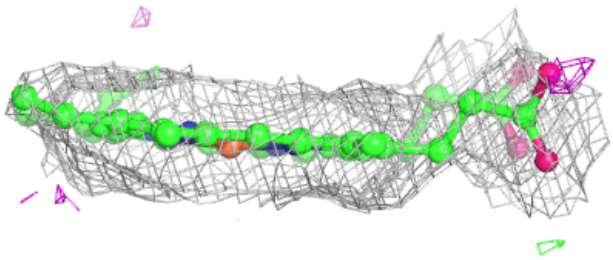




Electron density around HEM F 601:

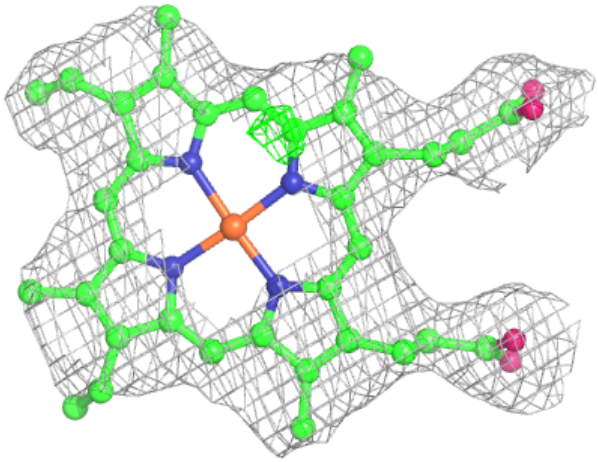
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

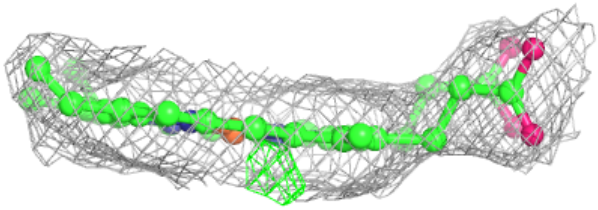


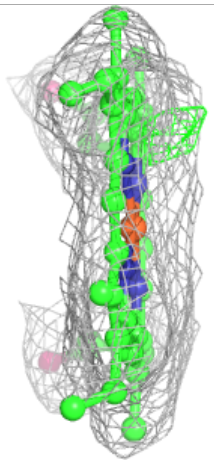


Electron density around HEM C 601:

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

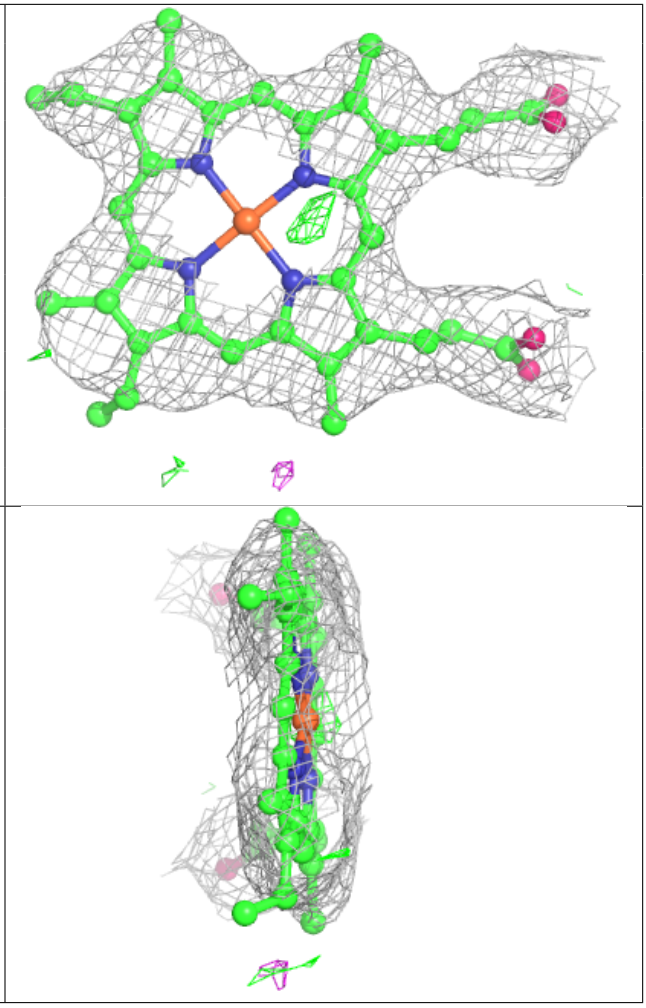






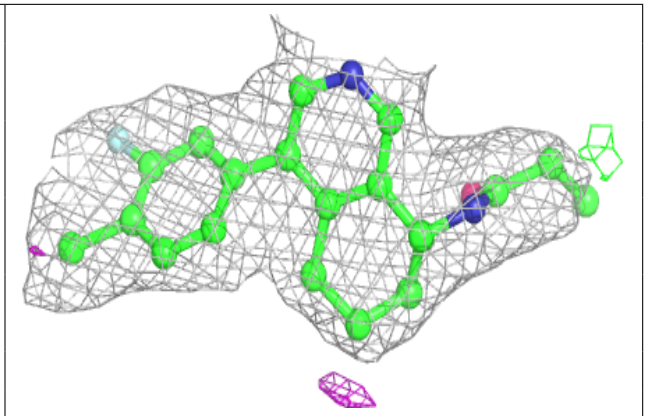
Electron density around HEM E 601:

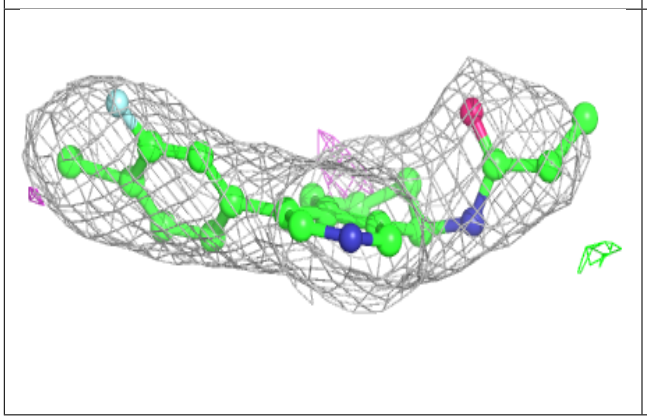
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

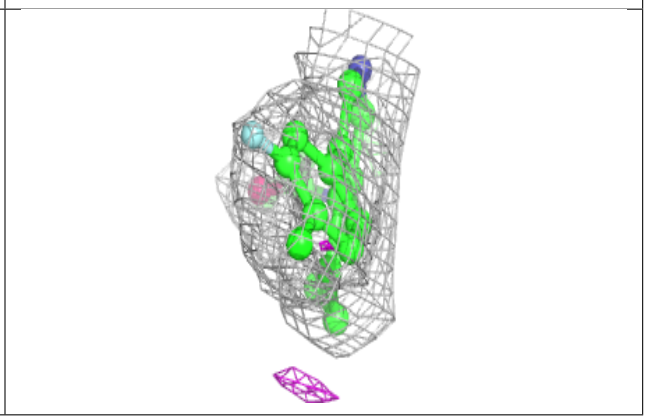


Electron density around QHC A 602:

$2mF_o$-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.