Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:26 PM EDT

PDB ID	:	6VLT
Title	:	Crystal Structure of Human P450 2C9*2 Genetic Variant in Complex with Losartan
Authors	:	Shah, M.B.
Deposited on	:	2020-01-25
Resolution	:	3.12 Å(reported)

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

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

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

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

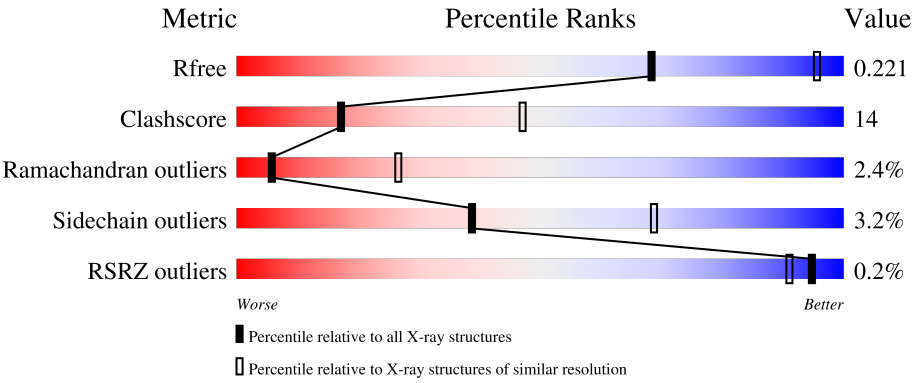
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.12 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	476	70% 25%
1	B	476	75% 19%
1	C	476	77% 16%
1	D	476	77% 17%
1	E	476	79% 16%

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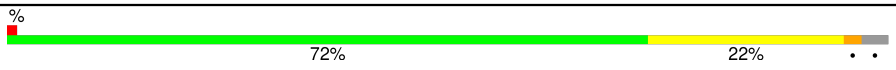
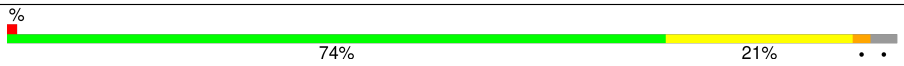
Mol	Chain	Length	Quality of chain
1	F	476	
1	G	476	
1	H	476	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CM5	E	501	-	-	-	X
4	CM5	E	504	-	-	-	X
4	CM5	F	501	-	-	-	X
4	CM5	G	501	-	-	-	X
4	CM5	H	501	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 29782 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 2C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3615	2337	599	656	23			
1	B	461	Total	C	N	O	S	0	0	0
			3639	2348	605	662	24			
1	C	460	Total	C	N	O	S	0	0	0
			3619	2340	601	655	23			
1	D	461	Total	C	N	O	S	0	0	0
			3586	2316	594	652	24			
1	E	460	Total	C	N	O	S	0	0	0
			3575	2310	588	654	23			
1	F	460	Total	C	N	O	S	0	0	0
			3583	2318	592	650	23			
1	G	462	Total	C	N	O	S	0	0	0
			3580	2315	588	653	24			
1	H	459	Total	C	N	O	S	0	0	0
			3571	2311	586	650	24			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P11712
A	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712
A	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
A	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
A	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
A	144	CYS	ARG	engineered mutation	UNP P11712
A	490	ILE	VAL	engineered mutation	UNP P11712
A	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
A	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
A	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
A	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
B	19	MET	-	initiating methionine	UNP P11712
B	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
B	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
B	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
B	144	CYS	ARG	engineered mutation	UNP P11712
B	490	ILE	VAL	engineered mutation	UNP P11712
B	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
B	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
B	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
B	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
C	19	MET	-	initiating methionine	UNP P11712
C	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712
C	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
C	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
C	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
C	144	CYS	ARG	engineered mutation	UNP P11712
C	490	ILE	VAL	engineered mutation	UNP P11712
C	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
C	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
C	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
C	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
D	19	MET	-	initiating methionine	UNP P11712
D	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712
D	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
D	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
D	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
D	144	CYS	ARG	engineered mutation	UNP P11712
D	490	ILE	VAL	engineered mutation	UNP P11712
D	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
D	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
D	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
D	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
E	19	MET	-	initiating methionine	UNP P11712
E	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712
E	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
E	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
E	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
E	144	CYS	ARG	engineered mutation	UNP P11712
E	490	ILE	VAL	engineered mutation	UNP P11712
E	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
E	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
E	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
E	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712

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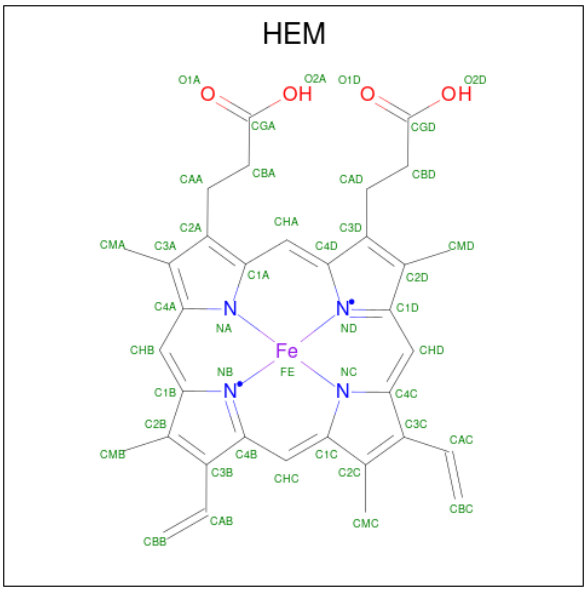
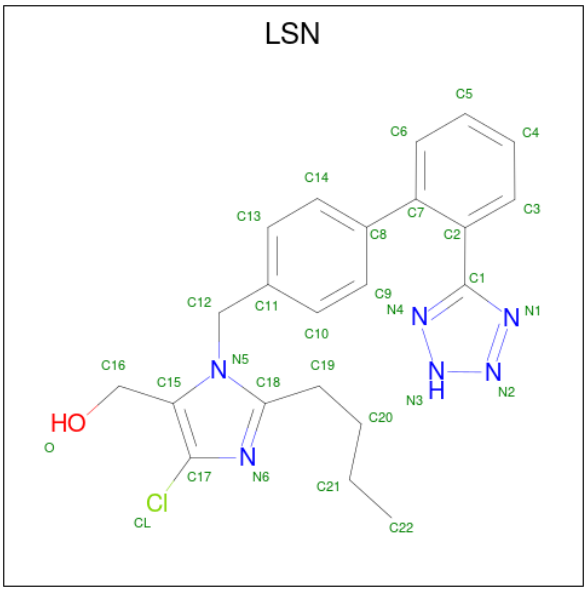
Chain	Residue	Modelled	Actual	Comment	Reference
F	19	MET	-	initiating methionine	UNP P11712
F	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712
F	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
F	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
F	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
F	144	CYS	ARG	engineered mutation	UNP P11712
F	490	ILE	VAL	engineered mutation	UNP P11712
F	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
F	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
F	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
F	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
G	19	MET	-	initiating methionine	UNP P11712
G	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712
G	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
G	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
G	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
G	144	CYS	ARG	engineered mutation	UNP P11712
G	490	ILE	VAL	engineered mutation	UNP P11712
G	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
G	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
G	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
G	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
H	19	MET	-	initiating methionine	UNP P11712
H	20	ALA	-	SEE SEQUENCE DETAILS	UNP P11712
H	21	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
H	22	LYS	-	SEE SEQUENCE DETAILS	UNP P11712
H	23	THR	-	SEE SEQUENCE DETAILS	UNP P11712
H	144	CYS	ARG	engineered mutation	UNP P11712
H	490	ILE	VAL	engineered mutation	UNP P11712
H	491	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
H	492	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
H	493	HIS	-	SEE SEQUENCE DETAILS	UNP P11712
H	494	HIS	-	SEE SEQUENCE DETAILS	UNP P11712

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



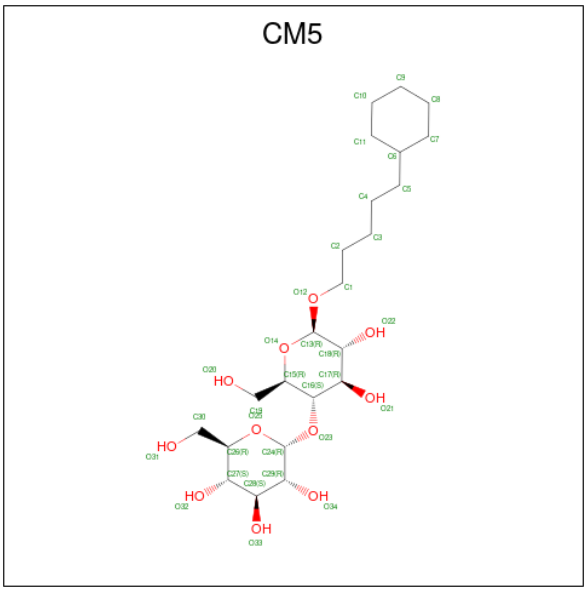
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G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

- Molecule 3 is [2-butyl-5-chloranyl-3-[[4-[2-(2H-1,2,3,4-tetrazol-5-yl)phenyl]phenyl]methyl]imidazol-4-yl]methanol (three-letter code: LSN) (formula: $C_{22}H_{23}ClN_6O$) (labeled as "Ligand of Interest" by depositor).



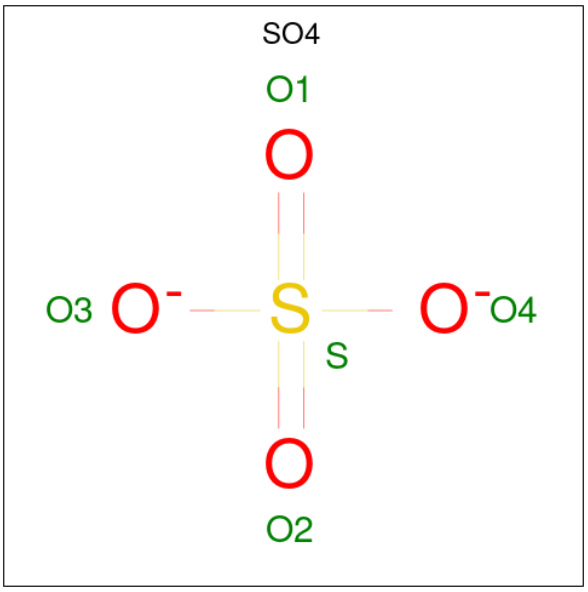
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		
3	B	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		
3	C	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		
3	D	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		
3	E	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		
3	F	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		
3	G	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		
3	H	1	Total	C	Cl	N	O	0	0
			30	22	1	6	1		

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 34 23 11	0	0
4	E	1	Total C O 34 23 11	0	0
4	F	1	Total C O 34 23 11	0	0
4	F	1	Total C O 34 23 11	0	0
4	G	1	Total C O 34 23 11	0	0
4	G	1	Total C O 34 23 11	0	0
4	H	1	Total C O 34 23 11	0	0
4	H	1	Total C O 34 23 11	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

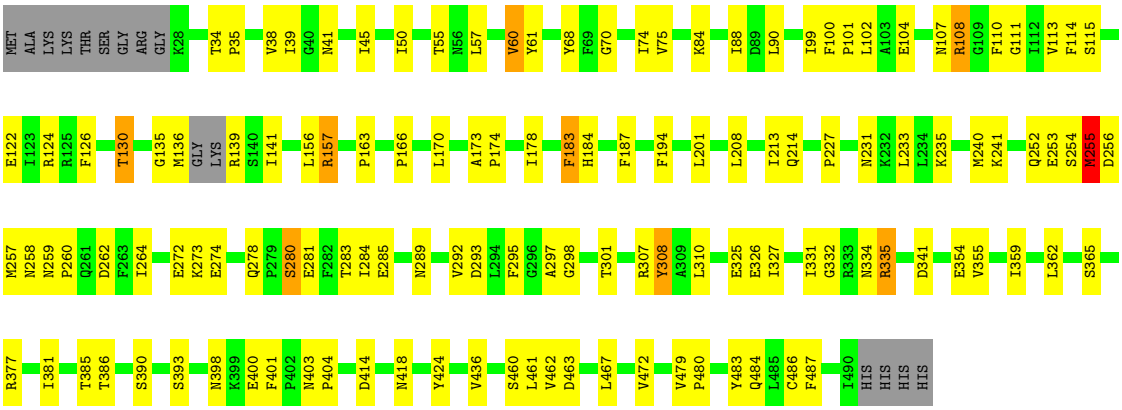
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	19	Total O 19 19	0	0
6	C	21	Total O 21 21	0	0
6	D	8	Total O 8 8	0	0
6	E	22	Total O 22 22	0	0
6	F	20	Total O 20 20	0	0
6	G	16	Total O 16 16	0	0
6	H	25	Total O 25 25	0	0

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 2C9

Chain A:

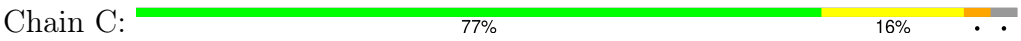


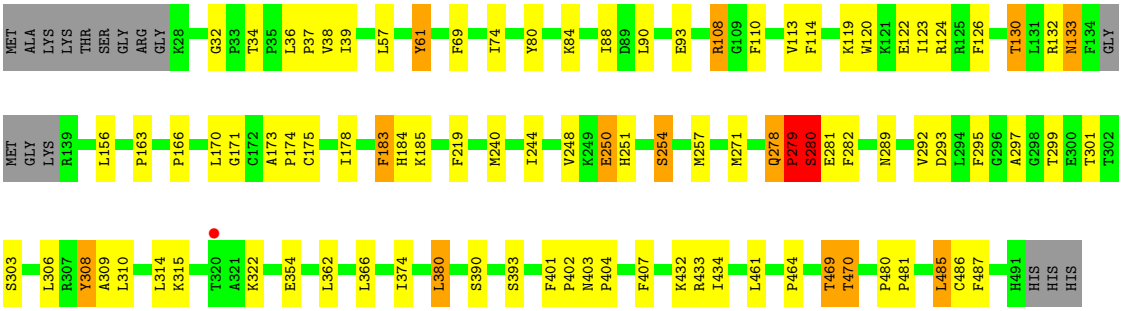
• Molecule 1: Cytochrome P450 2C9

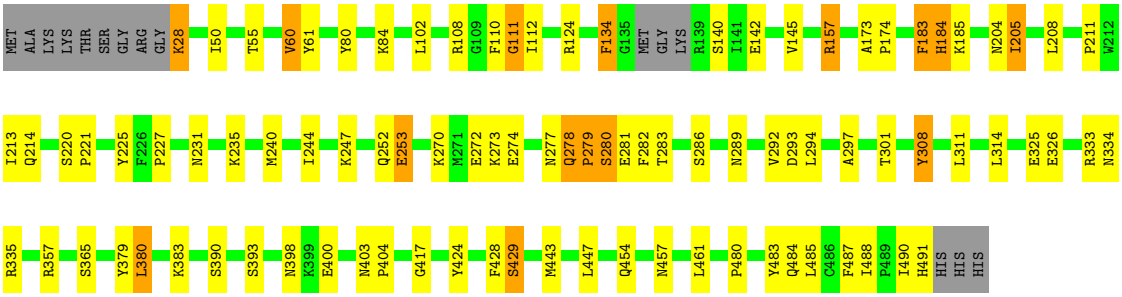
Chain B:

• Molecule 1: Cytochrome P450 2C9

Chain C:





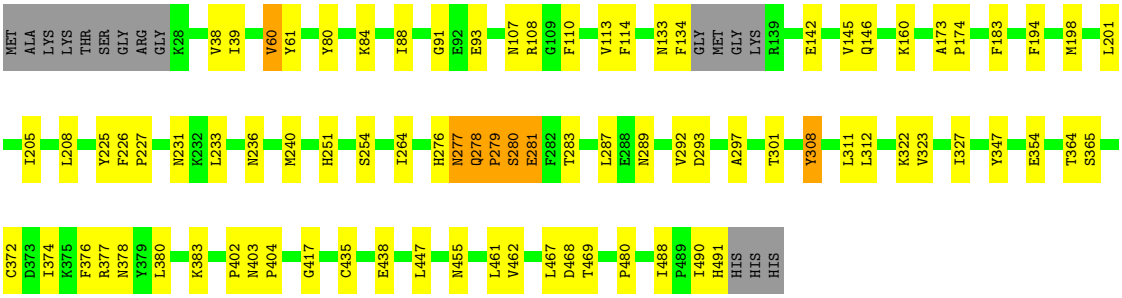


• Molecule 1: Cytochrome P450 2C9

Chain D:

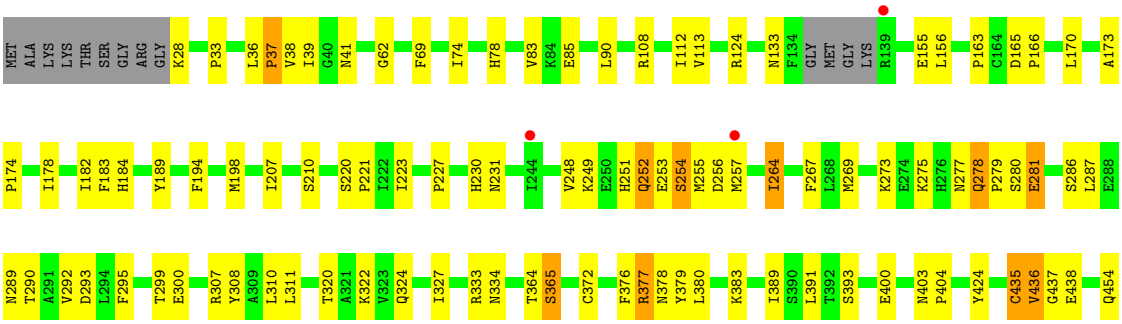
• Molecule 1: Cytochrome P450 2C9

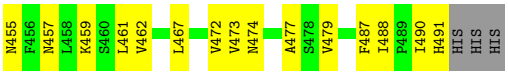
Chain E:



• Molecule 1: Cytochrome P450 2C9

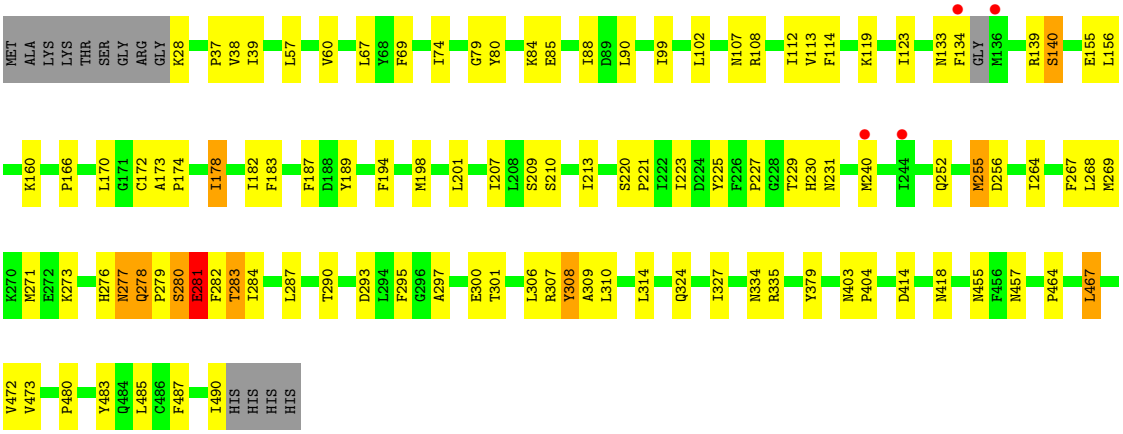
Chain F:





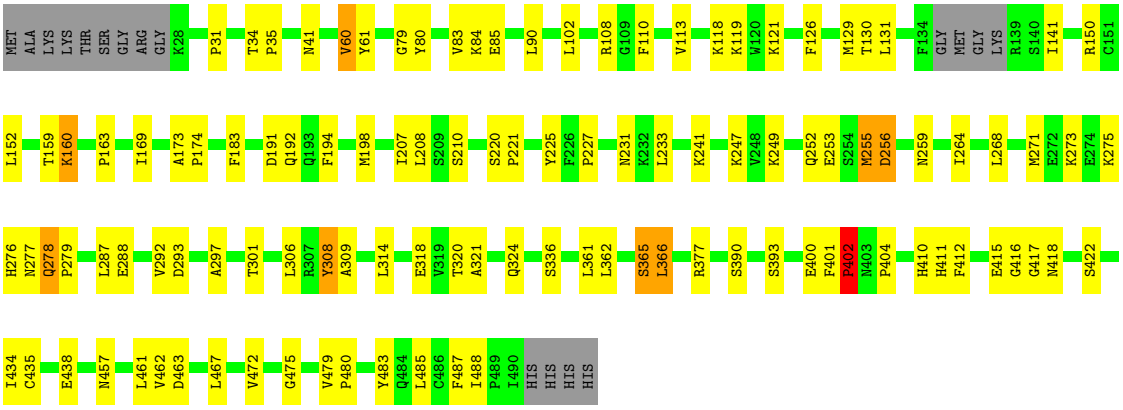
• Molecule 1: Cytochrome P450 2C9

Chain G:



• Molecule 1: Cytochrome P450 2C9

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	238.10Å 238.10Å 109.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 3.12 39.61 – 3.12	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.01-3.12) 99.3 (39.61-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.156 , 0.221 0.181 , 0.221	Depositor DCC
R_{free} test set	6047 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	80.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.457 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29782	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LSN, HEM, SO4, CM5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.62	0/3704	0.89	0/5028
1	B	0.63	0/3728	0.86	0/5057
1	C	0.63	0/3709	0.87	0/5034
1	D	0.62	0/3674	0.86	0/4995
1	E	0.63	0/3663	0.86	0/4981
1	F	0.62	0/3672	0.84	0/4991
1	G	0.62	0/3668	0.83	0/4988
1	H	0.63	0/3659	0.86	0/4973
All	All	0.62	0/29477	0.86	0/40047

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

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	3615	0	3577	123	0
1	B	3639	0	3613	81	0
1	C	3619	0	3588	92	0
1	D	3586	0	3514	79	0
1	E	3575	0	3498	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3583	0	3519	93	0
1	G	3580	0	3495	103	0
1	H	3571	0	3502	92	0
2	A	43	0	30	12	0
2	B	43	0	30	10	0
2	C	43	0	30	14	0
2	D	43	0	30	11	0
2	E	43	0	30	12	0
2	F	43	0	30	7	0
2	G	43	0	30	8	0
2	H	43	0	30	5	0
3	A	30	0	0	5	0
3	B	30	0	0	1	0
3	C	30	0	0	0	0
3	D	30	0	0	5	0
3	E	30	0	0	2	0
3	F	30	0	0	2	0
3	G	30	0	0	2	0
3	H	30	0	0	2	0
4	E	68	0	84	15	0
4	F	68	0	84	7	0
4	G	68	0	84	9	0
4	H	68	0	84	16	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
6	A	12	0	0	1	0
6	B	19	0	0	0	0
6	C	21	0	0	1	0
6	D	8	0	0	0	0
6	E	22	0	0	0	0
6	F	20	0	0	1	0
6	G	16	0	0	1	0
6	H	25	0	0	2	0
All	All	29782	0	28882	811	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 14.

All (811) 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:G:69:PHE:CD2	1:G:74:ILE:HD12	1.53	1.42
1:F:457:ASN:OD1	1:F:490:ILE:HD12	1.29	1.27
1:C:163:PRO:CB	1:C:461:LEU:HD11	1.66	1.24
1:D:277:ASN:O	1:D:279:PRO:HD2	1.39	1.19
1:E:461:LEU:HD12	1:E:461:LEU:O	1.42	1.18
1:H:278:GLN:HB2	1:H:279:PRO:HD3	1.19	1.13
1:B:380:LEU:HD23	1:B:380:LEU:O	1.48	1.10
1:C:163:PRO:HB2	1:C:461:LEU:HD11	1.20	1.10
2:F:502:HEM:HBC2	2:F:502:HEM:HHD	1.34	1.09
2:C:501:HEM:HBC2	2:C:501:HEM:HHD	1.33	1.09
1:C:124:ARG:HH12	1:C:433:ARG:HA	0.97	1.07
2:A:501:HEM:HBC2	2:A:501:HEM:HHD	1.34	1.06
1:G:69:PHE:CD2	1:G:74:ILE:CD1	2.39	1.05
1:H:278:GLN:HB2	1:H:279:PRO:CD	1.85	1.05
1:A:60:VAL:CG2	1:A:61:TYR:CD1	2.40	1.04
1:C:380:LEU:O	1:C:380:LEU:HD23	1.56	1.04
1:E:380:LEU:HD23	1:E:380:LEU:O	1.57	1.03
1:H:277:ASN:O	1:H:279:PRO:HD2	1.58	1.02
1:H:461:LEU:HD12	1:H:461:LEU:O	1.60	1.01
1:C:124:ARG:NH1	1:C:433:ARG:HA	1.75	1.00
1:F:227:PRO:HB2	4:F:504:CM5:O22	1.62	0.99
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.44	0.99
1:F:69:PHE:CD2	1:F:74:ILE:HD12	1.98	0.99
1:F:400:GLU:HG2	1:F:424:TYR:CD1	1.97	0.98
2:E:502:HEM:HHD	2:E:502:HEM:HBC2	1.42	0.97
1:B:163:PRO:HB3	1:B:461:LEU:HD21	1.47	0.97
1:G:69:PHE:HD2	1:G:74:ILE:HD12	0.89	0.96
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.46	0.95
1:A:108:ARG:HD2	1:A:241:LYS:HE2	1.49	0.94
1:D:273:LYS:O	1:D:274:GLU:HG2	1.68	0.94
1:C:163:PRO:HB3	1:C:461:LEU:HD11	1.47	0.94
2:E:502:HEM:HBB2	2:E:502:HEM:HMB2	1.48	0.94
1:F:364:THR:O	1:F:365:SER:O	1.86	0.94
1:C:280:SER:OG	1:C:281:GLU:N	2.01	0.91
1:H:278:GLN:CB	1:H:279:PRO:HD3	2.01	0.91
1:C:122:GLU:OE1	1:C:281:GLU:HG2	1.69	0.91
1:F:455:ASN:O	1:F:490:ILE:HG22	1.71	0.91
2:G:502:HEM:HBC2	2:G:502:HEM:HHD	1.52	0.91
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.52	0.91
1:D:28:LYS:HE2	1:D:380:LEU:HD23	1.53	0.91
1:G:306:LEU:O	1:G:309:ALA:HB3	1.72	0.90
1:F:459:LYS:HB2	1:F:488:ILE:HD11	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ARG:HH12	1:C:433:ARG:CA	1.83	0.90
1:C:163:PRO:HB2	1:C:461:LEU:CD1	2.00	0.90
1:F:457:ASN:OD1	1:F:490:ILE:CD1	2.20	0.89
1:H:461:LEU:O	1:H:462:VAL:HG23	1.72	0.89
1:B:119:LYS:HG2	1:B:281:GLU:OE1	1.71	0.89
1:D:277:ASN:OD1	1:D:279:PRO:HG2	1.70	0.89
4:E:501:CM5:H301	4:E:501:CM5:H29	1.54	0.89
1:H:208:LEU:HD21	1:H:233:LEU:HD21	1.54	0.88
1:A:283:THR:HG22	1:A:285:GLU:H	1.38	0.88
1:D:277:ASN:O	1:D:279:PRO:CD	2.22	0.87
1:A:108:ARG:O	1:A:114:PHE:HB2	1.73	0.87
1:B:186:ARG:HG3	1:B:186:ARG:HH11	1.39	0.87
1:H:401:PHE:O	1:H:402:PRO:O	1.92	0.86
1:D:277:ASN:OD1	1:D:279:PRO:CG	2.23	0.86
1:A:35:PRO:HG3	1:A:68:TYR:CD1	2.09	0.86
1:B:247:LYS:HD3	1:B:250:GLU:OE2	1.76	0.86
1:B:163:PRO:HB2	1:B:461:LEU:HD11	1.58	0.86
4:H:501:CM5:H29	4:H:501:CM5:H301	1.58	0.86
1:B:38:VAL:HG13	1:B:39:ILE:HG23	1.59	0.85
1:D:277:ASN:OD1	1:D:279:PRO:HD2	1.75	0.85
1:D:244:ILE:HG13	1:D:292:VAL:HG22	1.56	0.85
2:B:501:HEM:HBC2	2:B:501:HEM:HHD	1.57	0.84
1:A:60:VAL:HG23	1:A:61:TYR:CD1	2.11	0.83
1:F:253:GLU:O	1:F:254:SER:OG	1.95	0.83
1:G:297:ALA:O	1:G:301:THR:HG22	1.80	0.82
1:E:461:LEU:O	1:E:461:LEU:CD1	2.27	0.82
1:G:464:PRO:HA	1:G:467:LEU:HD11	1.58	0.82
2:E:502:HEM:HBB2	2:E:502:HEM:CMB	2.09	0.82
1:F:184:HIS:O	1:F:184:HIS:ND1	2.13	0.82
1:G:69:PHE:HD2	1:G:74:ILE:CD1	1.83	0.82
1:E:93:GLU:HG2	1:E:374:ILE:HD12	1.60	0.81
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.09	0.81
1:D:277:ASN:OD1	1:D:279:PRO:CD	2.28	0.81
4:F:501:CM5:H29	4:F:501:CM5:H301	1.63	0.80
1:B:380:LEU:O	1:B:380:LEU:CD2	2.29	0.79
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.13	0.79
1:D:280:SER:OG	1:D:281:GLU:N	2.16	0.79
1:B:183:PHE:O	1:B:184:HIS:HB3	1.81	0.79
2:D:501:HEM:HBC2	2:D:501:HEM:HHD	1.62	0.79
1:F:327:ILE:HG21	1:F:454:GLN:HB3	1.64	0.78
1:G:277:ASN:O	1:G:278:GLN:CB	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD21	1:A:240:MET:SD	2.24	0.78
1:G:227:PRO:HB2	4:G:504:CM5:O22	1.84	0.78
1:B:110:PHE:O	1:B:289:ASN:CB	2.32	0.77
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.66	0.77
1:G:467:LEU:N	1:G:467:LEU:HD12	1.98	0.77
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.10	0.77
1:G:134:PHE:CD1	1:G:139:ARG:HB3	2.19	0.77
1:C:163:PRO:CB	1:C:461:LEU:CD1	2.56	0.77
1:D:457:ASN:OD1	1:D:490:ILE:HG12	1.85	0.77
1:B:110:PHE:O	1:B:289:ASN:HB3	1.85	0.76
1:B:401:PHE:O	1:B:404:PRO:HG3	1.85	0.76
1:C:380:LEU:O	1:C:380:LEU:CD2	2.33	0.76
2:C:501:HEM:HBB2	2:C:501:HEM:CMB	2.14	0.76
1:G:170:LEU:HD21	1:G:310:LEU:HD12	1.68	0.75
1:G:281:GLU:HA	1:G:281:GLU:OE1	1.86	0.75
1:F:178:ILE:HD12	1:F:295:PHE:HA	1.67	0.75
1:C:120:TRP:HZ2	1:C:124:ARG:HH11	1.34	0.75
1:H:227:PRO:HB2	4:H:504:CM5:O22	1.87	0.75
1:C:485:LEU:O	1:C:485:LEU:HD23	1.86	0.75
1:F:461:LEU:O	1:F:461:LEU:HD12	1.85	0.75
1:A:110:PHE:HB2	1:A:289:ASN:HD22	1.52	0.74
1:F:377:ARG:O	1:F:378:ASN:OD1	2.04	0.74
1:C:132:ARG:O	1:C:133:ASN:OD1	2.05	0.74
1:H:231:ASN:CB	4:H:504:CM5:O34	2.35	0.74
1:C:124:ARG:NH1	1:C:432:LYS:O	2.21	0.74
1:F:113:VAL:HG22	2:F:502:HEM:HAD2	1.70	0.74
1:C:108:ARG:HH11	1:C:292:VAL:HG13	1.52	0.74
1:F:377:ARG:O	1:F:378:ASN:CG	2.26	0.74
1:G:457:ASN:OD1	1:G:490:ILE:HG21	1.88	0.74
1:F:277:ASN:O	1:F:278:GLN:CB	2.36	0.73
1:G:281:GLU:O	1:G:282:PHE:HB2	1.87	0.73
1:H:231:ASN:HB3	4:H:504:CM5:O34	1.88	0.73
1:D:28:LYS:HE2	1:D:380:LEU:CD2	2.17	0.73
1:E:173:ALA:HB3	1:E:174:PRO:HD3	1.69	0.73
2:F:502:HEM:HBC2	2:F:502:HEM:CHD	2.10	0.73
1:D:308:TYR:CD1	1:D:480:PRO:HB3	2.24	0.73
1:B:126:PHE:O	1:B:130:THR:HG23	1.89	0.72
1:H:108:ARG:NH1	1:H:293:ASP:OD1	2.23	0.72
1:G:113:VAL:HG22	2:G:502:HEM:HAD2	1.71	0.72
1:B:231:ASN:O	1:B:235:LYS:HG2	1.90	0.72
1:C:280:SER:O	1:C:281:GLU:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:461:LEU:O	1:H:462:VAL:CG2	2.38	0.72
1:B:108:ARG:NH1	1:B:293:ASP:OD1	2.23	0.71
1:C:32:GLY:HA2	1:C:61:TYR:CD2	2.25	0.71
1:F:251:HIS:O	1:F:252:GLN:C	2.26	0.71
4:E:501:CM5:H24	4:E:501:CM5:O21	1.89	0.71
1:G:134:PHE:HD1	1:G:139:ARG:HB3	1.55	0.71
1:C:108:ARG:NH1	1:C:292:VAL:HG13	2.06	0.71
1:G:324:GLN:HA	1:G:327:ILE:HD12	1.71	0.71
1:D:277:ASN:C	1:D:279:PRO:HD2	2.12	0.71
1:A:60:VAL:CG2	1:A:61:TYR:N	2.54	0.70
2:G:502:HEM:HHA	2:G:502:HEM:HBD1	1.73	0.70
2:A:501:HEM:HBC2	2:A:501:HEM:CHD	2.12	0.70
1:G:464:PRO:O	1:G:467:LEU:CD1	2.39	0.70
1:H:401:PHE:O	1:H:402:PRO:C	2.28	0.70
1:H:277:ASN:O	1:H:279:PRO:CD	2.39	0.69
2:H:502:HEM:HMB1	2:H:502:HEM:HBB2	1.73	0.69
1:D:461:LEU:HD21	1:D:484:GLN:HB2	1.74	0.69
1:F:400:GLU:HG2	1:F:424:TYR:CG	2.26	0.69
1:B:186:ARG:HG3	1:B:186:ARG:NH1	2.00	0.69
1:F:248:VAL:O	1:F:252:GLN:HG3	1.93	0.69
1:F:251:HIS:O	1:F:253:GLU:N	2.26	0.68
1:G:277:ASN:C	1:G:279:PRO:HD2	2.12	0.68
2:G:502:HEM:HBC2	2:G:502:HEM:CHD	2.20	0.68
1:G:225:TYR:CE1	4:G:501:CM5:O22	2.46	0.68
1:F:108:ARG:NH2	1:F:292:VAL:HG13	2.07	0.68
1:E:278:GLN:O	1:E:280:SER:N	2.27	0.68
4:H:501:CM5:O32	4:H:501:CM5:H191	1.94	0.68
1:A:208:LEU:HD21	1:A:233:LEU:HD11	1.74	0.68
1:D:485:LEU:HD11	1:D:487:PHE:CZ	2.30	0.67
4:E:501:CM5:H301	4:E:501:CM5:C29	2.25	0.67
1:H:276:HIS:O	1:H:278:GLN:HG2	1.92	0.67
1:B:170:LEU:HD11	1:B:310:LEU:HD12	1.75	0.67
1:C:297:ALA:O	1:C:301:THR:HG22	1.94	0.67
1:H:275:LYS:HA	6:H:614:HOH:O	1.95	0.67
1:H:314:LEU:HD11	1:H:485:LEU:CD2	2.25	0.67
1:A:201:LEU:CD2	1:A:240:MET:SD	2.82	0.67
1:E:108:ARG:O	1:E:114:PHE:HB2	1.95	0.67
4:H:501:CM5:O21	4:H:501:CM5:H24	1.94	0.67
1:A:283:THR:HG22	1:A:284:ILE:N	2.09	0.67
1:A:403:ASN:N	1:A:404:PRO:HD3	2.10	0.67
1:C:113:VAL:HG22	2:C:501:HEM:HAD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:LEU:CD1	1:F:467:LEU:HD13	2.25	0.66
1:H:461:LEU:O	1:H:461:LEU:CD1	2.40	0.66
1:F:173:ALA:HB3	1:F:174:PRO:HD3	1.75	0.66
1:A:183:PHE:HA	1:A:262:ASP:OD2	1.96	0.66
1:E:231:ASN:HB2	4:E:504:CM5:O34	1.96	0.66
1:A:38:VAL:HG13	1:A:39:ILE:H	1.61	0.66
1:G:255:MET:HG3	1:G:256:ASP:N	2.11	0.66
1:H:173:ALA:HB3	1:H:174:PRO:HD3	1.78	0.66
1:A:60:VAL:HG22	1:A:61:TYR:CD1	2.28	0.65
1:C:108:ARG:NH1	1:C:293:ASP:OD1	2.26	0.65
1:F:364:THR:C	1:F:365:SER:O	2.32	0.65
1:F:474:ASN:HA	1:F:477:ALA:O	1.97	0.65
1:G:403:ASN:N	1:G:404:PRO:HD3	2.10	0.65
1:A:60:VAL:CG2	1:A:61:TYR:CE1	2.80	0.65
1:D:124:ARG:NH1	2:D:501:HEM:O1D	2.30	0.65
1:A:401:PHE:O	1:A:404:PRO:HG3	1.97	0.65
1:F:124:ARG:NH1	2:F:502:HEM:O1D	2.30	0.65
1:F:163:PRO:HB3	1:F:461:LEU:CD2	2.28	0.64
1:A:283:THR:HG22	1:A:285:GLU:N	2.09	0.64
1:C:254:SER:O	1:C:254:SER:OG	2.09	0.64
1:B:277:ASN:O	1:B:279:PRO:HD2	1.98	0.64
1:C:166:PRO:HB2	1:C:170:LEU:CD1	2.28	0.64
1:E:380:LEU:O	1:E:380:LEU:CD2	2.40	0.64
1:A:308:TYR:CD1	1:A:480:PRO:HB3	2.32	0.64
1:A:174:PRO:O	1:A:178:ILE:HD12	1.99	0.63
1:E:84:LYS:HG3	1:E:88:ILE:HD12	1.81	0.63
2:A:501:HEM:HBA2	2:A:501:HEM:HHA	1.81	0.63
1:C:279:PRO:O	1:C:280:SER:HB3	1.97	0.63
1:B:163:PRO:CB	1:B:461:LEU:HD11	2.27	0.63
1:G:307:ARG:O	1:G:310:LEU:N	2.32	0.63
1:E:281:GLU:HA	1:E:281:GLU:OE1	1.98	0.63
1:F:307:ARG:HD2	6:F:615:HOH:O	1.98	0.63
1:F:320:THR:O	1:F:324:GLN:HG3	1.98	0.63
4:E:504:CM5:O21	4:E:504:CM5:H29	1.98	0.62
1:H:402:PRO:O	1:H:404:PRO:CD	2.47	0.62
1:A:38:VAL:HG13	1:A:39:ILE:N	2.14	0.62
1:C:166:PRO:HB2	1:C:170:LEU:HD12	1.81	0.62
1:F:69:PHE:CD2	1:F:74:ILE:CD1	2.80	0.62
1:G:69:PHE:CE2	1:G:74:ILE:HD12	2.25	0.62
1:A:252:GLN:OE1	1:A:284:ILE:HD11	2.00	0.62
1:B:108:ARG:NH1	1:B:293:ASP:CG	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:MET:O	1:B:256:ASP:HB3	1.99	0.62
1:C:119:LYS:O	1:C:123:ILE:HG13	1.98	0.62
1:F:36:LEU:HB3	1:F:37:PRO:HD2	1.81	0.62
1:H:152:LEU:HD11	1:H:169:ILE:HG22	1.80	0.62
2:D:501:HEM:HBC2	2:D:501:HEM:CHD	2.30	0.62
1:E:277:ASN:C	1:E:279:PRO:HD2	2.20	0.62
1:C:280:SER:O	1:C:281:GLU:CB	2.46	0.62
1:H:80:TYR:CZ	1:H:84:LYS:HD2	2.35	0.62
1:B:183:PHE:O	1:B:184:HIS:CB	2.47	0.62
1:C:124:ARG:NH2	1:C:434:ILE:O	2.33	0.62
1:F:364:THR:O	1:F:365:SER:C	2.39	0.62
1:A:60:VAL:HG21	1:A:61:TYR:CE1	2.35	0.62
1:G:307:ARG:HG2	1:G:483:TYR:OH	1.99	0.62
1:H:255:MET:HB3	6:H:605:HOH:O	2.00	0.61
1:D:325:GLU:OE1	1:D:326:GLU:N	2.32	0.61
1:B:485:LEU:HD11	1:B:487:PHE:CZ	2.36	0.61
1:C:38:VAL:HG13	1:C:39:ILE:HG23	1.82	0.61
1:E:205:ILE:HD11	3:E:503:LSN:N2	2.15	0.61
1:H:35:PRO:HA	1:H:41:ASN:ND2	2.15	0.61
1:C:171:GLY:HA2	1:C:303:SER:HB2	1.82	0.61
1:C:314:LEU:HD21	1:C:485:LEU:HD12	1.83	0.61
1:G:178:ILE:O	1:G:182:ILE:HG12	2.01	0.61
1:H:402:PRO:O	1:H:404:PRO:HD3	2.01	0.61
1:E:374:ILE:O	1:E:380:LEU:HA	2.00	0.61
1:E:403:ASN:N	1:E:404:PRO:HD3	2.15	0.61
1:G:173:ALA:HB3	1:G:174:PRO:HD3	1.83	0.61
1:A:157:ARG:HH11	1:A:157:ARG:CG	2.14	0.60
1:H:268:LEU:HA	1:H:271:MET:HG3	1.84	0.60
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.83	0.60
1:A:240:MET:HE1	3:A:502:LSN:CL	2.38	0.60
2:D:501:HEM:HBD1	2:D:501:HEM:HHA	1.83	0.60
1:A:60:VAL:HG22	1:A:61:TYR:HD1	1.64	0.60
1:A:231:ASN:O	1:A:235:LYS:HG2	1.99	0.60
1:C:362:LEU:HD12	2:C:501:HEM:HMA2	1.83	0.60
1:G:108:ARG:NH2	1:G:293:ASP:OD1	2.34	0.60
1:A:108:ARG:CZ	1:A:108:ARG:HB3	2.30	0.60
1:C:110:PHE:O	1:C:289:ASN:CB	2.50	0.60
1:C:163:PRO:HB3	1:C:461:LEU:CD1	2.27	0.60
1:G:307:ARG:CG	1:G:483:TYR:OH	2.50	0.60
1:A:60:VAL:HG23	1:A:61:TYR:N	2.16	0.60
1:D:111:GLY:O	1:D:293:ASP:OD2	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:PHE:CG	1:F:287:LEU:HD13	2.37	0.60
1:G:281:GLU:HB3	1:G:282:PHE:HD1	1.67	0.60
1:H:183:PHE:CE2	1:H:247:LYS:HE2	2.37	0.60
1:A:240:MET:CE	3:A:502:LSN:CL	2.87	0.59
1:B:120:TRP:CZ2	1:B:124:ARG:HD3	2.37	0.59
1:H:152:LEU:CD1	1:H:169:ILE:HG22	2.32	0.59
1:H:461:LEU:C	1:H:462:VAL:HG23	2.22	0.59
1:A:124:ARG:NH1	2:A:501:HEM:O1D	2.33	0.59
1:D:108:ARG:NH2	1:D:293:ASP:OD1	2.36	0.59
1:G:252:GLN:NE2	1:G:284:ILE:HD11	2.16	0.59
1:E:194:PHE:CE1	1:E:198:MET:HB2	2.38	0.59
1:C:280:SER:HG	1:C:281:GLU:H	1.48	0.59
1:F:281:GLU:OE1	1:F:281:GLU:HA	2.02	0.59
1:A:362:LEU:HD12	2:A:501:HEM:HMA3	1.84	0.59
1:D:398:ASN:OD1	1:D:398:ASN:O	2.20	0.59
1:E:108:ARG:NH2	1:E:293:ASP:OD1	2.35	0.59
1:C:69:PHE:CD1	1:C:74:ILE:HD12	2.38	0.59
2:F:502:HEM:HHA	2:F:502:HEM:CBD	2.33	0.59
1:C:308:TYR:CD1	1:C:480:PRO:HB3	2.37	0.58
1:G:280:SER:OG	1:G:281:GLU:N	2.34	0.58
1:E:93:GLU:CG	1:E:374:ILE:HD12	2.29	0.58
2:E:502:HEM:HMB2	2:E:502:HEM:CBB	2.28	0.58
1:D:28:LYS:O	1:D:379:TYR:O	2.22	0.58
1:H:208:LEU:CD2	1:H:233:LEU:HD21	2.29	0.58
1:A:50:ILE:HD11	1:A:214:GLN:HG2	1.85	0.58
1:D:428:PHE:O	1:D:429:SER:CB	2.52	0.58
1:G:207:ILE:O	1:G:210:SER:HB3	2.04	0.58
1:G:231:ASN:HB2	4:G:504:CM5:O34	2.04	0.58
4:F:501:CM5:H301	4:F:501:CM5:C29	2.29	0.58
1:G:252:GLN:HE22	1:G:284:ILE:HD11	1.69	0.57
1:H:108:ARG:NH2	3:H:503:LSN:N6	2.52	0.57
1:B:325:GLU:OE1	1:B:329:ARG:NH1	2.37	0.57
1:A:163:PRO:HB3	1:A:486:CYS:SG	2.43	0.57
1:G:209:SER:HB2	1:G:473:VAL:CG2	2.35	0.57
2:B:501:HEM:HMB2	2:B:501:HEM:CBB	2.26	0.57
2:C:501:HEM:HMB2	2:C:501:HEM:CBB	2.33	0.57
1:D:110:PHE:N	1:D:110:PHE:CD2	2.73	0.57
2:D:501:HEM:HMB2	2:D:501:HEM:CBB	2.27	0.57
1:H:255:MET:O	1:H:256:ASP:HB3	2.03	0.57
1:H:301:THR:HG21	2:H:502:HEM:CHC	2.35	0.57
1:F:377:ARG:O	1:F:377:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HD21	1:A:484:GLN:HB2	1.86	0.57
1:D:231:ASN:O	1:D:235:LYS:HG2	2.05	0.57
1:F:178:ILE:O	1:F:182:ILE:HG12	2.05	0.56
1:F:255:MET:HE2	1:F:257:MET:SD	2.44	0.56
1:G:455:ASN:C	1:G:490:ILE:HG12	2.25	0.56
2:F:502:HEM:HHA	2:F:502:HEM:HBD1	1.87	0.56
1:A:462:VAL:HG22	1:F:62:GLY:HA2	1.87	0.56
1:E:468:ASP:OD1	1:E:469:THR:N	2.37	0.56
1:F:467:LEU:HD12	1:F:467:LEU:O	2.06	0.56
1:G:273:LYS:O	1:G:273:LYS:HG2	2.06	0.56
1:G:276:HIS:O	1:G:277:ASN:O	2.22	0.56
4:H:501:CM5:H301	4:H:501:CM5:C29	2.26	0.56
1:A:108:ARG:HH21	1:A:292:VAL:HG13	1.70	0.56
1:H:183:PHE:HB3	1:H:264:ILE:HD12	1.88	0.56
1:C:108:ARG:O	1:C:114:PHE:HB2	2.06	0.56
1:B:112:ILE:HD12	1:B:124:ARG:HA	1.87	0.56
1:G:282:PHE:O	1:G:283:THR:C	2.44	0.56
1:G:301:THR:HG21	2:G:502:HEM:CHC	2.34	0.56
1:A:101:PRO:O	1:A:104:GLU:N	2.38	0.56
1:A:240:MET:HE1	3:A:502:LSN:C16	2.36	0.56
4:G:504:CM5:O21	4:G:504:CM5:H29	2.06	0.56
1:A:257:MET:O	1:A:259:ASN:N	2.39	0.56
1:A:136:MET:HA	1:A:139:ARG:N	2.21	0.56
1:H:207:ILE:O	1:H:210:SER:HB3	2.06	0.56
1:B:130:THR:O	1:B:132:ARG:N	2.39	0.55
1:B:253:GLU:C	1:B:255:MET:H	2.08	0.55
1:C:163:PRO:HA	1:C:486:CYS:HB3	1.88	0.55
1:C:61:TYR:N	1:C:61:TYR:CD1	2.73	0.55
1:F:273:LYS:O	1:F:273:LYS:HG2	2.05	0.55
1:G:280:SER:O	1:G:281:GLU:HB2	2.05	0.55
1:D:308:TYR:CE1	1:D:480:PRO:HB3	2.41	0.55
1:G:28:LYS:O	1:G:379:TYR:O	2.25	0.55
2:G:502:HEM:HHD	2:G:502:HEM:CBC	2.30	0.55
1:A:108:ARG:HD2	1:A:241:LYS:CE	2.31	0.55
1:H:485:LEU:HD11	1:H:487:PHE:CZ	2.41	0.55
1:D:272:GLU:C	1:D:274:GLU:H	2.09	0.55
1:H:457:ASN:HB2	1:H:488:ILE:HD11	1.87	0.55
1:E:93:GLU:CB	1:E:374:ILE:HD12	2.36	0.55
1:C:308:TYR:CE1	1:C:480:PRO:HB3	2.42	0.55
1:F:255:MET:CE	1:F:269:MET:HG3	2.37	0.55
1:G:223:ILE:HG23	1:G:230:HIS:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:PHE:O	1:F:377:ARG:C	2.45	0.54
1:G:187:PHE:CD2	1:G:194:PHE:HB2	2.42	0.54
1:A:126:PHE:CZ	1:A:130:THR:HG21	2.43	0.54
1:A:157:ARG:HH11	1:A:157:ARG:HG2	1.72	0.54
1:A:178:ILE:HG21	1:A:295:PHE:HA	1.88	0.54
1:B:112:ILE:CD1	1:B:124:ARG:HA	2.37	0.54
1:D:134:PHE:HD2	1:D:134:PHE:O	1.89	0.54
1:F:400:GLU:OE2	1:F:400:GLU:HA	2.07	0.54
1:H:297:ALA:O	1:H:301:THR:HG22	2.07	0.54
1:C:110:PHE:HD1	1:C:119:LYS:HZ3	1.51	0.54
1:C:469:THR:OG1	1:C:470:THR:N	2.40	0.54
1:D:280:SER:C	1:D:282:PHE:H	2.10	0.54
1:E:225:TYR:CD1	4:E:501:CM5:O22	2.59	0.54
4:F:501:CM5:H29	4:F:501:CM5:C30	2.35	0.54
1:A:301:THR:HG21	2:A:501:HEM:C4B	2.43	0.54
1:C:278:GLN:CB	1:C:279:PRO:CD	2.85	0.54
1:D:110:PHE:HB2	1:D:289:ASN:HD22	1.71	0.54
1:E:308:TYR:CE1	1:E:480:PRO:HB3	2.42	0.54
1:G:414:ASP:OD1	1:G:418:ASN:HB2	2.08	0.54
1:B:78:HIS:O	1:B:393:SER:OG	2.22	0.54
1:E:183:PHE:HB3	1:E:264:ILE:HD12	1.90	0.54
3:E:503:LSN:C14	3:E:503:LSN:C1	2.86	0.54
1:B:108:ARG:NH2	3:B:502:LSN:N6	2.53	0.54
1:C:163:PRO:HB3	1:C:461:LEU:HD21	1.89	0.54
1:D:227:PRO:HG3	4:H:501:CM5:H112	1.89	0.54
1:E:277:ASN:ND2	1:E:279:PRO:HG2	2.23	0.54
4:G:501:CM5:C30	4:G:501:CM5:H29	2.37	0.54
1:C:32:GLY:CA	1:C:61:TYR:CD2	2.91	0.54
1:C:301:THR:HG21	2:C:501:HEM:C4B	2.43	0.54
4:H:501:CM5:H191	4:H:501:CM5:H32	1.72	0.54
1:A:460:SER:OG	1:A:462:VAL:O	2.25	0.53
1:F:256:ASP:O	1:F:257:MET:HB2	2.07	0.53
2:A:501:HEM:HHA	2:A:501:HEM:HBD1	1.90	0.53
1:A:113:VAL:HG22	2:A:501:HEM:HAD2	1.89	0.53
1:B:288:GLU:O	1:B:292:VAL:HG12	2.08	0.53
1:G:209:SER:HB2	1:G:473:VAL:HG23	1.89	0.53
4:G:501:CM5:C30	4:G:501:CM5:C29	2.85	0.53
1:A:102:LEU:HD11	1:A:213:ILE:HD12	1.91	0.53
1:A:307:ARG:O	1:A:483:TYR:OH	2.21	0.53
1:E:278:GLN:C	1:E:280:SER:H	2.11	0.53
1:H:256:ASP:OD1	1:H:259:ASN:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASP:OD1	1:A:418:ASN:HB2	2.07	0.53
1:C:403:ASN:N	1:C:404:PRO:HD3	2.22	0.53
4:H:504:CM5:O21	4:H:504:CM5:H29	2.08	0.53
2:F:502:HEM:HHD	2:F:502:HEM:CBC	2.23	0.53
1:G:464:PRO:O	1:G:467:LEU:HD12	2.09	0.53
1:H:225:TYR:CD1	4:H:501:CM5:O22	2.61	0.53
1:H:410:HIS:O	1:H:411:HIS:C	2.43	0.53
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.74	0.53
1:A:325:GLU:OE1	1:A:326:GLU:N	2.42	0.53
1:B:156:LEU:HD22	1:B:487:PHE:CE2	2.43	0.53
1:F:112:ILE:HG13	1:F:290:THR:HG23	1.90	0.53
1:F:207:ILE:O	1:F:210:SER:HB3	2.08	0.53
1:G:279:PRO:O	1:G:279:PRO:HG2	2.08	0.53
1:A:38:VAL:CG1	1:A:39:ILE:H	2.21	0.53
1:H:126:PHE:CZ	1:H:130:THR:HG21	2.44	0.53
1:E:201:LEU:HG	1:E:240:MET:CE	2.39	0.52
1:F:223:ILE:HG23	1:F:230:HIS:HD2	1.75	0.52
1:F:311:LEU:HD11	1:F:467:LEU:HD13	1.91	0.52
1:A:257:MET:C	1:A:259:ASN:H	2.13	0.52
1:H:85:GLU:O	1:H:90:LEU:HD12	2.09	0.52
1:C:366:LEU:HD13	2:C:501:HEM:HAA1	1.91	0.52
1:G:485:LEU:HD11	1:G:487:PHE:CZ	2.45	0.52
1:A:253:GLU:C	1:A:255:MET:H	2.13	0.52
1:B:115:SER:O	1:B:433:ARG:NH2	2.37	0.52
1:E:227:PRO:HB2	4:E:504:CM5:O22	2.10	0.52
1:E:301:THR:HG21	2:E:502:HEM:CHC	2.39	0.52
1:F:38:VAL:HG23	1:F:39:ILE:HG23	1.91	0.52
1:F:255:MET:CE	1:F:257:MET:SD	2.98	0.52
1:F:403:ASN:N	1:F:404:PRO:HD3	2.25	0.52
4:H:501:CM5:O32	4:H:501:CM5:O23	2.28	0.52
1:C:120:TRP:HZ2	1:C:124:ARG:NH1	2.04	0.52
1:F:28:LYS:HD2	1:F:380:LEU:HD13	1.92	0.52
1:G:281:GLU:HB3	1:G:282:PHE:CD1	2.45	0.52
1:A:166:PRO:HB2	1:A:170:LEU:HD22	1.91	0.52
1:B:156:LEU:HD22	1:B:487:PHE:CD2	2.44	0.52
1:F:178:ILE:HD11	1:F:299:THR:OG1	2.10	0.52
1:G:166:PRO:HB2	1:G:170:LEU:HD22	1.92	0.52
1:H:314:LEU:HD11	1:H:485:LEU:HB3	1.90	0.52
1:A:334:ASN:OD1	1:A:334:ASN:C	2.46	0.52
1:A:183:PHE:HB3	1:A:264:ILE:HD12	1.91	0.52
1:E:308:TYR:CD1	1:E:480:PRO:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:SER:O	1:A:393:SER:OG	2.28	0.51
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.91	0.51
1:B:461:LEU:HD12	1:B:484:GLN:HB2	1.92	0.51
1:D:157:ARG:HH11	1:D:157:ARG:CG	2.23	0.51
1:C:244:ILE:O	1:C:248:VAL:HG23	2.10	0.51
1:D:390:SER:O	1:D:393:SER:OG	2.24	0.51
1:H:225:TYR:CG	4:H:501:CM5:O22	2.62	0.51
1:A:41:ASN:O	1:A:45:ILE:HG13	2.09	0.51
1:A:208:LEU:HD21	1:A:233:LEU:CD1	2.39	0.51
1:D:294:LEU:HD22	2:D:501:HEM:HBC1	1.91	0.51
1:E:435:CYS:HB2	2:E:502:HEM:NA	2.25	0.51
1:C:380:LEU:O	1:C:380:LEU:CG	2.55	0.51
1:D:205:ILE:CD1	3:D:502:LSN:N2	2.74	0.51
1:D:279:PRO:HG2	1:D:280:SER:H	1.75	0.51
1:F:170:LEU:HD21	1:F:310:LEU:HD12	1.93	0.51
1:G:464:PRO:O	1:G:467:LEU:HD11	2.08	0.51
1:A:283:THR:CG2	1:A:284:ILE:N	2.72	0.51
2:A:501:HEM:HMB2	2:A:501:HEM:CBB	2.32	0.51
2:B:501:HEM:HBC2	2:B:501:HEM:CHD	2.30	0.51
1:E:280:SER:OG	1:E:281:GLU:N	2.42	0.51
1:C:173:ALA:HB3	1:C:174:PRO:HD3	1.92	0.51
2:C:501:HEM:CBD	2:C:501:HEM:HHA	2.41	0.51
1:E:280:SER:OG	1:E:283:THR:CG2	2.59	0.51
1:A:208:LEU:CD2	1:A:233:LEU:HD11	2.41	0.51
1:B:139:ARG:HH21	1:B:144:CYS:HA	1.75	0.51
1:C:80:TYR:OH	1:C:84:LYS:HD3	2.10	0.51
1:C:271:MET:HG2	1:C:282:PHE:O	2.10	0.51
2:A:501:HEM:HHD	2:A:501:HEM:CBC	2.23	0.51
1:C:309:ALA:O	1:C:310:LEU:C	2.49	0.51
1:D:173:ALA:HB3	1:D:174:PRO:HD3	1.93	0.51
1:D:297:ALA:O	1:D:301:THR:HG22	2.11	0.51
1:H:402:PRO:O	1:H:404:PRO:N	2.44	0.51
1:F:163:PRO:HB3	1:F:461:LEU:HD21	1.92	0.51
1:G:134:PHE:CE1	1:G:139:ARG:HB3	2.45	0.51
1:H:194:PHE:CE1	1:H:198:MET:HB2	2.46	0.51
1:B:428:PHE:HB3	1:B:435:CYS:HB2	1.94	0.50
1:C:126:PHE:O	1:C:130:THR:HG23	2.11	0.50
1:E:231:ASN:CB	4:E:504:CM5:O34	2.59	0.50
1:G:306:LEU:O	1:G:309:ALA:CB	2.54	0.50
1:D:252:GLN:O	1:D:253:GLU:CB	2.58	0.50
1:A:108:ARG:NH2	1:A:292:VAL:HG13	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:O	1:A:130:THR:HG23	2.10	0.50
1:F:220:SER:N	1:F:221:PRO:HD2	2.27	0.50
1:A:60:VAL:HG22	1:A:61:TYR:H	1.76	0.50
1:A:297:ALA:O	1:A:301:THR:HG22	2.11	0.50
2:C:501:HEM:HHA	2:C:501:HEM:HBD1	1.93	0.50
1:E:403:ASN:H	1:E:404:PRO:HD3	1.76	0.50
1:F:178:ILE:CD1	1:F:299:THR:OG1	2.60	0.50
1:F:253:GLU:O	1:F:254:SER:CB	2.59	0.50
1:A:111:GLY:O	1:A:115:SER:HB3	2.12	0.50
1:F:156:LEU:HD22	1:F:487:PHE:CE2	2.47	0.50
1:G:301:THR:HG21	2:G:502:HEM:C4B	2.47	0.50
1:H:361:LEU:C	1:H:362:LEU:HD12	2.32	0.50
1:B:316:HIS:ND1	1:B:316:HIS:N	2.60	0.50
1:C:175:CYS:HB2	1:C:299:THR:HG23	1.93	0.50
1:B:301:THR:HG21	2:B:501:HEM:C4B	2.47	0.50
1:C:278:GLN:CB	1:C:279:PRO:HD3	2.41	0.50
1:G:281:GLU:C	1:G:282:PHE:HD1	2.15	0.50
1:A:398:ASN:OD1	1:A:398:ASN:O	2.30	0.50
2:C:501:HEM:HBC2	2:C:501:HEM:CHD	2.12	0.50
1:D:50:ILE:HD11	1:D:214:GLN:HG2	1.92	0.50
1:F:231:ASN:HB2	4:F:504:CM5:H29	1.94	0.50
1:F:255:MET:HE2	1:F:269:MET:HG3	1.93	0.50
1:F:289:ASN:HA	1:F:292:VAL:HG12	1.94	0.50
1:A:157:ARG:CG	1:A:157:ARG:NH1	2.73	0.50
1:B:187:PHE:CD2	1:B:194:PHE:HB2	2.47	0.50
1:F:166:PRO:O	1:F:170:LEU:HB2	2.11	0.50
1:H:163:PRO:HB3	1:H:461:LEU:HD23	1.94	0.50
2:H:502:HEM:HBB2	2:H:502:HEM:CMB	2.41	0.50
1:A:208:LEU:CD2	1:A:233:LEU:CD1	2.90	0.49
1:G:282:PHE:CD1	1:G:282:PHE:N	2.80	0.49
1:G:334:ASN:HB3	6:G:608:HOH:O	2.11	0.49
1:H:314:LEU:HD11	1:H:485:LEU:HD22	1.94	0.49
1:B:403:ASN:N	1:B:404:PRO:HD3	2.28	0.49
2:C:501:HEM:HHD	2:C:501:HEM:CBC	2.21	0.49
1:D:277:ASN:O	1:D:278:GLN:CB	2.60	0.49
1:B:319:VAL:HG12	1:B:347:TYR:OH	2.12	0.49
1:C:178:ILE:HG21	1:C:295:PHE:HA	1.94	0.49
1:C:390:SER:O	1:C:393:SER:OG	2.30	0.49
1:D:280:SER:O	1:D:281:GLU:CB	2.59	0.49
3:H:503:LSN:C14	3:H:503:LSN:C1	2.89	0.49
1:G:112:ILE:HG13	1:G:290:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:TYR:OH	1:D:84:LYS:HD3	2.11	0.49
1:E:311:LEU:HD11	1:E:467:LEU:HD13	1.94	0.49
2:G:502:HEM:HHA	2:G:502:HEM:CBD	2.40	0.49
1:E:490:ILE:HG23	1:E:490:ILE:O	2.12	0.49
3:G:503:LSN:C14	3:G:503:LSN:C1	2.90	0.49
1:G:231:ASN:CB	4:G:504:CM5:O34	2.61	0.49
1:H:314:LEU:HD11	1:H:485:LEU:HD23	1.94	0.49
1:A:332:GLY:HA3	6:A:602:HOH:O	2.12	0.49
1:B:362:LEU:HD12	2:B:501:HEM:HMA2	1.94	0.49
1:H:35:PRO:CA	1:H:41:ASN:HD21	2.26	0.49
1:H:297:ALA:O	1:H:301:THR:CG2	2.61	0.49
1:A:308:TYR:CE1	1:A:480:PRO:HB3	2.47	0.49
1:E:488:ILE:O	1:E:488:ILE:HG13	2.13	0.49
1:B:491:HIS:O	1:B:491:HIS:ND1	2.46	0.48
1:F:36:LEU:HD12	1:F:39:ILE:HD11	1.95	0.48
1:G:139:ARG:O	1:G:140:SER:CB	2.60	0.48
1:A:354:GLU:HA	1:A:354:GLU:OE1	2.14	0.48
1:A:467:LEU:HD12	1:A:467:LEU:O	2.13	0.48
1:D:333:ARG:NH1	1:D:491:HIS:HA	2.29	0.48
1:F:333:ARG:O	1:F:334:ASN:OD1	2.31	0.48
1:B:221:PRO:O	1:B:222:ILE:C	2.50	0.48
2:B:501:HEM:HHD	2:B:501:HEM:CBC	2.37	0.48
1:E:133:ASN:OD1	1:E:134:PHE:N	2.46	0.48
1:E:455:ASN:C	1:E:490:ILE:HG22	2.34	0.48
1:F:178:ILE:CD1	1:F:295:PHE:O	2.61	0.48
1:A:461:LEU:O	1:A:462:VAL:HG23	2.14	0.48
1:F:455:ASN:C	1:F:490:ILE:HG22	2.33	0.48
1:G:255:MET:O	1:G:256:ASP:HB3	2.14	0.48
1:C:401:PHE:O	1:C:404:PRO:HG3	2.13	0.48
1:E:60:VAL:HG22	1:E:61:TYR:CD1	2.49	0.48
1:E:201:LEU:HG	1:E:240:MET:HE1	1.95	0.48
1:E:208:LEU:HD21	1:E:233:LEU:HD21	1.96	0.48
1:F:365:SER:HB2	1:F:391:LEU:HD11	1.96	0.48
1:H:457:ASN:HB2	1:H:488:ILE:CD1	2.43	0.48
1:D:145:VAL:HG11	1:D:447:LEU:HD12	1.95	0.48
1:C:108:ARG:HB3	1:C:108:ARG:CZ	2.44	0.48
1:F:83:VAL:HG22	1:F:389:ILE:HG23	1.95	0.48
1:F:300:GLU:HB3	3:F:503:LSN:N3	2.28	0.48
1:G:267:PHE:CE1	1:G:287:LEU:HB2	2.49	0.48
1:H:231:ASN:HB2	4:H:504:CM5:O34	2.11	0.48
1:A:38:VAL:CG1	1:A:39:ILE:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:HD13	1:A:386:THR:HB	1.95	0.47
1:B:255:MET:O	1:B:256:ASP:CB	2.62	0.47
1:B:278:GLN:CB	1:D:253:GLU:H	2.27	0.47
1:B:297:ALA:O	1:B:301:THR:HG22	2.14	0.47
1:G:140:SER:O	1:G:140:SER:OG	2.32	0.47
1:H:318:GLU:O	1:H:321:ALA:HB3	2.15	0.47
1:D:60:VAL:HG22	1:D:61:TYR:CD1	2.49	0.47
1:E:225:TYR:CG	4:E:501:CM5:O22	2.68	0.47
1:E:376:PHE:O	1:E:378:ASN:N	2.46	0.47
1:F:435:CYS:O	1:F:436:VAL:C	2.52	0.47
1:E:402:PRO:O	1:E:403:ASN:HB2	2.14	0.47
1:A:403:ASN:N	1:A:404:PRO:CD	2.76	0.47
1:B:49:ASP:OD2	1:B:52:LYS:HB2	2.15	0.47
1:D:183:PHE:O	1:D:185:LYS:N	2.47	0.47
1:H:249:LYS:HE3	1:H:252:GLN:OE1	2.14	0.47
1:E:201:LEU:HD23	1:E:240:MET:HE3	1.96	0.47
1:A:187:PHE:CD2	1:A:194:PHE:HB2	2.49	0.47
1:A:227:PRO:HB3	1:E:226:PHE:CD2	2.50	0.47
1:C:315:LYS:NZ	1:C:464:PRO:O	2.48	0.47
1:C:401:PHE:O	1:C:402:PRO:C	2.50	0.47
1:D:205:ILE:HD12	3:D:502:LSN:N2	2.29	0.47
1:E:308:TYR:O	1:E:312:LEU:HD12	2.15	0.47
1:B:170:LEU:HD11	1:B:310:LEU:CD1	2.45	0.47
1:B:247:LYS:CD	1:B:250:GLU:OE2	2.55	0.47
1:C:36:LEU:HB3	1:C:37:PRO:HD2	1.97	0.47
1:D:204:ASN:O	1:D:208:LEU:HG	2.15	0.47
1:D:279:PRO:CG	1:D:280:SER:H	2.28	0.47
1:D:301:THR:HG21	2:D:501:HEM:C4B	2.48	0.47
2:E:502:HEM:HHA	2:E:502:HEM:HBD1	1.97	0.47
1:H:410:HIS:O	1:H:412:PHE:N	2.48	0.47
1:A:400:GLU:HG2	1:A:424:TYR:HB2	1.97	0.47
1:B:175:CYS:HB2	1:B:299:THR:HG23	1.95	0.47
1:E:280:SER:O	1:E:281:GLU:HB2	2.14	0.47
1:A:461:LEU:HD21	1:A:484:GLN:CB	2.45	0.47
1:B:301:THR:HG21	2:B:501:HEM:CHC	2.45	0.47
1:H:60:VAL:HG22	1:H:61:TYR:CD1	2.50	0.47
1:G:99:ILE:HD11	1:G:114:PHE:HB3	1.97	0.47
1:G:455:ASN:O	1:G:490:ILE:HG12	2.15	0.47
1:H:150:ARG:NH1	1:H:336:SER:OG	2.48	0.47
1:H:472:VAL:HG12	1:H:479:VAL:HG22	1.96	0.47
1:A:60:VAL:CG2	1:A:61:TYR:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PRO:HG3	4:E:504:CM5:H21A	1.96	0.46
2:B:501:HEM:HBD1	2:B:501:HEM:HHA	1.97	0.46
1:D:314:LEU:HD11	1:D:485:LEU:HD23	1.97	0.46
3:D:502:LSN:C14	3:D:502:LSN:C1	2.93	0.46
1:B:251:HIS:C	1:B:253:GLU:H	2.18	0.46
1:B:125:ARG:NH2	1:H:253:GLU:OE1	2.47	0.46
1:B:483:TYR:HE1	1:B:485:LEU:HD23	1.79	0.46
1:F:311:LEU:CD1	1:F:467:LEU:CD1	2.93	0.46
1:F:461:LEU:O	1:F:461:LEU:CD1	2.60	0.46
4:F:501:CM5:O21	4:F:501:CM5:H24	2.15	0.46
1:E:297:ALA:O	1:E:301:THR:HG22	2.14	0.46
1:G:119:LYS:O	1:G:123:ILE:HG13	2.15	0.46
1:H:390:SER:O	1:H:393:SER:OG	2.33	0.46
1:A:335:ARG:NH2	1:A:341:ASP:OD1	2.48	0.46
1:C:183:PHE:O	1:C:184:HIS:CB	2.63	0.46
1:C:280:SER:HA	6:C:607:HOH:O	2.15	0.46
1:A:253:GLU:C	1:A:255:MET:N	2.69	0.46
1:F:28:LYS:O	1:F:379:TYR:O	2.34	0.46
4:F:504:CM5:H24	4:F:504:CM5:O21	2.16	0.46
1:F:36:LEU:HB3	1:F:37:PRO:CD	2.45	0.46
1:G:307:ARG:HG3	1:G:483:TYR:OH	2.16	0.46
1:G:314:LEU:HD11	1:G:485:LEU:HD23	1.97	0.46
1:H:110:PHE:N	1:H:110:PHE:CD2	2.82	0.46
1:A:57:LEU:O	1:A:60:VAL:HG22	2.15	0.46
1:E:93:GLU:HB3	1:E:374:ILE:HD12	1.98	0.46
1:G:225:TYR:CE1	4:G:501:CM5:C18	2.98	0.46
1:A:170:LEU:HD21	1:A:310:LEU:CD1	2.46	0.46
1:D:225:TYR:O	4:H:504:CM5:H6	2.16	0.46
2:D:501:HEM:HHD	2:D:501:HEM:CBC	2.38	0.46
2:E:502:HEM:HBC2	2:E:502:HEM:CHD	2.17	0.46
1:F:372:CYS:HA	1:F:383:LYS:HD3	1.98	0.46
1:C:110:PHE:CD1	1:C:119:LYS:NZ	2.76	0.45
1:C:110:PHE:O	1:C:289:ASN:HB3	2.16	0.45
1:D:428:PHE:O	1:D:429:SER:HB3	2.16	0.45
1:F:155:GLU:HG3	1:F:189:TYR:CD2	2.51	0.45
1:G:281:GLU:C	1:G:282:PHE:CD1	2.90	0.45
1:A:108:ARG:HH11	1:A:108:ARG:CG	2.29	0.45
1:D:314:LEU:HD11	1:D:485:LEU:HB3	1.98	0.45
1:E:403:ASN:N	1:E:404:PRO:CD	2.79	0.45
3:F:503:LSN:C14	3:F:503:LSN:C1	2.94	0.45
1:H:113:VAL:HG22	2:H:502:HEM:CAD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HG3	4:E:501:CM5:H112	1.98	0.45
1:A:233:LEU:C	1:A:233:LEU:HD23	2.36	0.45
1:C:306:LEU:O	1:C:309:ALA:HB3	2.16	0.45
2:E:502:HEM:HHA	2:E:502:HEM:HBA2	1.97	0.45
1:F:280:SER:O	1:F:281:GLU:CB	2.65	0.45
1:H:416:GLY:O	1:H:418:ASN:N	2.49	0.45
1:H:483:TYR:HE1	1:H:485:LEU:HD23	1.81	0.45
1:E:264:ILE:HG23	1:E:287:LEU:HD21	1.99	0.45
1:G:170:LEU:HD21	1:G:310:LEU:CD1	2.44	0.45
1:G:307:ARG:HH11	1:G:480:PRO:HG2	1.81	0.45
1:A:122:GLU:HG3	1:A:281:GLU:HG2	1.99	0.45
1:B:106:ALA:O	1:B:107:ASN:CB	2.64	0.45
1:C:122:GLU:OE1	1:C:281:GLU:CG	2.54	0.45
1:C:250:GLU:HG2	1:C:251:HIS:N	2.32	0.45
1:E:289:ASN:HA	1:E:292:VAL:HG12	1.99	0.45
1:G:220:SER:N	1:G:221:PRO:HD2	2.32	0.45
1:H:108:ARG:HD2	1:H:241:LYS:HE2	1.97	0.45
1:D:461:LEU:HD23	1:D:461:LEU:H	1.81	0.45
1:H:306:LEU:O	1:H:309:ALA:HB3	2.17	0.45
1:A:257:MET:C	1:A:259:ASN:N	2.70	0.44
1:D:157:ARG:CG	1:D:157:ARG:NH1	2.80	0.44
1:D:270:LYS:O	1:D:274:GLU:CG	2.65	0.44
1:G:194:PHE:CE1	1:G:198:MET:HB2	2.51	0.44
1:G:201:LEU:HD21	1:G:240:MET:SD	2.57	0.44
1:G:178:ILE:HD13	1:G:295:PHE:HA	1.99	0.44
1:H:264:ILE:HG23	1:H:287:LEU:HD21	1.99	0.44
1:A:108:ARG:NH2	1:A:293:ASP:OD1	2.50	0.44
1:A:327:ILE:O	1:A:331:ILE:O	2.36	0.44
1:A:156:LEU:HD22	1:A:487:PHE:CE2	2.52	0.44
1:F:183:PHE:HB3	1:F:264:ILE:HD13	2.00	0.44
1:F:194:PHE:CE1	1:F:198:MET:HB2	2.53	0.44
1:A:110:PHE:HB2	1:A:289:ASN:ND2	2.28	0.44
1:B:78:HIS:O	1:B:393:SER:CB	2.65	0.44
4:G:501:CM5:H24	4:G:501:CM5:H301	1.91	0.44
1:H:288:GLU:O	1:H:292:VAL:HG13	2.17	0.44
1:D:80:TYR:CZ	1:D:84:LYS:HD3	2.52	0.44
1:D:272:GLU:C	1:D:274:GLU:N	2.70	0.44
1:F:437:GLY:O	1:F:438:GLU:C	2.56	0.44
1:G:183:PHE:HB3	1:G:264:ILE:HD12	1.99	0.44
1:H:35:PRO:CA	1:H:41:ASN:ND2	2.80	0.44
1:H:278:GLN:CB	1:H:279:PRO:CD	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PHE:O	1:C:289:ASN:HB2	2.18	0.44
1:E:38:VAL:HG13	1:E:39:ILE:HG23	1.99	0.44
1:E:110:PHE:CD2	1:E:110:PHE:N	2.85	0.44
1:G:209:SER:CB	1:G:473:VAL:HG23	2.47	0.44
1:G:277:ASN:C	1:G:279:PRO:CD	2.85	0.44
1:A:227:PRO:HG3	4:E:501:CM5:C11	2.48	0.44
1:C:32:GLY:C	1:C:61:TYR:CE2	2.91	0.44
1:D:145:VAL:CG1	1:D:447:LEU:HD12	2.48	0.44
2:D:501:HEM:HHA	2:D:501:HEM:CBD	2.48	0.44
1:B:277:ASN:OD1	1:B:279:PRO:O	2.35	0.44
1:D:400:GLU:HG2	1:D:424:TYR:HB2	2.00	0.44
1:G:276:HIS:O	1:G:277:ASN:C	2.56	0.44
1:A:170:LEU:HD21	1:A:310:LEU:HD12	2.00	0.43
1:A:227:PRO:CG	4:E:501:CM5:H112	2.48	0.43
1:B:380:LEU:O	1:B:380:LEU:CG	2.61	0.43
1:C:93:GLU:HG2	1:C:374:ILE:HD13	2.00	0.43
1:D:244:ILE:CG1	1:D:292:VAL:HG22	2.38	0.43
1:G:156:LEU:HD22	1:G:487:PHE:CE2	2.53	0.43
1:B:124:ARG:NH1	1:B:436:VAL:HG23	2.33	0.43
1:C:374:ILE:O	1:C:380:LEU:HA	2.17	0.43
1:D:157:ARG:HH11	1:D:157:ARG:HG2	1.82	0.43
1:D:270:LYS:O	1:D:274:GLU:HG2	2.18	0.43
1:F:182:ILE:O	1:F:264:ILE:HD12	2.17	0.43
1:A:99:ILE:HG22	1:A:100:PHE:O	2.19	0.43
1:C:84:LYS:HG3	1:C:88:ILE:CG1	2.48	0.43
1:A:240:MET:HE3	3:A:502:LSN:CL	2.55	0.43
1:B:32:GLY:HA2	1:B:61:TYR:CD2	2.54	0.43
1:B:302:THR:HG21	1:B:444:GLU:OE1	2.17	0.43
1:E:113:VAL:HG22	2:E:502:HEM:CAD	2.49	0.43
1:A:174:PRO:C	1:A:178:ILE:HD12	2.38	0.43
1:C:171:GLY:HA2	1:C:303:SER:CB	2.48	0.43
1:D:102:LEU:HD11	1:D:213:ILE:HD12	1.99	0.43
1:E:364:THR:O	1:E:364:THR:HG22	2.18	0.43
1:D:311:LEU:HD13	1:D:483:TYR:CD2	2.54	0.43
1:C:301:THR:HG21	2:C:501:HEM:CHC	2.49	0.43
4:E:501:CM5:O23	4:E:501:CM5:O32	2.32	0.43
1:F:78:HIS:O	1:F:393:SER:CB	2.66	0.43
1:F:472:VAL:HG12	1:F:479:VAL:HG13	2.01	0.43
1:G:85:GLU:O	1:G:90:LEU:HD13	2.19	0.43
1:G:403:ASN:N	1:G:404:PRO:CD	2.80	0.43
1:H:113:VAL:HG22	2:H:502:HEM:HAD1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:308:TYR:CE1	1:H:480:PRO:HB3	2.54	0.43
1:E:323:VAL:O	1:E:327:ILE:HG13	2.19	0.43
1:A:178:ILE:HD11	1:A:298:GLY:C	2.38	0.43
1:D:134:PHE:O	1:D:134:PHE:CD2	2.71	0.43
1:E:145:VAL:HG11	1:E:447:LEU:HD12	2.00	0.43
1:H:472:VAL:CG1	1:H:479:VAL:HG22	2.47	0.43
2:E:502:HEM:HHD	2:E:502:HEM:CBC	2.28	0.42
1:B:390:SER:O	1:B:393:SER:OG	2.37	0.42
1:B:460:SER:OG	1:B:467:LEU:CD2	2.67	0.42
1:D:403:ASN:N	1:D:404:PRO:HD3	2.33	0.42
1:D:461:LEU:HD21	1:D:484:GLN:CB	2.47	0.42
1:E:354:GLU:OE1	1:E:354:GLU:HA	2.19	0.42
1:G:102:LEU:HD11	1:G:213:ILE:HD12	2.00	0.42
1:G:308:TYR:CD1	1:G:480:PRO:HB3	2.55	0.42
1:B:250:GLU:O	1:B:254:SER:OG	2.38	0.42
1:B:308:TYR:CD1	1:B:480:PRO:HB3	2.54	0.42
1:C:132:ARG:O	1:C:133:ASN:CG	2.57	0.42
1:F:156:LEU:HD22	1:F:487:PHE:CD2	2.54	0.42
1:H:79:GLY:O	1:H:83:VAL:HG23	2.19	0.42
1:E:142:GLU:O	1:E:146:GLN:HB2	2.19	0.42
1:F:267:PHE:CE1	1:F:287:LEU:HB2	2.54	0.42
1:G:277:ASN:O	1:G:279:PRO:HD2	2.19	0.42
1:H:434:ILE:O	1:H:435:CYS:C	2.56	0.42
1:G:255:MET:CE	1:G:269:MET:HG3	2.50	0.42
1:H:462:VAL:HG12	1:H:463:ASP:N	2.35	0.42
1:C:156:LEU:HD22	1:C:487:PHE:CD2	2.55	0.42
1:G:38:VAL:HG13	1:G:39:ILE:HG23	2.02	0.42
1:G:134:PHE:CE1	1:G:139:ARG:CB	3.03	0.42
1:H:400:GLU:OE1	1:H:422:SER:OG	2.23	0.42
1:A:462:VAL:O	1:A:463:ASP:C	2.57	0.42
1:D:247:LYS:H	1:D:247:LYS:HG2	1.69	0.42
1:D:333:ARG:HH12	1:D:491:HIS:HA	1.83	0.42
1:A:256:ASP:OD2	1:A:259:ASN:HB3	2.19	0.42
1:A:272:GLU:C	1:A:274:GLU:H	2.22	0.42
1:F:435:CYS:O	1:F:437:GLY:N	2.52	0.42
1:G:85:GLU:O	1:G:85:GLU:HG2	2.19	0.42
1:H:365:SER:OG	1:H:366:LEU:N	2.52	0.42
1:B:184:HIS:HB2	1:B:262:ASP:HB3	2.02	0.41
1:B:247:LYS:HA	1:B:250:GLU:OE2	2.19	0.41
1:C:289:ASN:HA	1:C:292:VAL:HG12	2.02	0.41
1:D:357:ARG:NH1	1:D:404:PRO:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:LEU:CD2	1:E:240:MET:HE3	2.50	0.41
1:E:236:ASN:O	1:E:240:MET:HG2	2.20	0.41
1:F:281:GLU:OE1	1:F:281:GLU:CA	2.68	0.41
1:G:268:LEU:HA	1:G:271:MET:HG3	2.01	0.41
1:E:277:ASN:HD21	1:E:279:PRO:HG2	1.83	0.41
1:A:101:PRO:O	1:A:102:LEU:C	2.58	0.41
1:B:253:GLU:C	1:B:255:MET:N	2.73	0.41
1:F:249:LYS:HA	1:F:252:GLN:HE21	1.84	0.41
1:B:106:ALA:O	1:B:107:ASN:HB2	2.21	0.41
1:B:280:SER:OG	1:B:281:GLU:N	2.53	0.41
1:C:61:TYR:N	1:C:61:TYR:HD1	2.17	0.41
1:C:480:PRO:HA	1:C:481:PRO:HD3	1.95	0.41
1:D:220:SER:N	1:D:221:PRO:HD2	2.36	0.41
1:E:278:GLN:C	1:E:280:SER:N	2.73	0.41
1:G:57:LEU:HD13	1:G:67:LEU:HD21	2.03	0.41
1:G:300:GLU:HB3	3:G:503:LSN:N3	2.35	0.41
1:H:118:LYS:O	1:H:121:LYS:N	2.52	0.41
1:H:191:ASP:OD1	1:H:192:GLN:N	2.53	0.41
1:A:335:ARG:NH2	1:A:341:ASP:OD2	2.54	0.41
1:C:32:GLY:CA	1:C:61:TYR:CE2	3.04	0.41
1:H:225:TYR:CZ	4:H:501:CM5:O21	2.59	0.41
1:A:108:ARG:CD	1:A:241:LYS:HE2	2.35	0.41
1:A:108:ARG:NH1	3:A:502:LSN:N6	2.69	0.41
1:B:325:GLU:O	1:B:326:GLU:C	2.59	0.41
1:B:485:LEU:C	1:B:485:LEU:HD12	2.41	0.41
1:D:454:GLN:O	1:D:490:ILE:HD12	2.19	0.41
1:E:145:VAL:CG1	1:E:447:LEU:HD12	2.51	0.41
1:E:364:THR:O	1:E:364:THR:CG2	2.69	0.41
1:F:108:ARG:NH2	1:F:293:ASP:OD1	2.54	0.41
1:G:464:PRO:CA	1:G:467:LEU:HD11	2.40	0.41
1:H:320:THR:O	1:H:324:GLN:HG3	2.21	0.41
1:A:381:ILE:CG2	1:A:385:THR:HB	2.51	0.41
1:B:108:ARG:O	1:B:110:PHE:N	2.54	0.41
1:D:283:THR:OG1	1:D:286:SER:N	2.49	0.41
1:H:118:LYS:O	1:H:119:LYS:C	2.58	0.41
1:A:75:VAL:HG21	1:A:381:ILE:HG12	2.03	0.41
1:A:472:VAL:HG12	1:A:479:VAL:HG22	2.03	0.41
1:B:166:PRO:HB2	1:B:170:LEU:HD12	2.03	0.41
1:D:205:ILE:HD12	3:D:502:LSN:N3	2.36	0.41
1:E:113:VAL:HG22	2:E:502:HEM:HAD1	2.03	0.41
1:E:277:ASN:O	1:E:278:GLN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:SER:O	1:E:281:GLU:CB	2.68	0.41
1:G:84:LYS:HG3	1:G:88:ILE:HD12	2.03	0.41
1:G:156:LEU:HD22	1:G:487:PHE:CD2	2.55	0.41
1:G:201:LEU:CD2	1:G:240:MET:SD	3.09	0.41
1:G:282:PHE:O	1:G:283:THR:O	2.39	0.41
1:G:308:TYR:CE1	1:G:480:PRO:HB3	2.55	0.41
1:F:33:PRO:HB2	1:F:41:ASN:ND2	2.36	0.41
1:H:159:THR:O	1:H:160:LYS:C	2.59	0.41
1:C:354:GLU:HG3	1:C:407:PHE:CD1	2.56	0.40
1:E:322:LYS:HE3	1:E:347:TYR:CZ	2.56	0.40
1:E:372:CYS:HA	1:E:383:LYS:HD3	2.03	0.40
1:G:155:GLU:HG3	1:G:189:TYR:CG	2.57	0.40
1:H:102:LEU:HD13	1:H:233:LEU:HD23	2.03	0.40
1:H:131:LEU:HD23	1:H:131:LEU:O	2.22	0.40
1:A:461:LEU:O	1:A:462:VAL:CG2	2.69	0.40
1:B:207:ILE:O	1:B:210:SER:HB3	2.21	0.40
1:C:39:ILE:HG22	1:C:219:PHE:CZ	2.56	0.40
1:C:61:TYR:HD1	1:C:61:TYR:H	1.69	0.40
1:C:113:VAL:HG22	2:C:501:HEM:CAD	2.50	0.40
1:A:84:LYS:HG3	1:A:88:ILE:HD12	2.02	0.40
1:D:142:GLU:HB2	1:D:443:MET:HE1	2.03	0.40
3:D:502:LSN:C14	3:D:502:LSN:N4	2.84	0.40
1:E:225:TYR:CZ	4:E:501:CM5:O21	2.72	0.40
1:A:108:ARG:O	1:A:114:PHE:CB	2.58	0.40
1:A:253:GLU:O	1:A:255:MET:N	2.45	0.40
1:B:304:THR:HG21	1:B:361:LEU:HD11	2.03	0.40
1:H:80:TYR:OH	1:H:84:LYS:HD2	2.20	0.40
1:A:280:SER:OG	1:A:281:GLU:N	2.54	0.40
1:A:355:VAL:O	1:A:359:ILE:HG12	2.21	0.40
1:F:85:GLU:O	1:F:90:LEU:HD13	2.21	0.40
1:H:220:SER:N	1:H:221:PRO:HD2	2.36	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	457/476 (96%)	386 (84%)	62 (14%)	9 (2%)	7	30
1	B	457/476 (96%)	396 (87%)	52 (11%)	9 (2%)	7	30
1	C	456/476 (96%)	409 (90%)	40 (9%)	7 (2%)	10	38
1	D	457/476 (96%)	403 (88%)	42 (9%)	12 (3%)	5	25
1	E	456/476 (96%)	397 (87%)	44 (10%)	15 (3%)	4	20
1	F	456/476 (96%)	391 (86%)	53 (12%)	12 (3%)	5	25
1	G	458/476 (96%)	398 (87%)	50 (11%)	10 (2%)	6	28
1	H	455/476 (96%)	396 (87%)	46 (10%)	13 (3%)	4	23
All	All	3652/3808 (96%)	3176 (87%)	389 (11%)	87 (2%)	6	26

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	280	SER
1	B	255	MET
1	B	278	GLN
1	C	278	GLN
1	C	279	PRO
1	C	280	SER
1	D	112	ILE
1	D	278	GLN
1	D	279	PRO
1	D	280	SER
1	E	80	TYR
1	E	277	ASN
1	E	278	GLN
1	E	281	GLU
1	E	417	GLY
1	E	462	VAL
1	F	133	ASN
1	F	252	GLN
1	F	278	GLN
1	F	281	GLU
1	F	365	SER
1	G	277	ASN
1	G	278	GLN

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Mol	Chain	Res	Type
1	H	255	MET
1	H	278	GLN
1	H	402	PRO
1	H	415	GLU
1	H	417	GLY
1	A	70	GLY
1	A	135	GLY
1	A	255	MET
1	A	258	ASN
1	B	131	LEU
1	B	184	HIS
1	C	470	THR
1	D	111	GLY
1	D	417	GLY
1	E	91	GLY
1	E	254	SER
1	F	37	PRO
1	F	254	SER
1	F	377	ARG
1	F	435	CYS
1	G	255	MET
1	G	280	SER
1	H	365	SER
1	H	438	GLU
1	H	475	GLY
1	A	273	LYS
1	B	256	ASP
1	B	380	LEU
1	C	133	ASN
1	C	257	MET
1	C	380	LEU
1	D	184	HIS
1	D	253	GLU
1	D	380	LEU
1	D	429	SER
1	E	107	ASN
1	E	438	GLU
1	G	160	LYS
1	G	281	GLU
1	H	256	ASP
1	H	273	LYS
1	H	377	ARG

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Mol	Chain	Res	Type
1	E	276	HIS
1	E	280	SER
1	E	365	SER
1	F	462	VAL
1	G	283	THR
1	A	365	SER
1	D	365	SER
1	E	160	LYS
1	F	436	VAL
1	G	79	GLY
1	G	107	ASN
1	H	160	LYS
1	D	211	PRO
1	E	279	PRO
1	F	279	PRO
1	G	140	SER
1	B	417	GLY
1	B	464	PRO
1	A	260	PRO
1	B	109	GLY
1	H	31	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/429 (93%)	383 (96%)	17 (4%)	29	61
1	B	406/429 (95%)	386 (95%)	20 (5%)	25	57
1	C	402/429 (94%)	385 (96%)	17 (4%)	30	62
1	D	393/429 (92%)	378 (96%)	15 (4%)	33	65
1	E	392/429 (91%)	387 (99%)	5 (1%)	69	86
1	F	393/429 (92%)	385 (98%)	8 (2%)	55	79
1	G	390/429 (91%)	378 (97%)	12 (3%)	40	69
1	H	391/429 (91%)	383 (98%)	8 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3167/3432 (92%)	3065 (97%)	102 (3%)	39 69

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	55	THR
1	A	60	VAL
1	A	90	LEU
1	A	107	ASN
1	A	108	ARG
1	A	130	THR
1	A	141	ILE
1	A	157	ARG
1	A	183	PHE
1	A	184	HIS
1	A	254	SER
1	A	255	MET
1	A	308	TYR
1	A	335	ARG
1	A	377	ARG
1	A	436	VAL
1	B	55	THR
1	B	107	ASN
1	B	108	ARG
1	B	130	THR
1	B	131	LEU
1	B	164	CYS
1	B	186	ARG
1	B	197	LEU
1	B	221	PRO
1	B	240	MET
1	B	242	SER
1	B	254	SER
1	B	255	MET
1	B	257	MET
1	B	308	TYR
1	B	316	HIS
1	B	377	ARG
1	B	402	PRO
1	B	436	VAL
1	B	479	VAL

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Mol	Chain	Res	Type
1	C	34	THR
1	C	57	LEU
1	C	61	TYR
1	C	90	LEU
1	C	108	ARG
1	C	130	THR
1	C	183	PHE
1	C	185	LYS
1	C	240	MET
1	C	250	GLU
1	C	254	SER
1	C	279	PRO
1	C	280	SER
1	C	308	TYR
1	C	322	LYS
1	C	469	THR
1	C	485	LEU
1	D	28	LYS
1	D	55	THR
1	D	60	VAL
1	D	134	PHE
1	D	140	SER
1	D	157	ARG
1	D	183	PHE
1	D	184	HIS
1	D	205	ILE
1	D	240	MET
1	D	308	TYR
1	D	334	ASN
1	D	335	ARG
1	D	383	LYS
1	D	488	ILE
1	E	60	VAL
1	E	251	HIS
1	E	308	TYR
1	E	377	ARG
1	E	491	HIS
1	F	165	ASP
1	F	264	ILE
1	F	275	LYS
1	F	286	SER
1	F	308	TYR

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Mol	Chain	Res	Type
1	F	322	LYS
1	F	473	VAL
1	F	491	HIS
1	G	37	PRO
1	G	60	VAL
1	G	80	TYR
1	G	133	ASN
1	G	172	CYS
1	G	178	ILE
1	G	229	THR
1	G	281	GLU
1	G	308	TYR
1	G	335	ARG
1	G	467	LEU
1	G	472	VAL
1	H	34	THR
1	H	60	VAL
1	H	129	MET
1	H	141	ILE
1	H	308	TYR
1	H	366	LEU
1	H	402	PRO
1	H	467	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	202	ASN
1	A	418	ASN
1	F	230	HIS
1	F	231	ASN
1	G	41	ASN
1	G	252	GLN
1	G	344	HIS
1	H	41	ASN

5.3.3 RNA

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)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	LSN	C	502	-	30,33,33	0.64	0	34,45,45	1.36	3 (8%)
3	LSN	H	503	-	30,33,33	0.64	0	34,45,45	1.38	3 (8%)
4	CM5	E	504	-	36,36,36	0.14	0	49,49,49	0.21	0
3	LSN	A	502	-	30,33,33	0.64	0	34,45,45	1.37	3 (8%)
3	LSN	F	503	-	30,33,33	0.64	0	34,45,45	1.38	3 (8%)
2	HEM	G	502	1	42,50,50	1.96	12 (28%)	46,82,82	2.17	13 (28%)
5	SO4	E	505	-	4,4,4	0.37	0	6,6,6	0.06	0
5	SO4	F	505	-	4,4,4	0.39	0	6,6,6	0.10	0
5	SO4	G	505	-	4,4,4	0.35	0	6,6,6	0.10	0
4	CM5	F	501	-	36,36,36	0.14	0	49,49,49	0.21	0
4	CM5	G	501	-	36,36,36	0.14	0	49,49,49	0.23	0
2	HEM	F	502	1	42,50,50	1.90	11 (26%)	46,82,82	2.30	18 (39%)
2	HEM	B	501	1	42,50,50	1.84	9 (21%)	46,82,82	2.03	8 (17%)
3	LSN	G	503	-	30,33,33	0.63	0	34,45,45	1.38	3 (8%)
2	HEM	C	501	1	42,50,50	1.86	12 (28%)	46,82,82	2.13	14 (30%)
3	LSN	E	503	-	30,33,33	0.64	0	34,45,45	1.38	3 (8%)
2	HEM	D	501	1	42,50,50	1.92	12 (28%)	46,82,82	2.06	11 (23%)
4	CM5	H	504	-	36,36,36	0.13	0	49,49,49	0.21	0
2	HEM	H	502	1	42,50,50	1.57	7 (16%)	46,82,82	1.84	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	E	502	1	42,50,50	1.97	14 (33%)	46,82,82	2.07	11 (23%)
2	HEM	A	501	1	42,50,50	1.94	10 (23%)	46,82,82	2.09	12 (26%)
4	CM5	F	504	-	36,36,36	0.14	0	49,49,49	0.22	0
4	CM5	G	504	-	36,36,36	0.13	0	49,49,49	0.21	0
3	LSN	D	502	-	30,33,33	0.65	0	34,45,45	1.37	3 (8%)
4	CM5	H	501	-	36,36,36	0.14	0	49,49,49	0.22	0
3	LSN	B	502	-	30,33,33	0.64	0	34,45,45	1.36	3 (8%)
4	CM5	E	501	-	36,36,36	0.14	0	49,49,49	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LSN	C	502	-	-	7/16/18/18	0/4/4/4
3	LSN	H	503	-	-	7/16/18/18	0/4/4/4
4	CM5	E	504	-	-	12/17/65/65	0/3/3/3
3	LSN	A	502	-	-	6/16/18/18	0/4/4/4
3	LSN	F	503	-	-	6/16/18/18	0/4/4/4
2	HEM	G	502	1	-	4/12/54/54	-
4	CM5	F	501	-	-	12/17/65/65	0/3/3/3
4	CM5	G	501	-	-	11/17/65/65	0/3/3/3
2	HEM	F	502	1	-	7/12/54/54	-
2	HEM	B	501	1	-	4/12/54/54	-
3	LSN	G	503	-	-	5/16/18/18	0/4/4/4
2	HEM	C	501	1	-	7/12/54/54	-
3	LSN	E	503	-	-	7/16/18/18	0/4/4/4
2	HEM	D	501	1	-	4/12/54/54	-
4	CM5	H	504	-	-	11/17/65/65	0/3/3/3
2	HEM	H	502	1	-	2/12/54/54	-
2	HEM	E	502	1	-	6/12/54/54	-
2	HEM	A	501	1	-	9/12/54/54	-
4	CM5	F	504	-	-	10/17/65/65	0/3/3/3
4	CM5	G	504	-	-	9/17/65/65	0/3/3/3
3	LSN	D	502	-	-	4/16/18/18	0/4/4/4
4	CM5	H	501	-	-	8/17/65/65	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LSN	B	502	-	-	5/16/18/18	0/4/4/4
4	CM5	E	501	-	-	10/17/65/65	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	502	HEM	C1B-NB	-4.95	1.31	1.40
2	A	501	HEM	C3C-C2C	-4.92	1.33	1.40
2	E	502	HEM	C4D-ND	-4.77	1.32	1.40
2	G	502	HEM	C1B-NB	-4.69	1.32	1.40
2	B	501	HEM	C1B-NB	-4.63	1.32	1.40
2	C	501	HEM	C1B-NB	-4.62	1.32	1.40
2	F	502	HEM	C3C-C2C	-4.60	1.34	1.40
2	D	501	HEM	C3C-C2C	-4.59	1.34	1.40
2	A	501	HEM	C4D-ND	-4.58	1.32	1.40
2	E	502	HEM	C1B-NB	-4.56	1.32	1.40
2	D	501	HEM	C4D-ND	-4.51	1.32	1.40
2	A	501	HEM	C1B-NB	-4.49	1.32	1.40
2	G	502	HEM	C4D-ND	-4.45	1.32	1.40
2	G	502	HEM	C3C-C2C	-4.40	1.34	1.40
2	D	501	HEM	C1B-NB	-4.40	1.32	1.40
2	E	502	HEM	FE-ND	-4.18	1.74	1.98
2	B	501	HEM	C4D-ND	-4.09	1.33	1.40
2	C	501	HEM	C4D-ND	-4.08	1.33	1.40
2	F	502	HEM	C4D-ND	-4.07	1.33	1.40
2	G	502	HEM	FE-ND	-3.97	1.75	1.98
2	H	502	HEM	C1B-NB	-3.96	1.33	1.40
2	G	502	HEM	C4B-NB	-3.94	1.31	1.38
2	H	502	HEM	C4B-NB	-3.87	1.31	1.38
2	E	502	HEM	C3C-C2C	-3.86	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.82	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.81	1.35	1.40
2	F	502	HEM	C1D-ND	-3.76	1.31	1.38
2	E	502	HEM	C4B-NB	-3.68	1.31	1.38
2	F	502	HEM	C4B-NB	-3.62	1.31	1.38
2	D	501	HEM	C4B-NB	-3.60	1.31	1.38
2	A	501	HEM	C4B-NB	-3.54	1.31	1.38
2	D	501	HEM	C1D-ND	-3.53	1.31	1.38
2	B	501	HEM	C1D-ND	-3.52	1.31	1.38
2	C	501	HEM	C4B-NB	-3.48	1.32	1.38
2	E	502	HEM	C1D-ND	-3.48	1.32	1.38
2	A	501	HEM	C1D-ND	-3.46	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C1D-ND	-3.45	1.32	1.38
2	B	501	HEM	C4B-NB	-3.42	1.32	1.38
2	G	502	HEM	C1D-ND	-3.37	1.32	1.38
2	H	502	HEM	C4D-ND	-3.35	1.34	1.40
2	B	501	HEM	FE-ND	-3.29	1.79	1.98
2	A	501	HEM	FE-ND	-3.05	1.81	1.98
2	C	501	HEM	FE-ND	-3.00	1.81	1.98
2	D	501	HEM	FE-ND	-2.98	1.81	1.98
2	D	501	HEM	O2D-CGD	-2.80	1.21	1.30
2	H	502	HEM	C3C-C4C	2.75	1.45	1.41
2	F	502	HEM	FE-ND	-2.70	1.82	1.98
2	C	501	HEM	O2D-CGD	-2.65	1.22	1.30
2	A	501	HEM	O2D-CGD	-2.62	1.22	1.30
2	B	501	HEM	O2D-CGD	-2.57	1.22	1.30
2	A	501	HEM	C3D-C2D	-2.54	1.31	1.36
2	G	502	HEM	C3D-C2D	-2.42	1.31	1.36
2	F	502	HEM	C2C-C1C	-2.41	1.37	1.42
2	H	502	HEM	FE-NB	2.37	2.11	1.98
2	A	501	HEM	O2A-CGA	-2.35	1.23	1.30
2	G	502	HEM	O2D-CGD	-2.32	1.23	1.30
2	E	502	HEM	C2C-C1C	-2.31	1.37	1.42
2	D	501	HEM	O2A-CGA	-2.31	1.23	1.30
2	B	501	HEM	C2C-C1C	-2.30	1.37	1.42
2	E	502	HEM	FE-NB	2.30	2.10	1.98
2	E	502	HEM	O2D-CGD	-2.27	1.23	1.30
2	B	501	HEM	C3D-C2D	-2.27	1.31	1.36
2	C	501	HEM	C3D-C2D	-2.27	1.31	1.36
2	D	501	HEM	C2C-C1C	-2.26	1.37	1.42
2	F	502	HEM	O2D-CGD	-2.26	1.23	1.30
2	E	502	HEM	C3D-C2D	-2.25	1.31	1.36
2	F	502	HEM	C3D-C2D	-2.22	1.32	1.36
2	C	501	HEM	C1B-C2B	-2.21	1.40	1.44
2	G	502	HEM	C2C-C1C	-2.21	1.37	1.42
2	E	502	HEM	C1B-C2B	-2.20	1.40	1.44
2	G	502	HEM	FE-NB	2.19	2.10	1.98
2	E	502	HEM	O2A-CGA	-2.16	1.23	1.30
2	H	502	HEM	C1D-ND	-2.16	1.34	1.38
2	C	501	HEM	O2A-CGA	-2.14	1.23	1.30
2	C	501	HEM	C3B-C2B	-2.13	1.32	1.37
2	C	501	HEM	C2C-C1C	-2.12	1.37	1.42
2	F	502	HEM	O2A-CGA	-2.12	1.23	1.30
2	E	502	HEM	C4A-CHB	-2.11	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	502	HEM	C1A-CHA	-2.11	1.35	1.41
2	G	502	HEM	O2A-CGA	-2.11	1.23	1.30
2	D	501	HEM	C3D-C2D	-2.09	1.32	1.36
2	A	501	HEM	C1B-C2B	-2.07	1.40	1.44
2	F	502	HEM	C3B-C2B	-2.06	1.33	1.37
2	H	502	HEM	CHB-C1B	2.06	1.39	1.34
2	G	502	HEM	C1A-CHA	-2.05	1.35	1.41
2	D	501	HEM	C1A-CHA	-2.01	1.35	1.41
2	D	501	HEM	C1B-C2B	-2.01	1.40	1.44

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	502	HEM	CHC-C4B-NB	7.21	132.20	124.44
2	F	502	HEM	CHC-C4B-NB	6.71	131.65	124.44
2	A	501	HEM	CHC-C4B-NB	6.65	131.59	124.44
2	C	501	HEM	CHC-C4B-NB	6.41	131.34	124.44
2	D	501	HEM	CHC-C4B-NB	6.39	131.31	124.44
2	E	502	HEM	CHC-C4B-NB	6.37	131.29	124.44
2	B	501	HEM	CHC-C4B-NB	6.32	131.24	124.44
2	C	501	HEM	CHD-C1D-ND	5.95	130.83	124.44
2	F	502	HEM	CHD-C1D-ND	5.61	130.47	124.44
2	B	501	HEM	CHD-C1D-ND	5.46	130.31	124.44
2	G	502	HEM	CHD-C1D-ND	5.46	130.31	124.44
2	A	501	HEM	CHD-C1D-ND	5.35	130.19	124.44
2	E	502	HEM	CHD-C1D-ND	5.33	130.17	124.44
2	D	501	HEM	CHD-C1D-ND	5.30	130.13	124.44
2	H	502	HEM	CHD-C1D-ND	5.10	129.93	124.44
2	E	502	HEM	CHA-C4D-ND	4.47	129.91	124.37
2	F	502	HEM	CHA-C4D-ND	4.38	129.80	124.37
3	G	503	LSN	N4-N3-N2	4.32	112.34	109.54
3	D	502	LSN	N4-N3-N2	4.32	112.34	109.54
3	E	503	LSN	N4-N3-N2	4.31	112.34	109.54
3	F	503	LSN	N4-N3-N2	4.29	112.32	109.54
3	H	503	LSN	N4-N3-N2	4.29	112.32	109.54
3	C	502	LSN	N4-N3-N2	4.27	112.31	109.54
3	A	502	LSN	N4-N3-N2	4.26	112.30	109.54
3	B	502	LSN	N4-N3-N2	4.23	112.28	109.54
2	D	501	HEM	CHA-C4D-ND	4.16	129.53	124.37
3	H	503	LSN	N1-N2-N3	-4.12	106.86	109.54
3	B	502	LSN	C15-N5-C18	-4.10	106.18	109.76
2	A	501	HEM	CHA-C4D-ND	4.08	129.43	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CHA-C4D-ND	4.07	129.42	124.37
3	G	503	LSN	N1-N2-N3	-4.07	106.89	109.54
3	E	503	LSN	C15-N5-C18	-4.07	106.20	109.76
3	G	503	LSN	C15-N5-C18	-4.07	106.21	109.76
2	G	502	HEM	CHC-C4B-C3B	-4.07	118.35	124.57
3	A	502	LSN	N1-N2-N3	-4.05	106.91	109.54
3	H	503	LSN	C15-N5-C18	-4.05	106.22	109.76
3	D	502	LSN	C15-N5-C18	-4.04	106.22	109.76
3	F	503	LSN	C15-N5-C18	-4.04	106.22	109.76
3	F	503	LSN	N1-N2-N3	-4.03	106.92	109.54
3	A	502	LSN	C15-N5-C18	-4.01	106.26	109.76
3	B	502	LSN	N1-N2-N3	-4.00	106.94	109.54
3	E	503	LSN	N1-N2-N3	-4.00	106.94	109.54
3	C	502	LSN	C15-N5-C18	-4.00	106.27	109.76
3	C	502	LSN	N1-N2-N3	-3.96	106.97	109.54
3	D	502	LSN	N1-N2-N3	-3.95	106.97	109.54
2	E	502	HEM	CHB-C1B-NB	3.82	129.10	124.37
2	C	501	HEM	CHD-C1D-C2D	-3.79	119.05	125.03
2	A	501	HEM	CHD-C1D-C2D	-3.75	119.11	125.03
2	G	502	HEM	CHA-C4D-ND	3.74	129.01	124.37
2	H	502	HEM	CHA-C4D-ND	3.74	129.00	124.37
2	C	501	HEM	CHA-C4D-ND	3.71	128.97	124.37
2	F	502	HEM	CHC-C4B-C3B	-3.64	119.00	124.57
2	C	501	HEM	CHB-C1B-NB	3.58	128.81	124.37
2	F	502	HEM	CHB-C1B-NB	3.56	128.79	124.37
2	B	501	HEM	CHD-C1D-C2D	-3.53	119.45	125.03
2	D	501	HEM	CHB-C1B-NB	3.52	128.73	124.37
2	G	502	HEM	CHD-C1D-C2D	-3.51	119.49	125.03
2	H	502	HEM	C4B-CHC-C1C	3.44	127.09	122.56
2	D	501	HEM	CHD-C1D-C2D	-3.41	119.65	125.03
2	F	502	HEM	CHD-C1D-C2D	-3.39	119.68	125.03
2	H	502	HEM	CHC-C4B-NB	3.33	128.01	124.44
2	H	502	HEM	CMB-C2B-C1B	3.30	130.19	125.03
2	D	501	HEM	CHC-C4B-C3B	-3.27	119.57	124.57
2	A	501	HEM	CHB-C1B-NB	3.25	128.40	124.37
2	E	502	HEM	CAA-CBA-CGA	-3.21	105.18	113.83
2	E	502	HEM	CHA-C4D-C3D	-3.17	119.38	125.23
2	A	501	HEM	CHC-C4B-C3B	-3.12	119.80	124.57
2	B	501	HEM	CHA-C4D-C3D	-3.11	119.50	125.23
2	D	501	HEM	CAA-CBA-CGA	-3.10	105.47	113.83
2	F	502	HEM	CHA-C4D-C3D	-3.08	119.54	125.23
2	B	501	HEM	CHC-C4B-C3B	-3.06	119.88	124.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	502	HEM	CHD-C1D-C2D	-3.05	120.21	125.03
2	H	502	HEM	CHD-C1D-C2D	-3.03	120.25	125.03
2	C	501	HEM	CHC-C4B-C3B	-3.00	119.97	124.57
2	H	502	HEM	CHA-C4D-C3D	-3.00	119.69	125.23
2	F	502	HEM	CAD-C3D-C4D	2.94	129.82	124.70
2	C	501	HEM	CAD-C3D-C4D	2.90	129.76	124.70
2	B	501	HEM	CHB-C1B-NB	2.89	127.95	124.37
2	A	501	HEM	CAA-CBA-CGA	-2.89	106.06	113.83
2	H	502	HEM	CAA-CBA-CGA	-2.87	106.09	113.83
2	G	502	HEM	CHB-C1B-NB	2.87	127.93	124.37
2	G	502	HEM	CHA-C4D-C3D	-2.84	119.98	125.23
2	C	501	HEM	CAA-CBA-CGA	-2.84	106.19	113.83
2	A	501	HEM	CHA-C4D-C3D	-2.78	120.10	125.23
2	D	501	HEM	CHA-C4D-C3D	-2.77	120.11	125.23
2	E	502	HEM	C1B-NB-C4B	2.77	108.49	105.21
2	G	502	HEM	C1B-NB-C4B	2.75	108.46	105.21
2	F	502	HEM	C1B-NB-C4B	2.71	108.42	105.21
2	G	502	HEM	O2D-CGD-CBD	2.66	122.40	114.00
2	G	502	HEM	CAD-C3D-C4D	2.64	129.29	124.70
2	F	502	HEM	O2D-CGD-CBD	2.63	122.30	114.00
2	E	502	HEM	CHC-C4B-C3B	-2.62	120.56	124.57
2	H	502	HEM	C1B-NB-C4B	2.59	108.27	105.21
2	A	501	HEM	C1B-NB-C4B	2.54	108.21	105.21
2	B	501	HEM	C1B-NB-C4B	2.46	108.12	105.21
2	C	501	HEM	CHA-C4D-C3D	-2.44	120.73	125.23
2	F	502	HEM	C4B-C3B-C2B	-2.44	105.04	107.28
2	F	502	HEM	C4B-CHC-C1C	-2.43	119.35	122.56
2	D	501	HEM	C1B-NB-C4B	2.41	108.06	105.21
2	F	502	HEM	CMA-C3A-C4A	-2.36	124.99	128.46
2	F	502	HEM	CAA-CBA-CGA	-2.34	107.52	113.83
2	G	502	HEM	CMA-C3A-C4A	-2.33	125.04	128.46
2	E	502	HEM	CHB-C1B-C2B	-2.32	120.37	126.94
2	C	501	HEM	CHB-C1B-C2B	-2.27	120.51	126.94
2	G	502	HEM	O2D-CGD-O1D	-2.26	117.53	123.33
2	F	502	HEM	C4A-C3A-C2A	2.24	108.55	107.00
2	H	502	HEM	O2D-CGD-CBD	2.21	120.98	114.00
2	C	501	HEM	C4C-CHD-C1D	-2.18	119.68	122.56
2	F	502	HEM	CBA-CAA-C2A	2.18	116.20	112.54
2	F	502	HEM	O2D-CGD-O1D	-2.16	117.77	123.33
2	C	501	HEM	C1B-NB-C4B	2.16	107.77	105.21
2	C	501	HEM	O2D-CGD-CBD	2.14	120.78	114.00
2	A	501	HEM	CBD-CAD-C3D	-2.13	106.63	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	O2D-CGD-O1D	-2.11	117.92	123.33
2	D	501	HEM	CBD-CAD-C3D	-2.09	106.77	112.53
2	H	502	HEM	C3C-C4C-NC	-2.07	107.04	110.94
2	A	501	HEM	CHB-C1B-C2B	-2.07	121.09	126.94
2	D	501	HEM	CHB-C1B-C2B	-2.06	121.12	126.94
2	G	502	HEM	CMB-C2B-C1B	2.03	128.21	125.03
2	A	501	HEM	CAD-C3D-C4D	2.03	128.24	124.70
2	F	502	HEM	C3B-C2B-C1B	2.03	107.93	106.41
2	E	502	HEM	O2D-CGD-CBD	2.02	120.39	114.00

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
3	A	502	LSN	C18-C19-C20-C21
3	B	502	LSN	C18-C19-C20-C21
3	C	502	LSN	N6-C18-C19-C20
3	C	502	LSN	C18-C19-C20-C21
3	E	503	LSN	C18-C19-C20-C21
3	F	503	LSN	C18-C19-C20-C21
3	H	503	LSN	C18-C19-C20-C21
3	H	503	LSN	N1-C1-C2-C3
3	H	503	LSN	N4-C1-C2-C3
4	E	504	CM5	C18-C13-O12-C1
4	E	504	CM5	O14-C13-O12-C1
2	F	502	HEM	C4D-C3D-CAD-CBD
4	F	504	CM5	C16-C15-C19-O20
4	F	504	CM5	O14-C15-C19-O20
4	G	501	CM5	C27-C26-C30-O31
4	F	504	CM5	O14-C13-O12-C1
4	G	504	CM5	O14-C13-O12-C1
4	H	504	CM5	O14-C13-O12-C1
4	G	501	CM5	O25-C26-C30-O31
4	H	504	CM5	C16-C15-C19-O20
4	F	504	CM5	C18-C13-O12-C1
4	G	504	CM5	C18-C13-O12-C1
4	H	504	CM5	C18-C13-O12-C1
4	F	501	CM5	C4-C5-C6-C11
4	F	501	CM5	O12-C1-C2-C3
4	H	501	CM5	O12-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	H	501	CM5	C15-C16-O23-C24
4	E	504	CM5	O14-C15-C19-O20
4	H	504	CM5	O14-C15-C19-O20
4	E	501	CM5	C4-C5-C6-C11
4	E	501	CM5	O14-C13-O12-C1
4	F	501	CM5	O14-C13-O12-C1
4	H	501	CM5	O14-C13-O12-C1
4	E	501	CM5	C15-C16-O23-C24
4	E	501	CM5	O12-C1-C2-C3
4	F	504	CM5	O12-C1-C2-C3
4	G	501	CM5	O12-C1-C2-C3
2	C	501	HEM	C4D-C3D-CAD-CBD
3	A	502	LSN	N1-C1-C2-C3
3	A	502	LSN	N4-C1-C2-C3
3	C	502	LSN	N1-C1-C2-C3
3	C	502	LSN	N4-C1-C2-C3
3	E	503	LSN	N1-C1-C2-C3
3	E	503	LSN	N4-C1-C2-C3
3	F	503	LSN	N1-C1-C2-C3
3	F	503	LSN	N4-C1-C2-C3
3	G	503	LSN	N1-C1-C2-C3
3	G	503	LSN	N4-C1-C2-C3
4	E	504	CM5	C3-C4-C5-C6
4	E	501	CM5	C18-C13-O12-C1
4	F	501	CM5	C18-C13-O12-C1
4	H	501	CM5	C18-C13-O12-C1
4	G	501	CM5	C16-C15-C19-O20
4	G	504	CM5	C16-C15-C19-O20
2	C	501	HEM	C2D-C3D-CAD-CBD
2	F	502	HEM	C2D-C3D-CAD-CBD
4	H	501	CM5	C17-C16-O23-C24
4	E	501	CM5	C17-C16-O23-C24
4	E	504	CM5	O25-C26-C30-O31
4	F	504	CM5	C2-C1-O12-C13
4	H	504	CM5	C1-C2-C3-C4
4	G	504	CM5	C1-C2-C3-C4
4	E	504	CM5	O12-C1-C2-C3
2	G	502	HEM	C4D-C3D-CAD-CBD
4	G	504	CM5	C2-C3-C4-C5
4	G	501	CM5	C15-C16-O23-C24
2	G	502	HEM	C2D-C3D-CAD-CBD
4	G	501	CM5	C17-C16-O23-C24

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Mol	Chain	Res	Type	Atoms
4	G	501	CM5	O14-C15-C19-O20
4	E	504	CM5	C1-C2-C3-C4
4	G	501	CM5	C2-C3-C4-C5
4	G	504	CM5	O14-C15-C19-O20
4	G	504	CM5	O25-C24-O23-C16
4	F	501	CM5	C15-C16-O23-C24
4	F	501	CM5	C16-C15-C19-O20
4	G	504	CM5	C29-C24-O23-C16
3	B	502	LSN	N1-C1-C2-C3
4	F	501	CM5	C17-C16-O23-C24
4	F	504	CM5	C1-C2-C3-C4
4	F	501	CM5	C2-C3-C4-C5
4	H	501	CM5	C2-C3-C4-C5
4	H	504	CM5	C2-C3-C4-C5
4	F	504	CM5	C2-C3-C4-C5
4	G	504	CM5	C2-C1-O12-C13
4	E	504	CM5	C15-C16-O23-C24
4	E	504	CM5	C17-C16-O23-C24
4	E	501	CM5	C2-C3-C4-C5
4	F	501	CM5	C3-C4-C5-C6
4	F	504	CM5	C15-C16-O23-C24
4	F	501	CM5	O14-C15-C19-O20
4	F	504	CM5	C17-C16-O23-C24
3	B	502	LSN	C10-C11-C12-N5
2	E	502	HEM	C3A-C2A-CAA-CBA
4	G	501	CM5	O14-C13-O12-C1
3	B	502	LSN	C13-C11-C12-N5
4	G	501	CM5	C18-C13-O12-C1
4	H	504	CM5	C29-C24-O23-C16
4	H	504	CM5	O25-C24-O23-C16
3	D	502	LSN	C10-C11-C12-N5
4	E	504	CM5	C29-C24-O23-C16
4	E	504	CM5	O25-C24-O23-C16
3	F	503	LSN	C10-C11-C12-N5
2	A	501	HEM	C4D-C3D-CAD-CBD
3	C	502	LSN	C10-C11-C12-N5
3	G	503	LSN	C13-C11-C12-N5
3	H	503	LSN	C10-C11-C12-N5
3	G	503	LSN	C10-C11-C12-N5
3	A	502	LSN	C10-C11-C12-N5
3	A	502	LSN	N1-C1-C2-C7
3	C	502	LSN	N1-C1-C2-C7

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Mol	Chain	Res	Type	Atoms
3	G	503	LSN	N1-C1-C2-C7
3	H	503	LSN	N1-C1-C2-C7
3	E	503	LSN	C10-C11-C12-N5
3	D	502	LSN	C13-C11-C12-N5
3	F	503	LSN	C13-C11-C12-N5
3	H	503	LSN	C13-C11-C12-N5
3	E	503	LSN	C13-C11-C12-N5
3	A	502	LSN	C13-C11-C12-N5
3	C	502	LSN	C13-C11-C12-N5
4	H	504	CM5	C4-C5-C6-C11
4	H	504	CM5	C4-C5-C6-C7
4	H	501	CM5	C16-C15-C19-O20
4	H	504	CM5	O12-C1-C2-C3
4	E	501	CM5	C16-C15-C19-O20
4	E	504	CM5	C2-C3-C4-C5
3	B	502	LSN	N4-C1-C2-C3
3	D	502	LSN	N1-C1-C2-C3
2	C	501	HEM	C3D-CAD-CBD-CGD
4	E	501	CM5	C4-C5-C6-C7
4	G	501	CM5	C3-C4-C5-C6
2	F	502	HEM	C3D-CAD-CBD-CGD
2	D	501	HEM	CAA-CBA-CGA-O2A
2	F	502	HEM	CAA-CBA-CGA-O1A
4	H	501	CM5	O14-C15-C19-O20
2	B	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	G	502	HEM	CAD-CBD-CGD-O1D
2	F	502	HEM	CAD-CBD-CGD-O2D
4	E	501	CM5	O14-C15-C19-O20
2	B	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	E	502	HEM	CAD-CBD-CGD-O1D
2	F	502	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
4	F	501	CM5	O25-C26-C30-O31
2	A	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O1D
2	F	502	HEM	CAD-CBD-CGD-O1D
2	H	502	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	E	502	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	G	502	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	C4D-C3D-CAD-CBD
2	E	502	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	C3D-CAD-CBD-CGD
2	E	502	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	H	502	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	C2D-C3D-CAD-CBD
2	E	502	HEM	C1A-C2A-CAA-CBA
4	F	501	CM5	C4-C5-C6-C7
3	E	503	LSN	C19-C20-C21-C22
3	D	502	LSN	N4-C1-C2-C3
3	E	503	LSN	N1-C1-C2-C7
3	F	503	LSN	N1-C1-C2-C7
3	H	503	LSN	N4-C1-C2-C7
2	D	501	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

23 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	503	LSN	2	0
4	E	504	CM5	5	0
3	A	502	LSN	5	0
3	F	503	LSN	2	0
2	G	502	HEM	8	0
4	F	501	CM5	4	0
4	G	501	CM5	5	0
2	F	502	HEM	7	0
2	B	501	HEM	10	0
3	G	503	LSN	2	0
2	C	501	HEM	14	0
3	E	503	LSN	2	0
2	D	501	HEM	11	0
4	H	504	CM5	6	0
2	H	502	HEM	5	0
2	E	502	HEM	12	0
2	A	501	HEM	12	0
4	F	504	CM5	3	0

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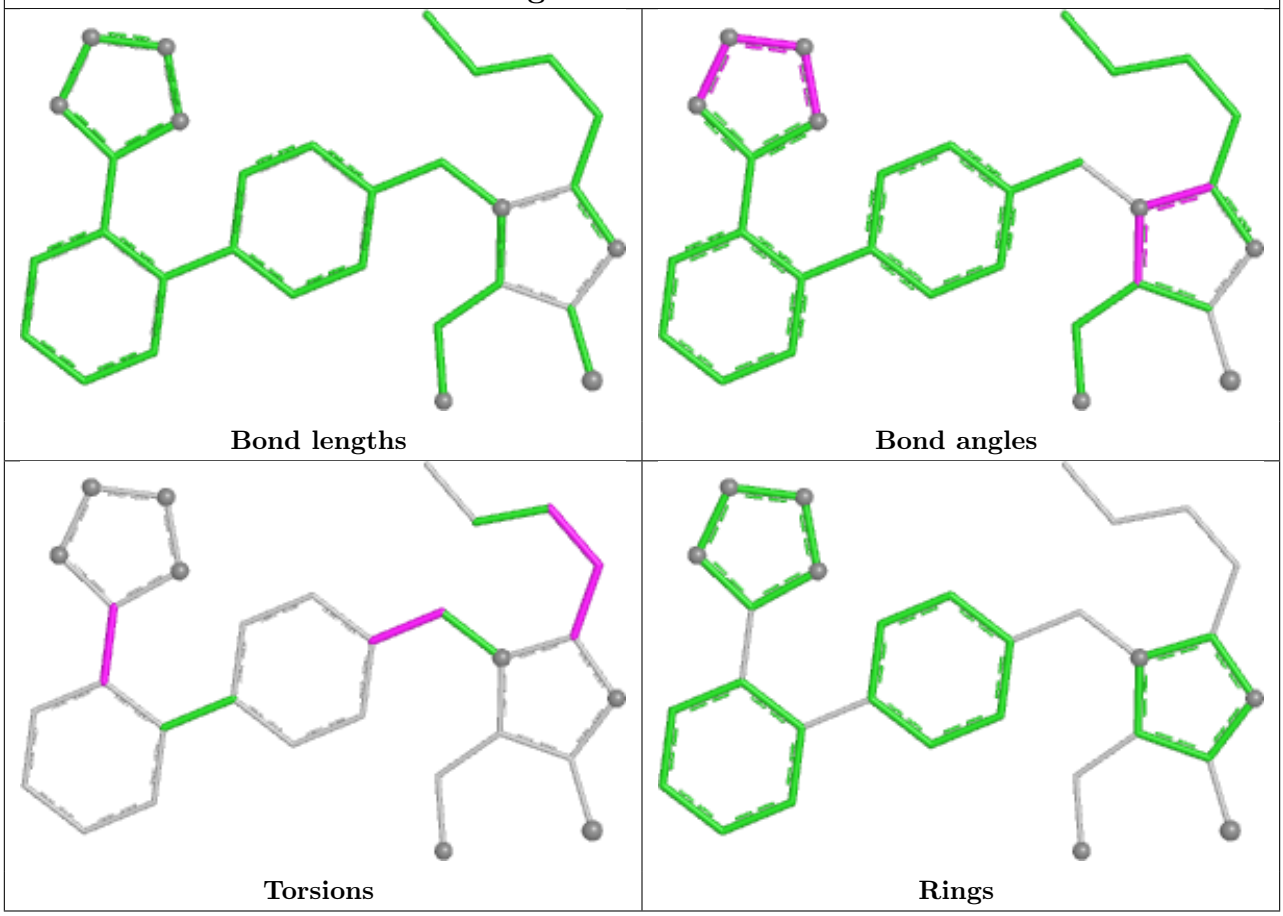
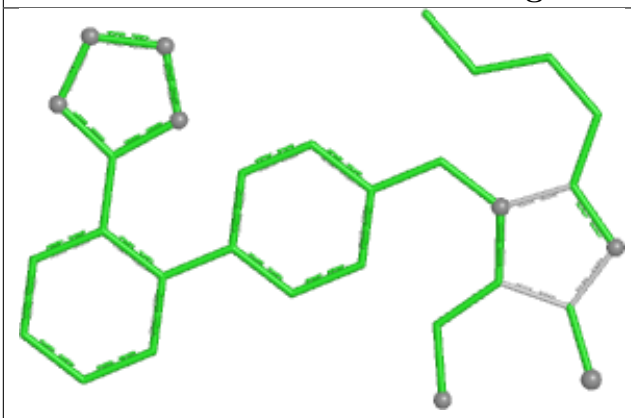
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	504	CM5	4	0
3	D	502	LSN	5	0
4	H	501	CM5	10	0
3	B	502	LSN	1	0
4	E	501	CM5	10	0

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

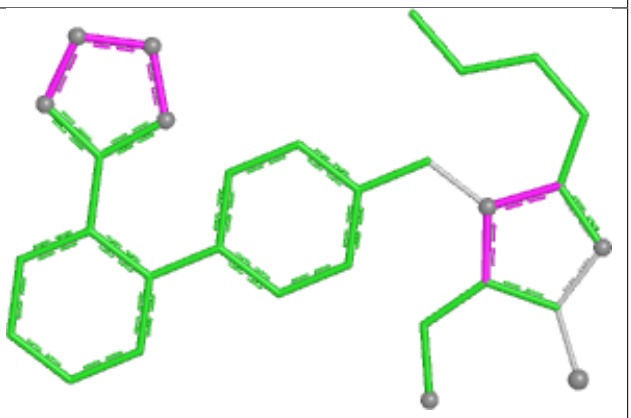
Ligand LSN C 502



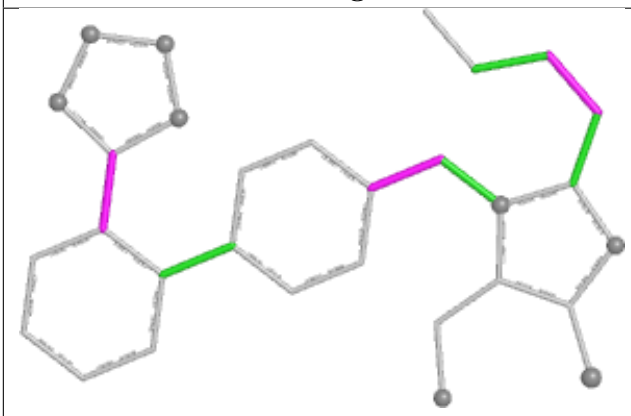
Ligand LSN H 503



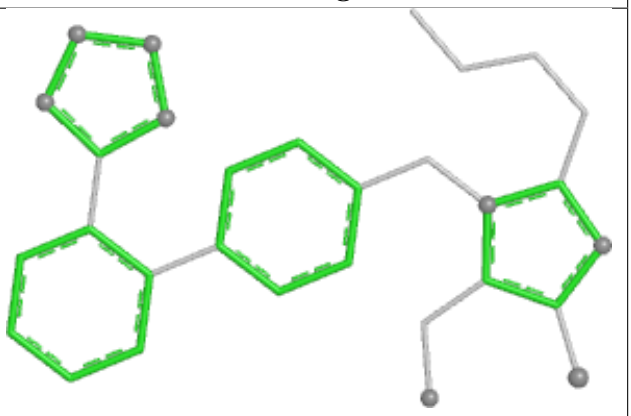
Bond lengths



Bond angles

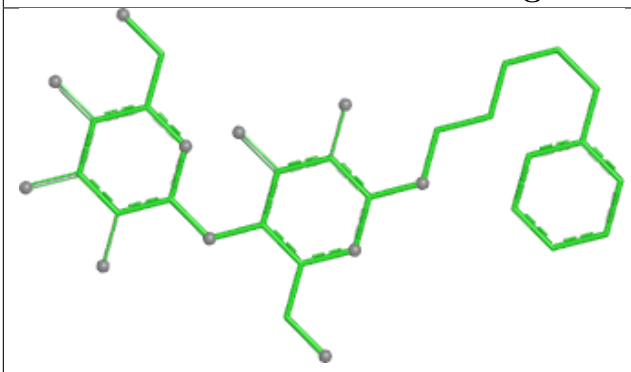


Torsions

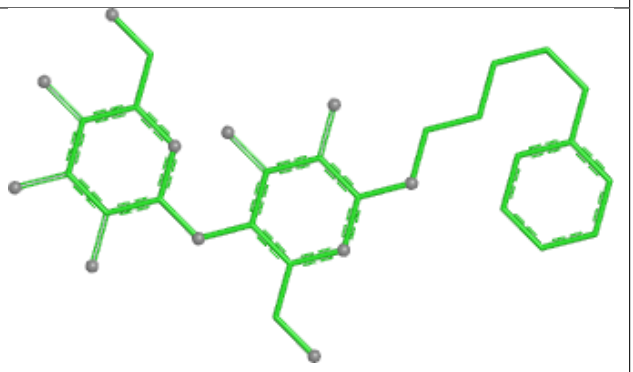


Rings

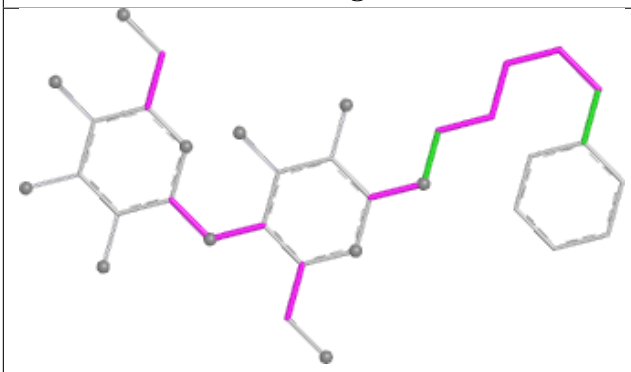
Ligand CM5 E 504



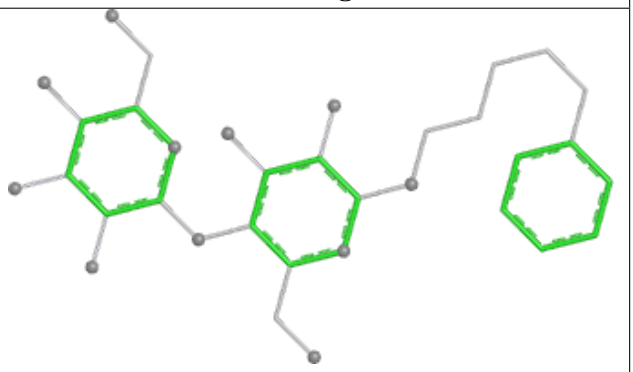
Bond lengths



Bond angles

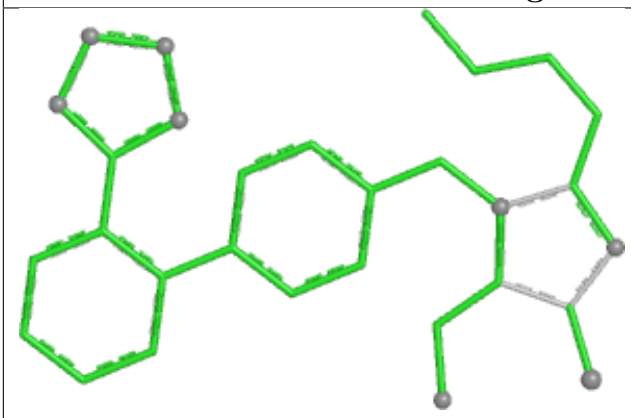


Torsions

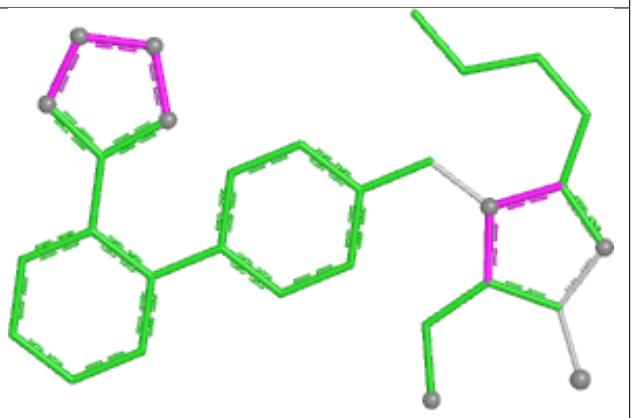


Rings

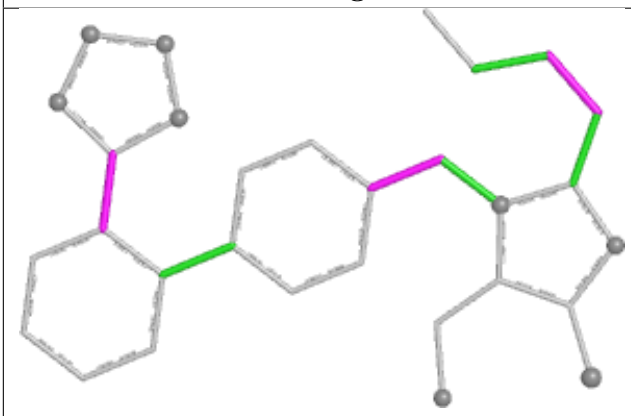
Ligand LSN A 502



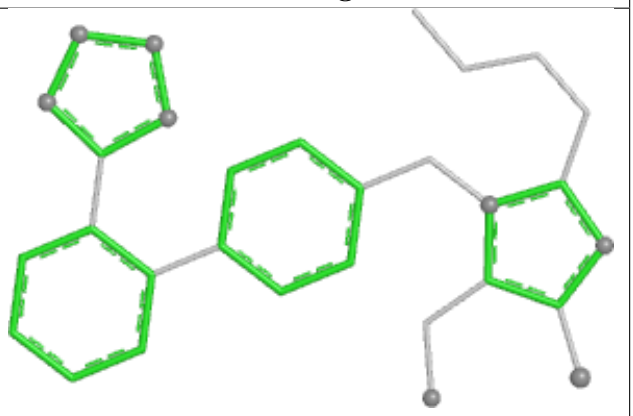
Bond lengths



Bond angles

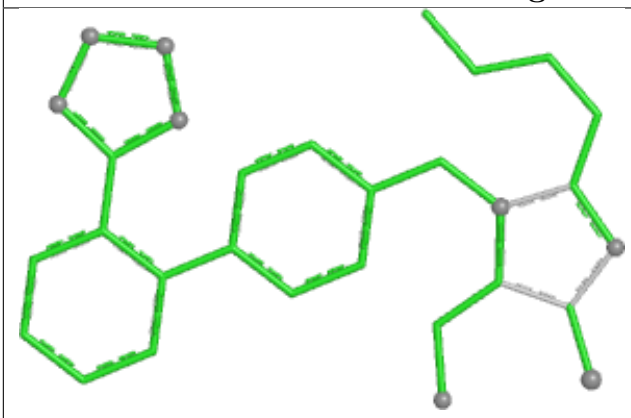


Torsions

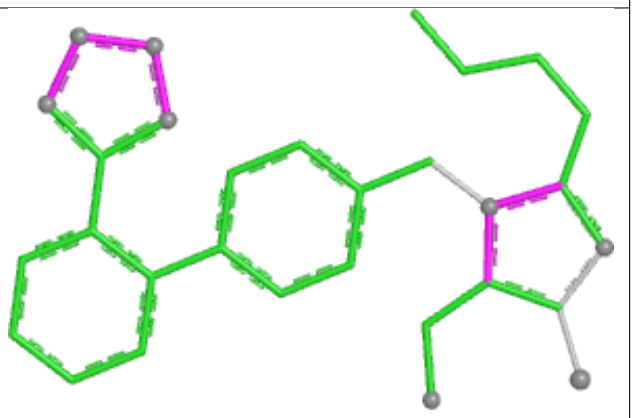


Rings

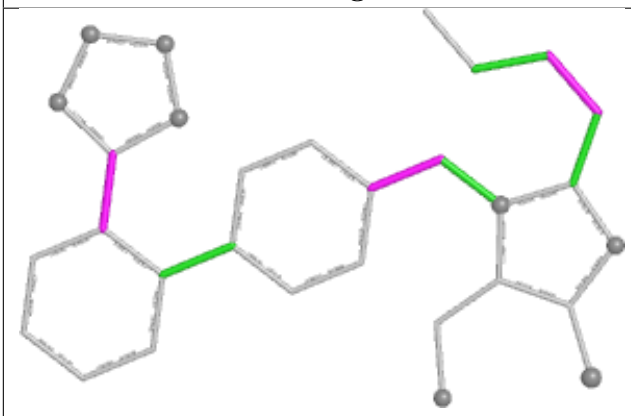
Ligand LSN F 503



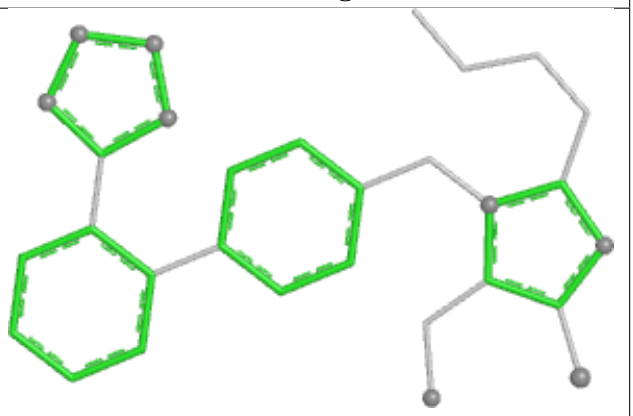
Bond lengths



Bond angles

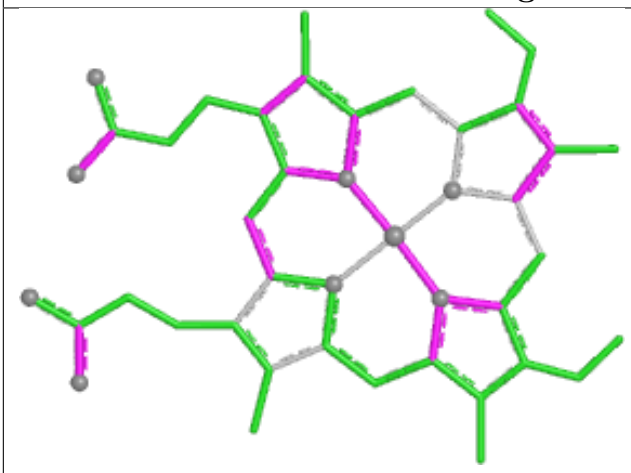


Torsions

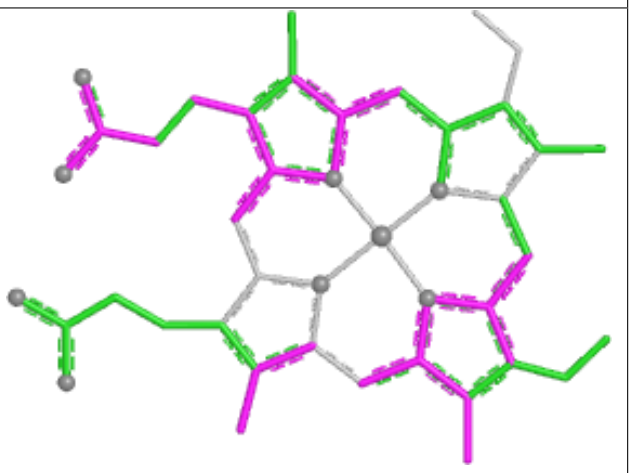


Rings

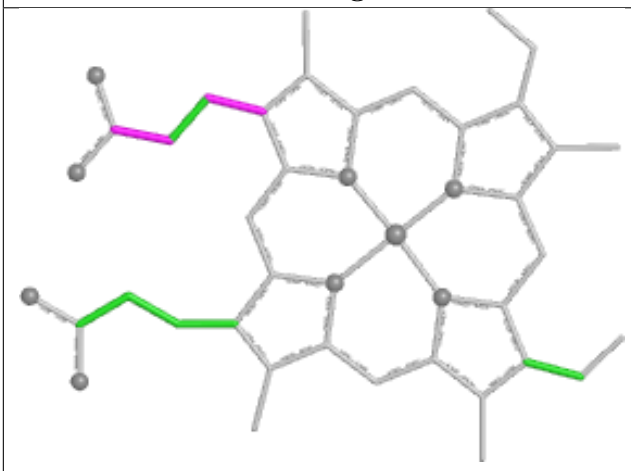
Ligand HEM G 502



Bond lengths



Bond angles



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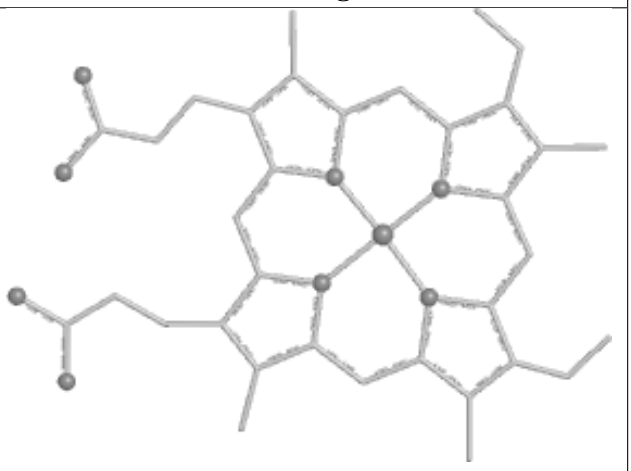
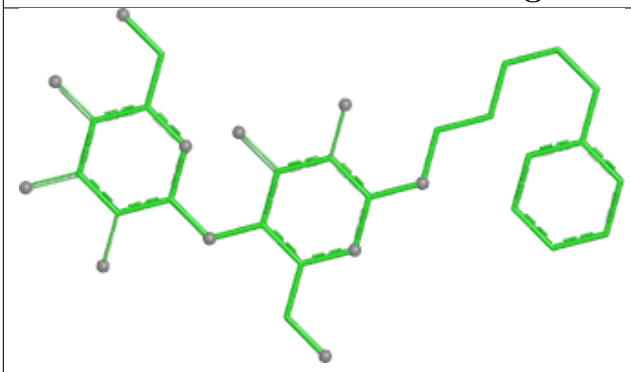


Rings

Ligand CM5 F 501



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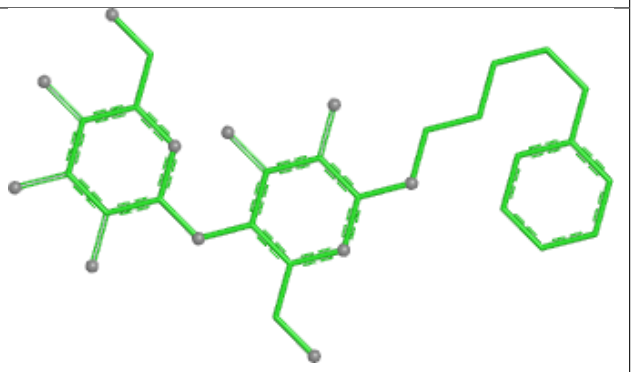
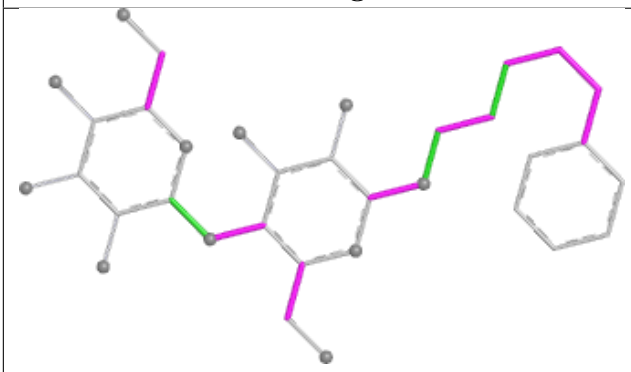


Bond angles



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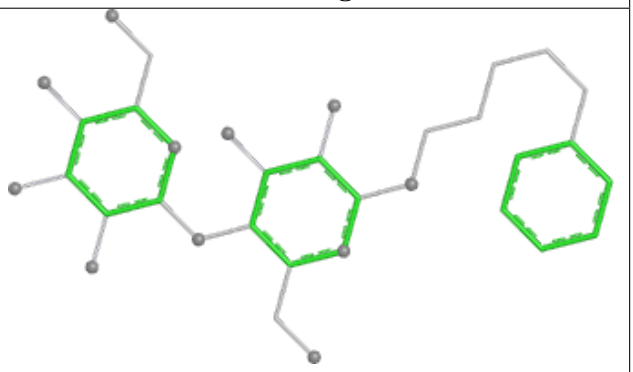
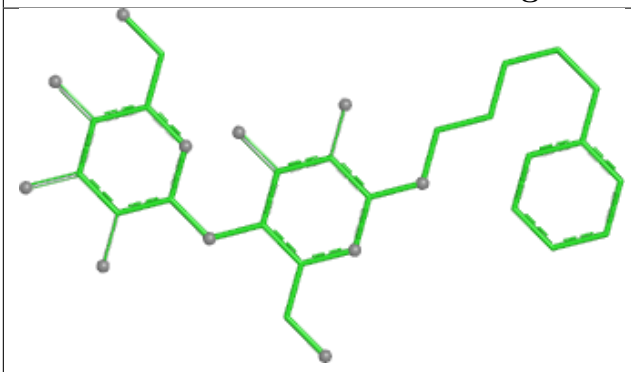
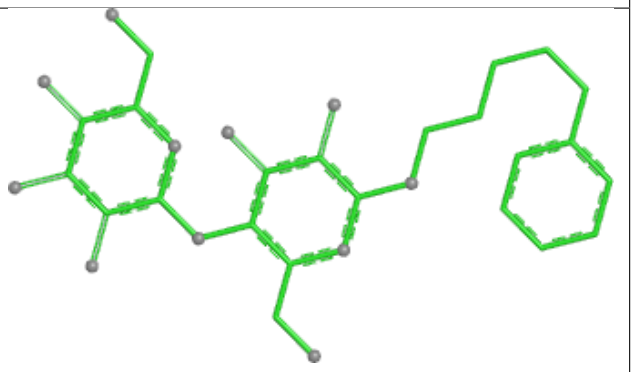


Rings

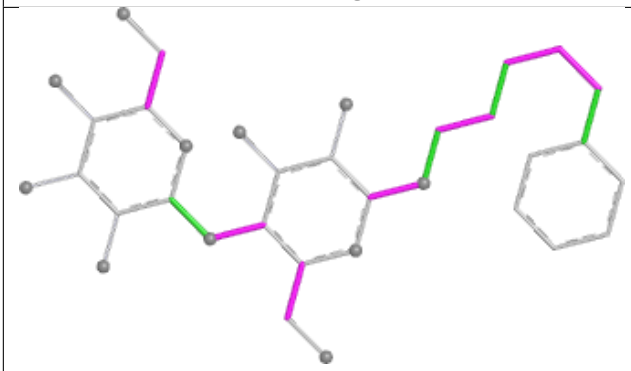
Ligand CM5 G 501



Bond lengths



Bond angles



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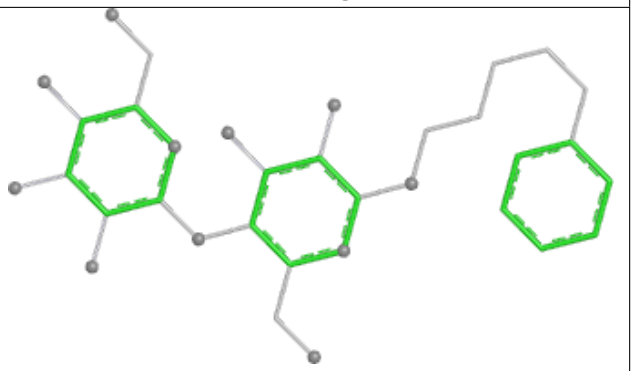
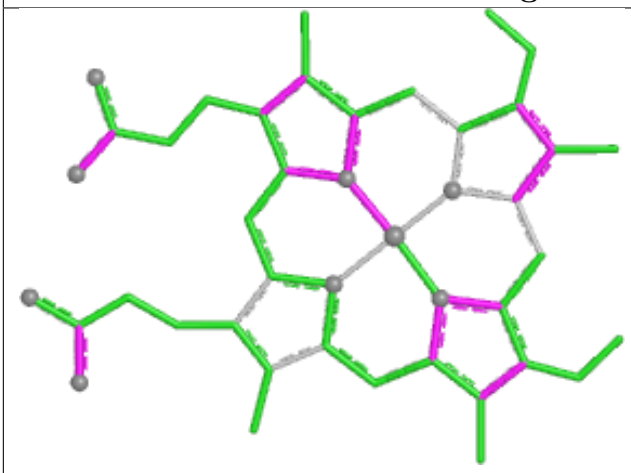
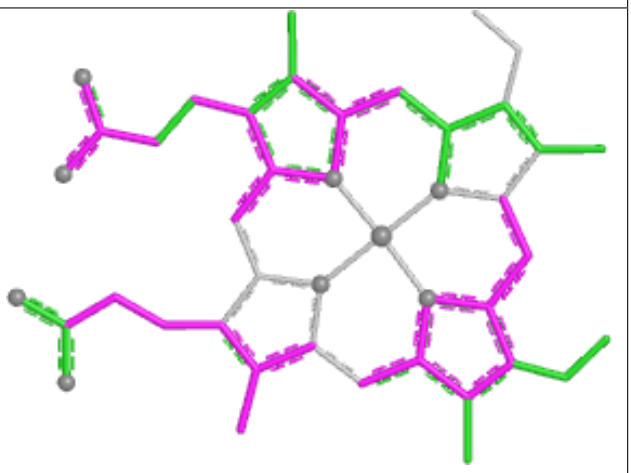


Rings

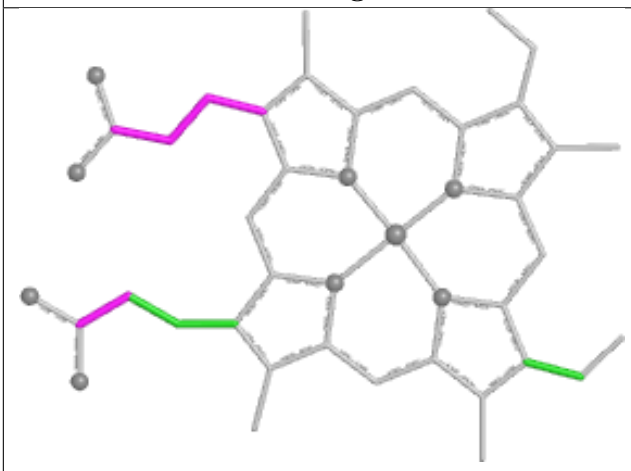
Ligand HEM F 502



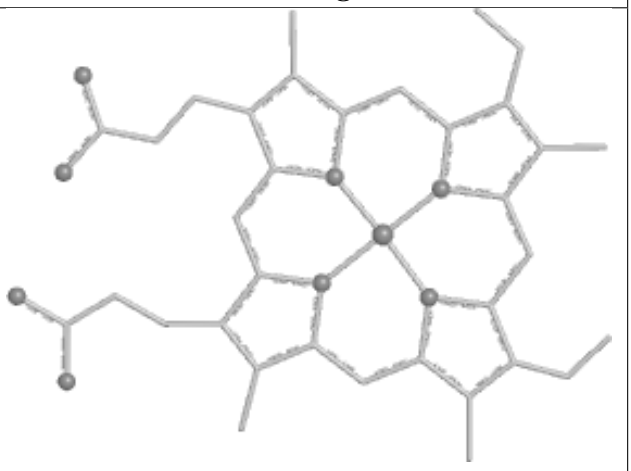
Bond lengths



Bond angles

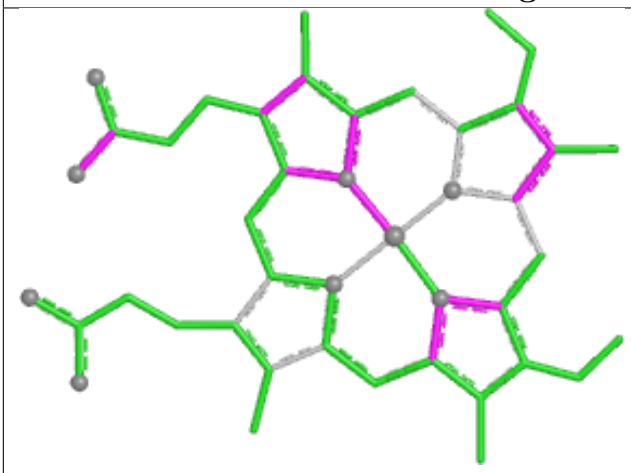


Torsions

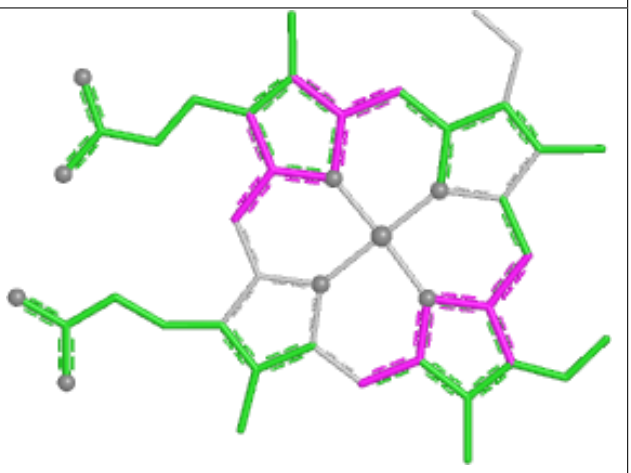


Rings

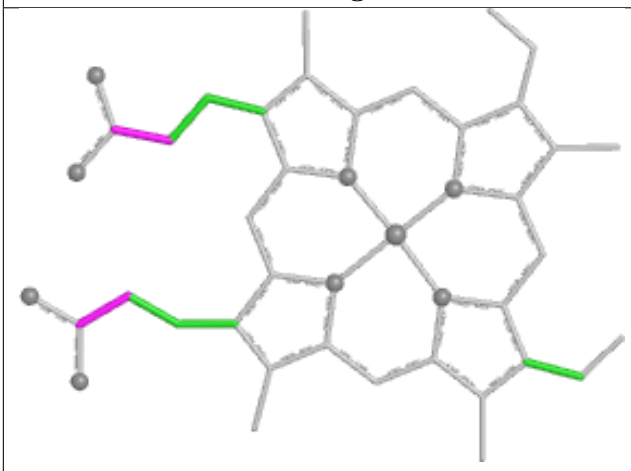
Ligand HEM B 501



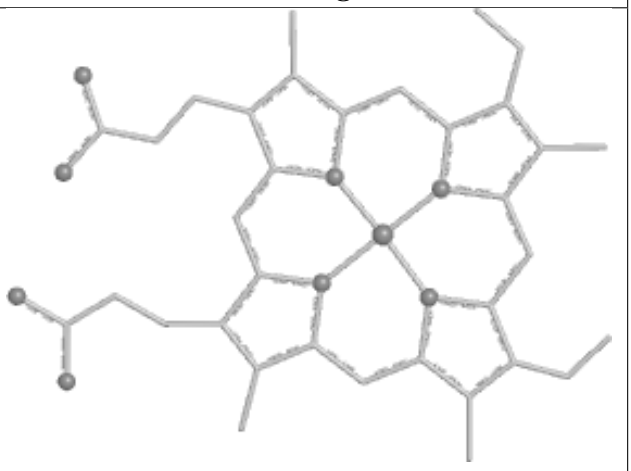
Bond lengths



Bond angles

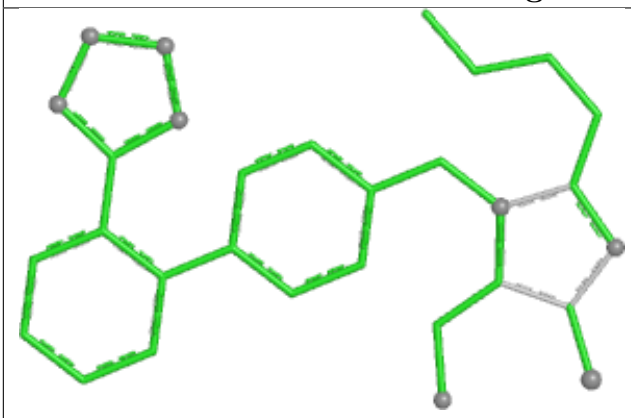


Torsions



Rings

Ligand LSN G 503



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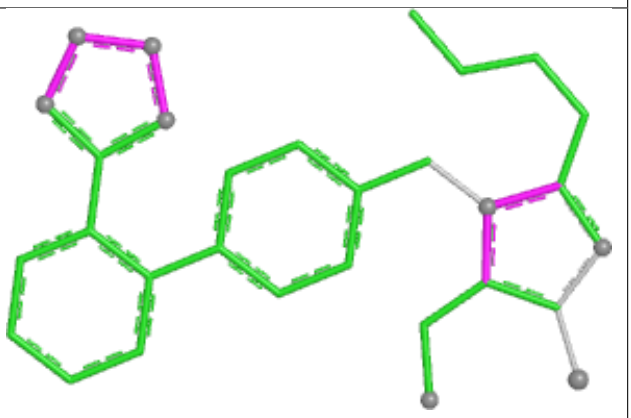

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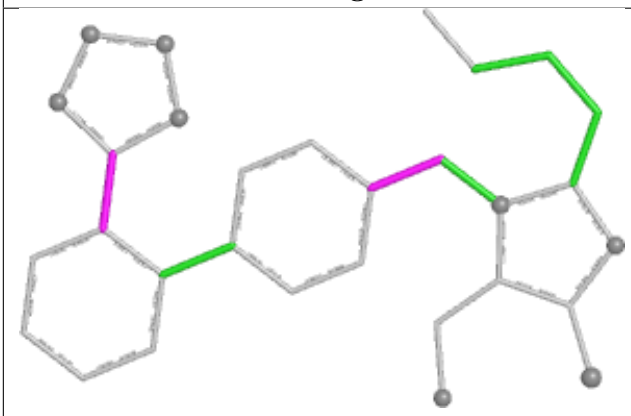

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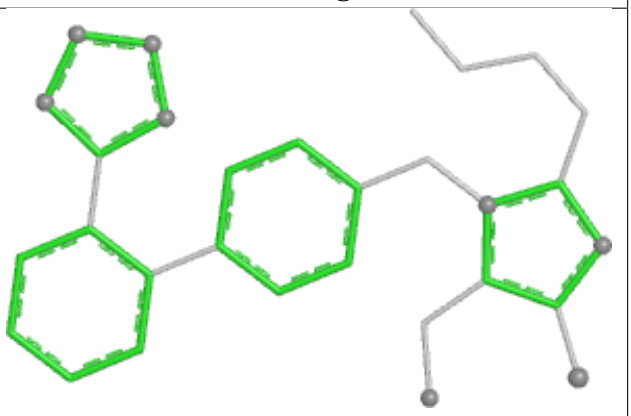
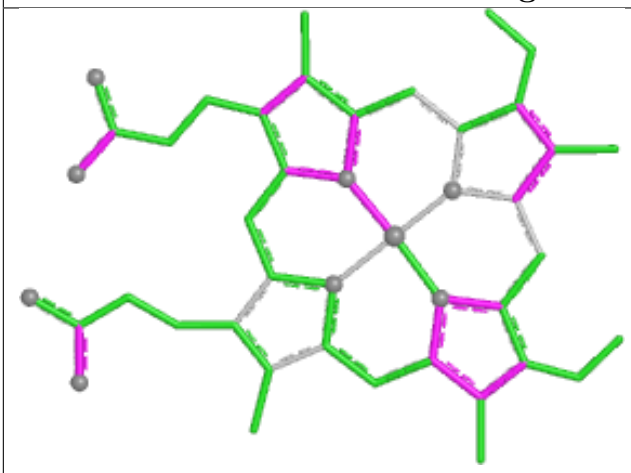


Rings

Ligand HEM C 501



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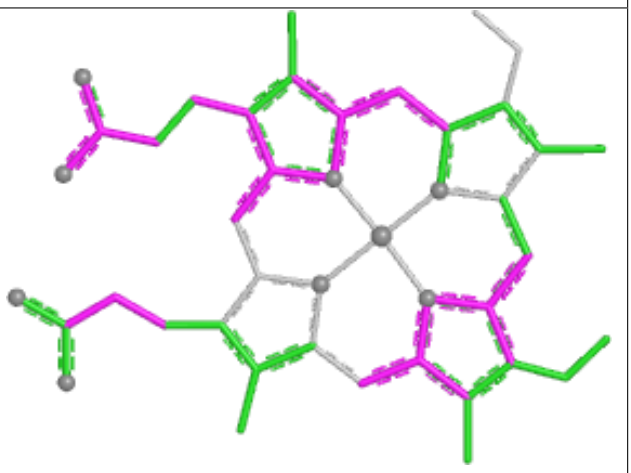

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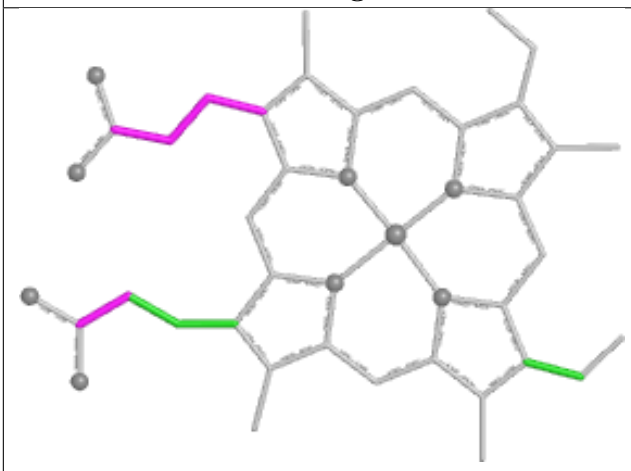

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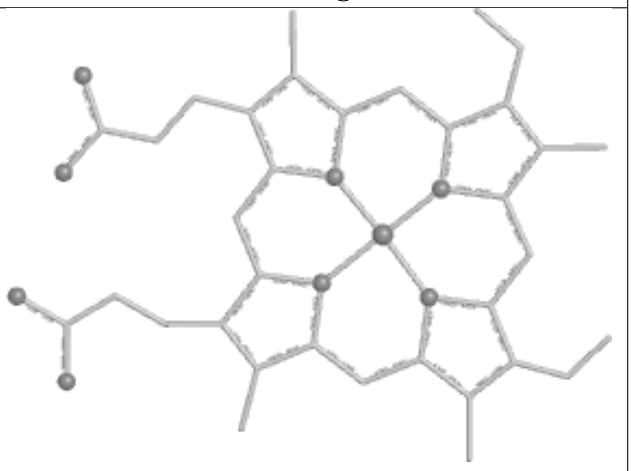
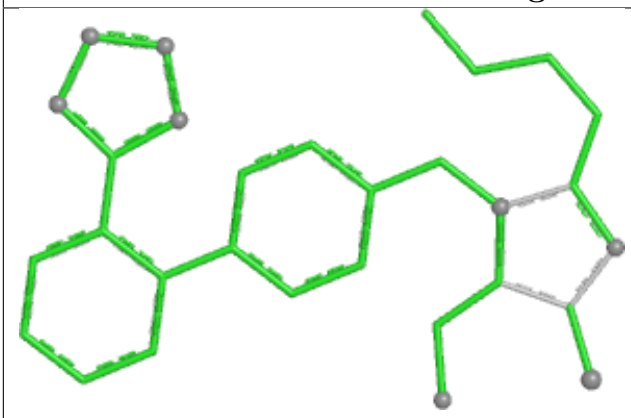


Rings

Ligand LSN E 503



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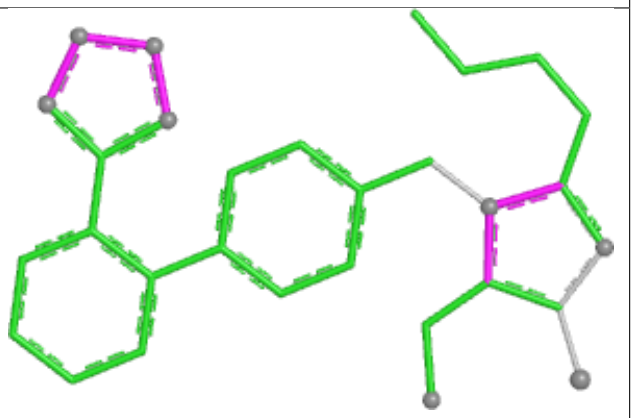

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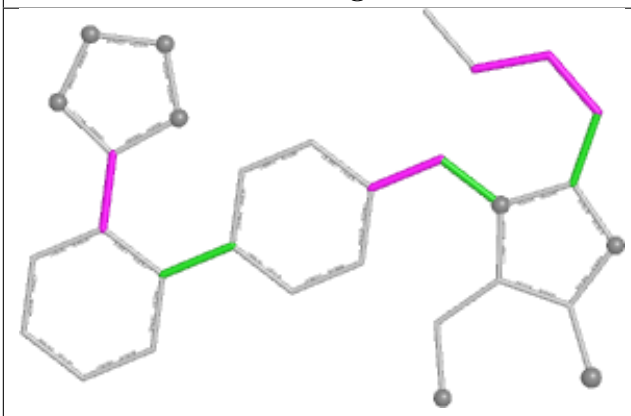

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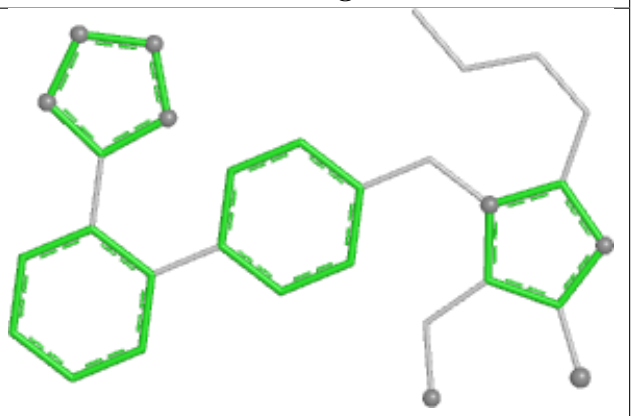
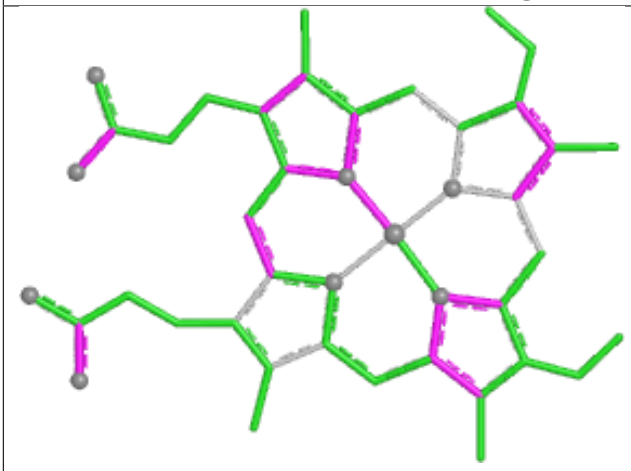


Rings

Ligand HEM D 501



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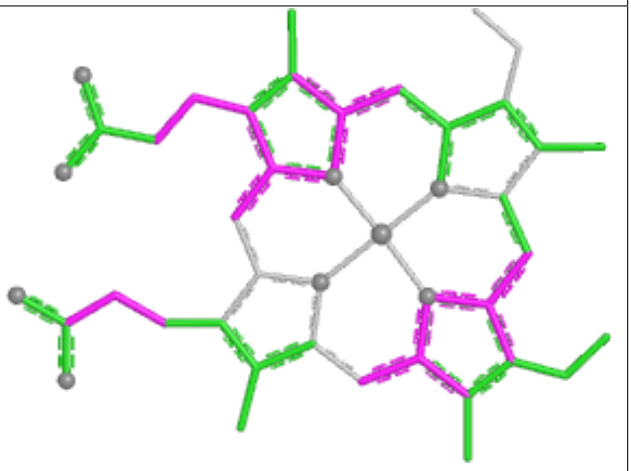

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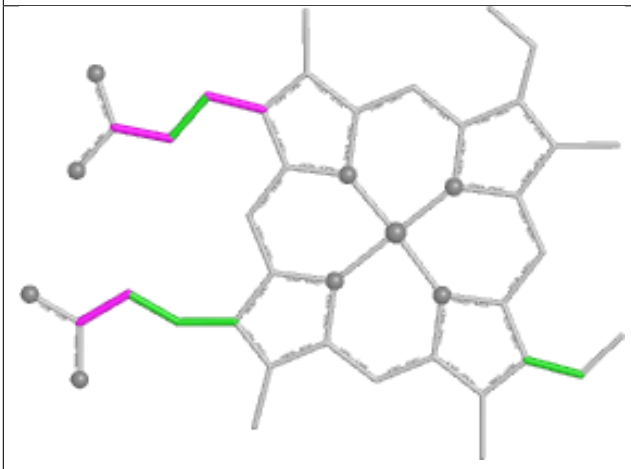

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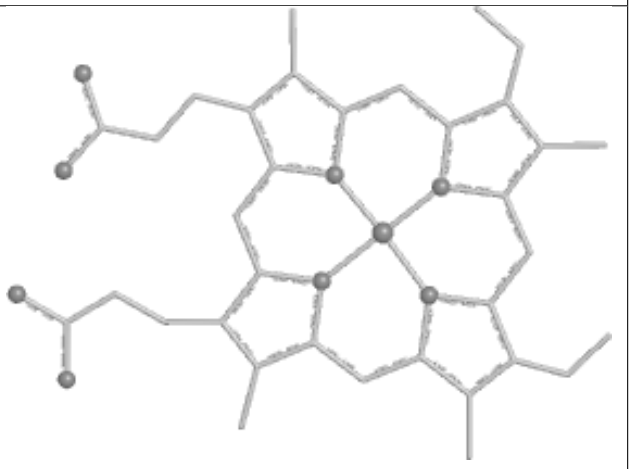
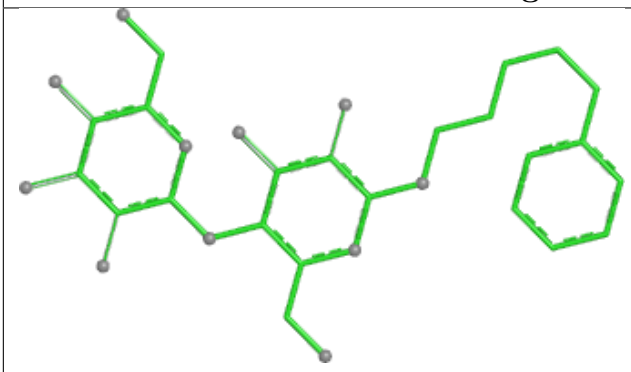


Rings

Ligand CM5 H 504



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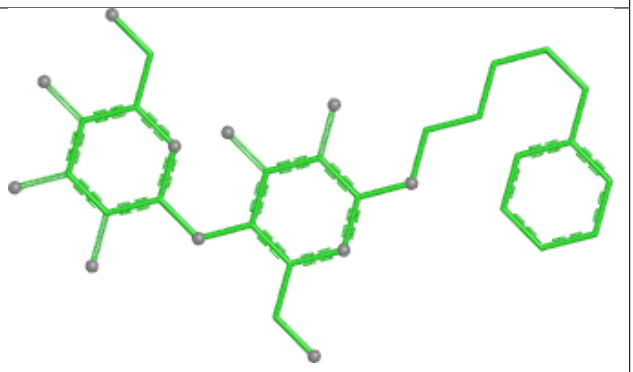

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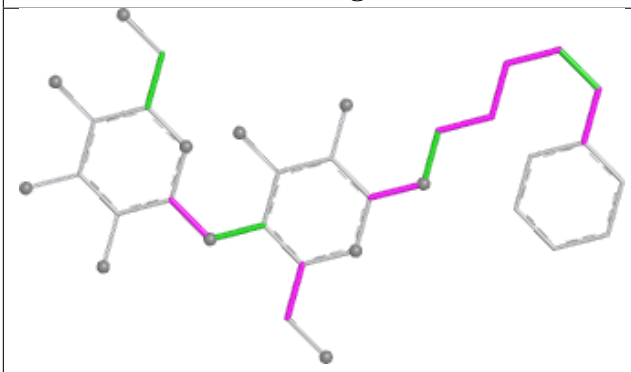

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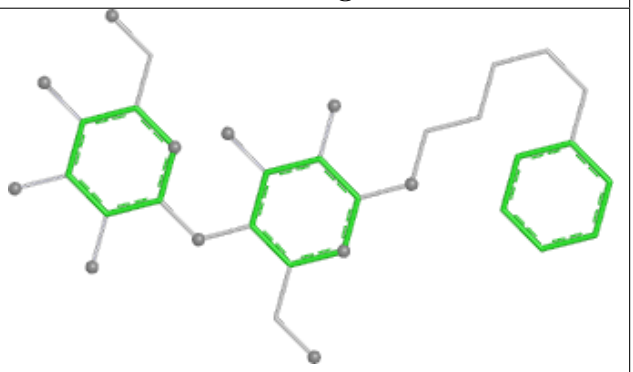
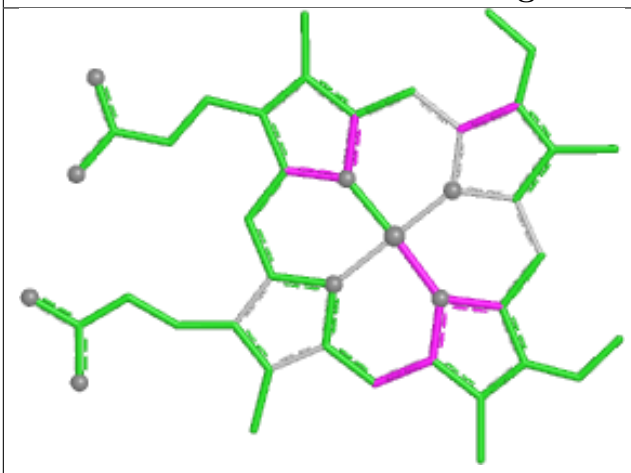


Rings

Ligand HEM H 502



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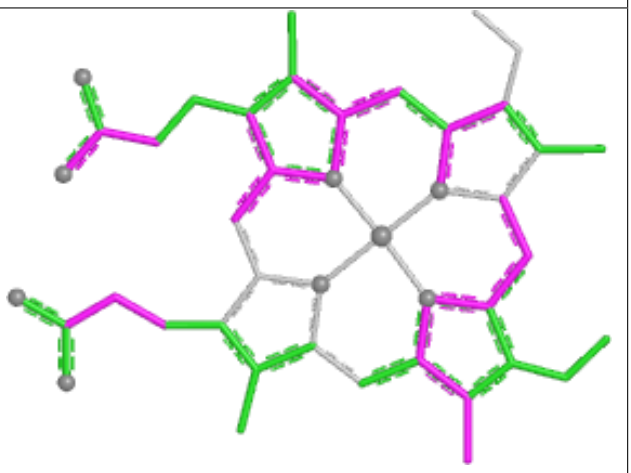

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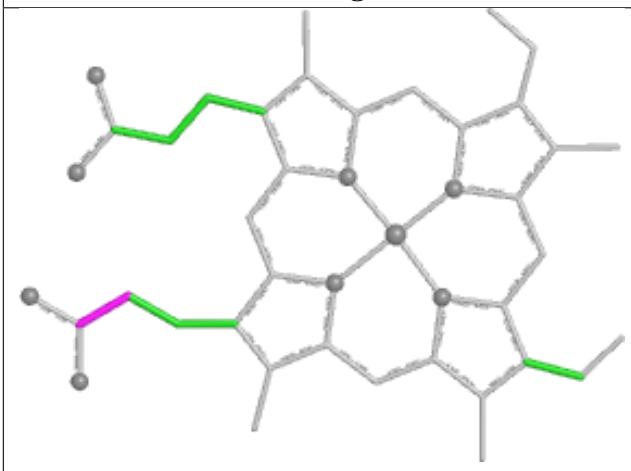

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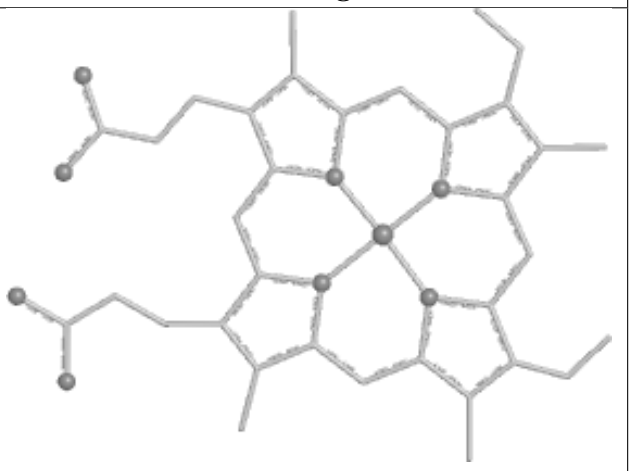
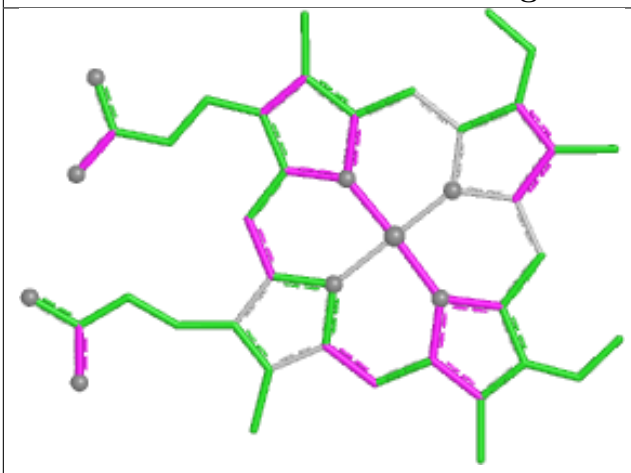


Rings

Ligand HEM E 502



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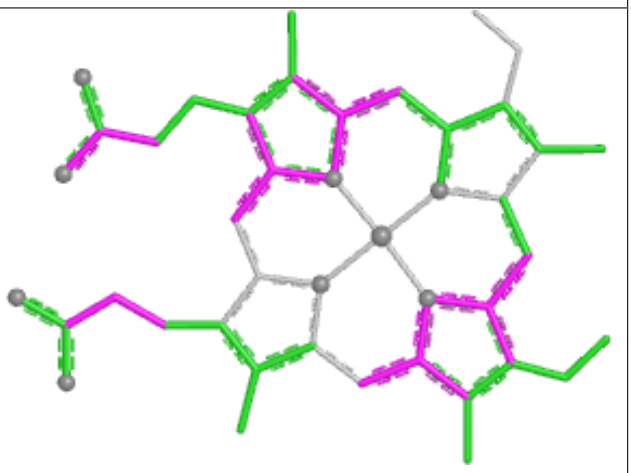

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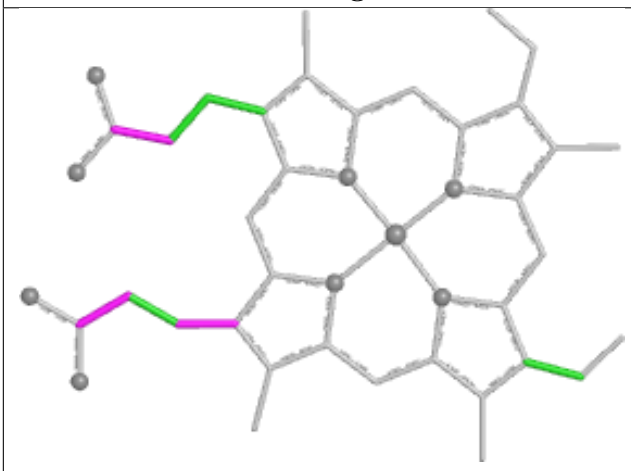

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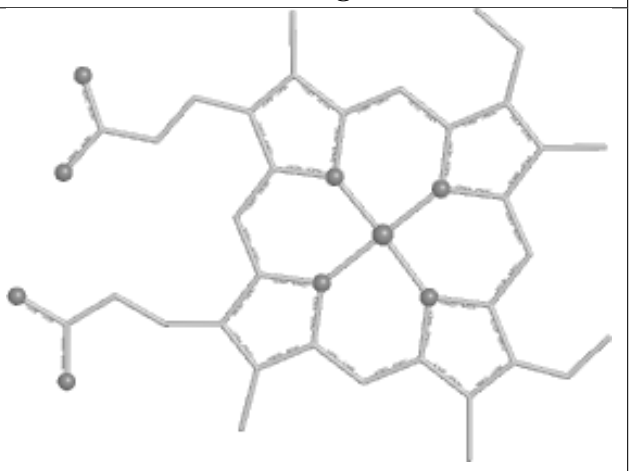
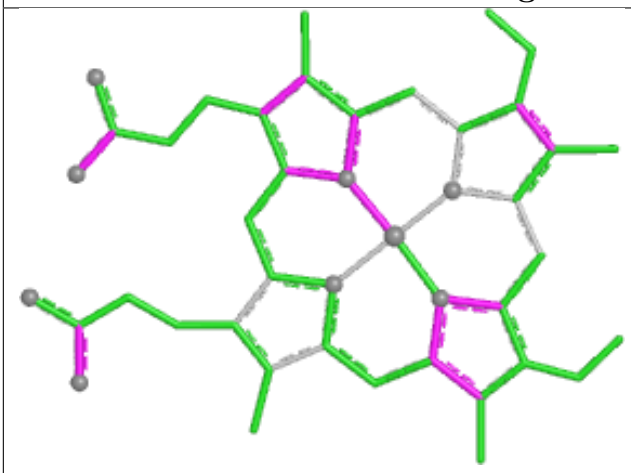


Rings

Ligand HEM A 501



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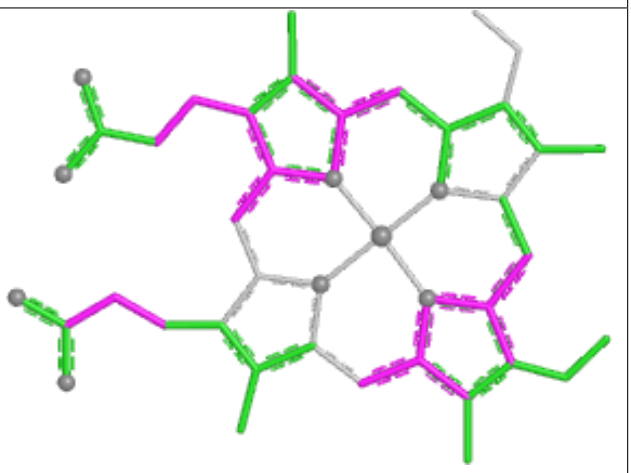

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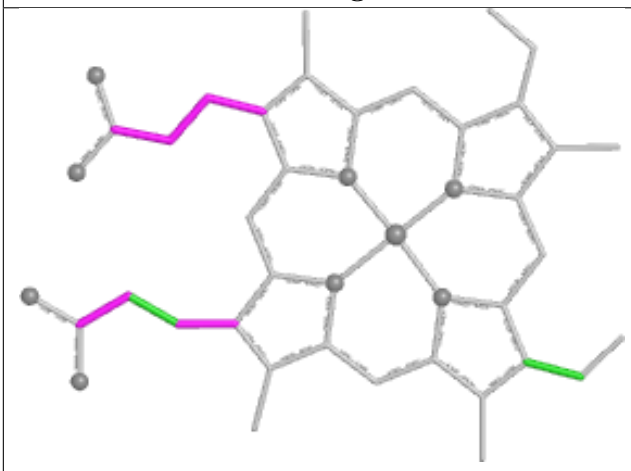

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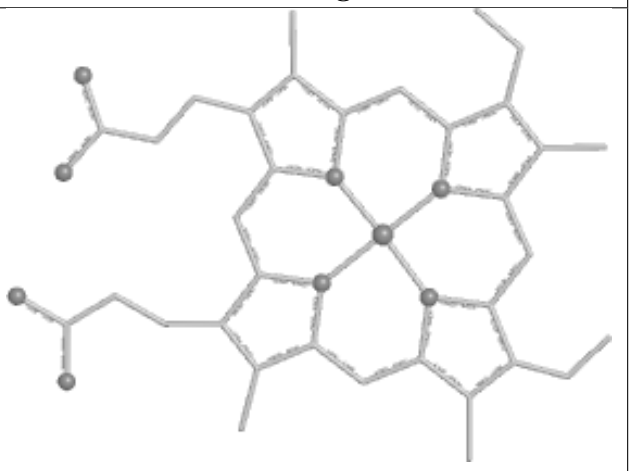
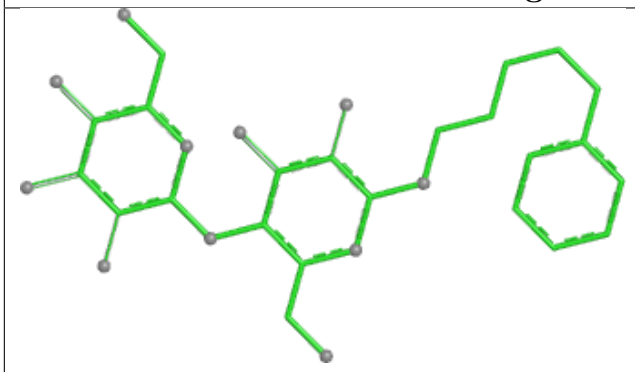


Rings

Ligand CM5 F 504



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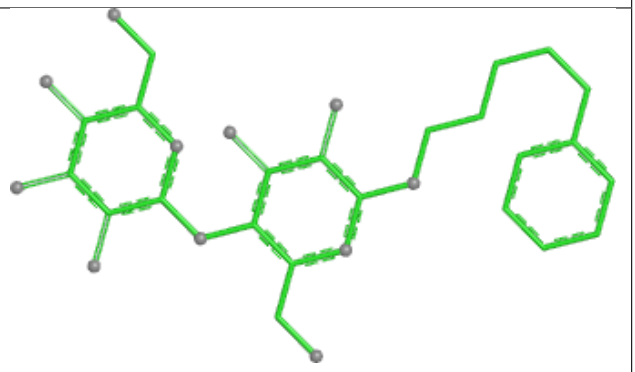

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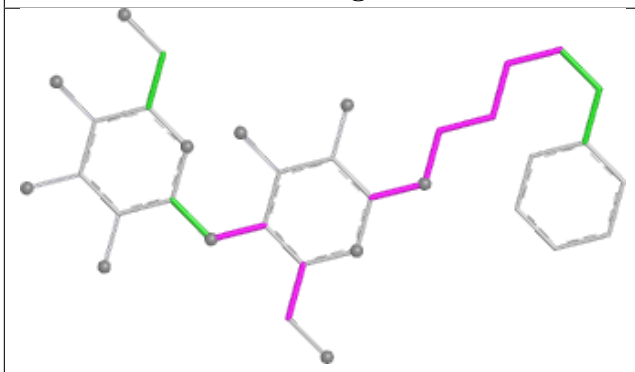

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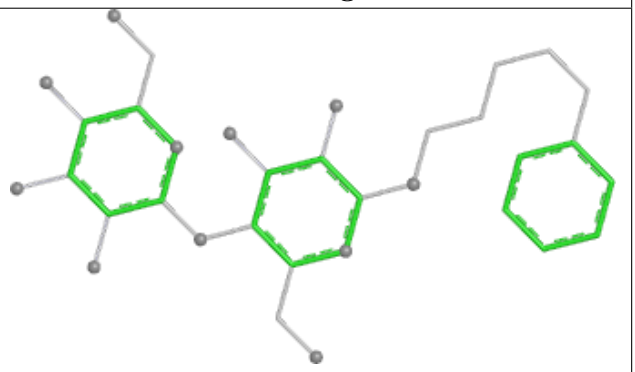
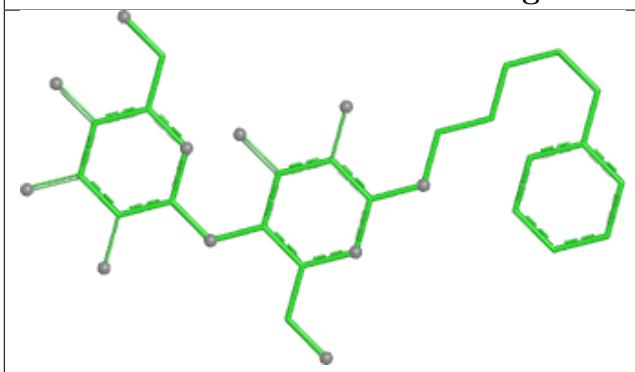


Rings

Ligand CM5 G 504



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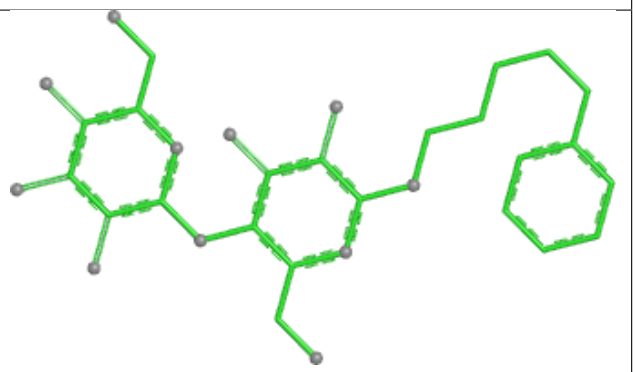

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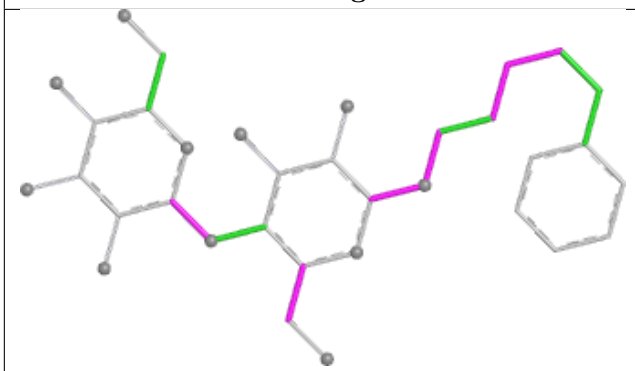

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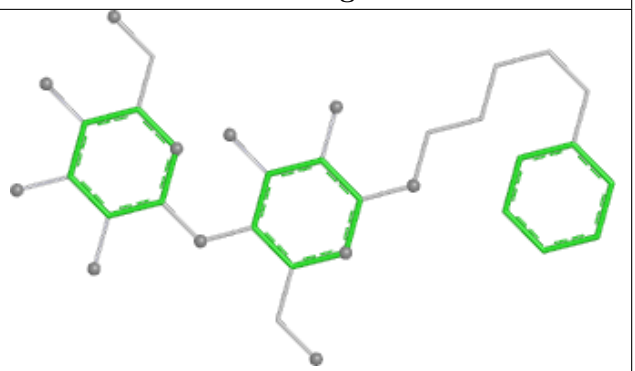
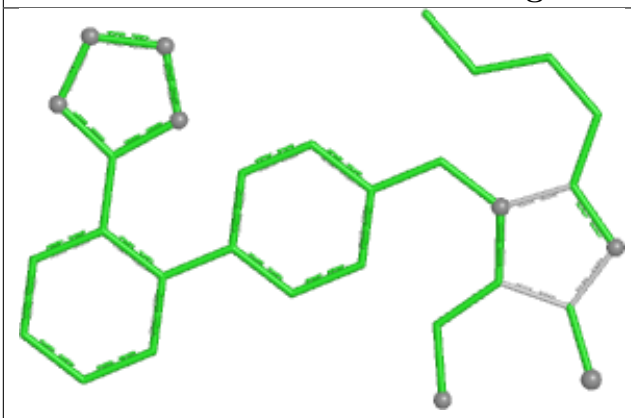


Rings

Ligand LSN D 502



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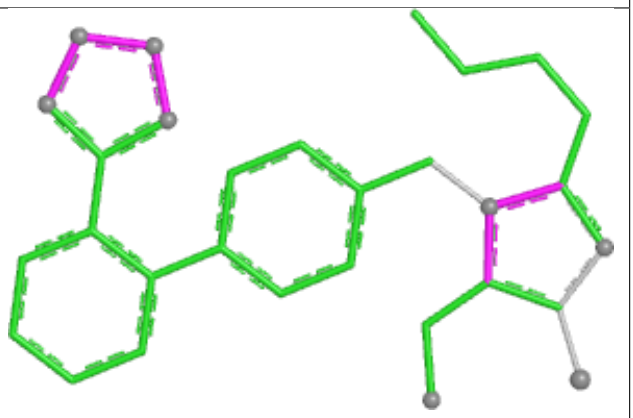

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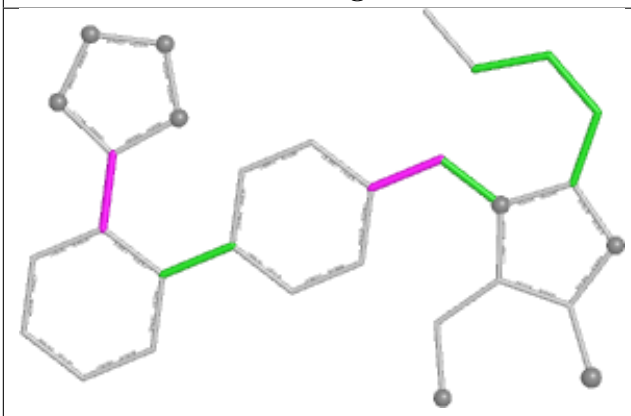

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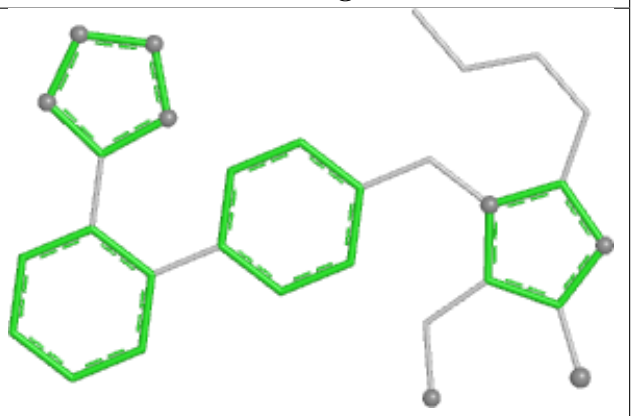
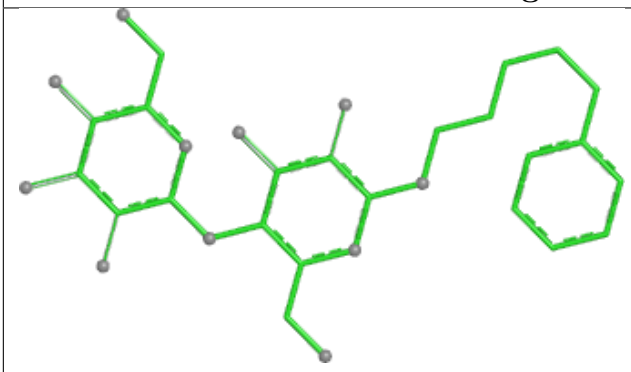


Rings

Ligand CM5 H 501



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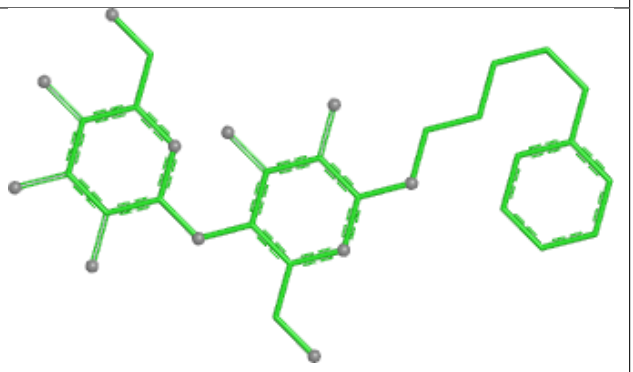

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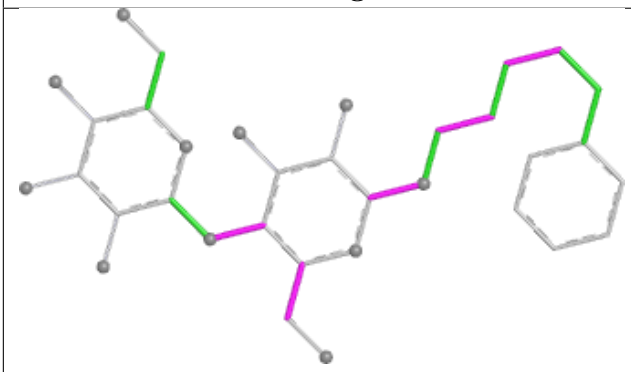

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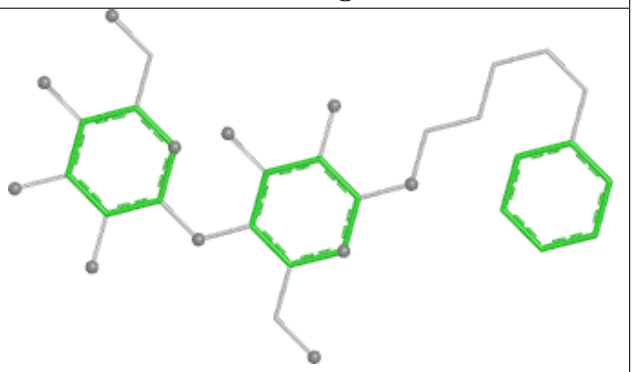
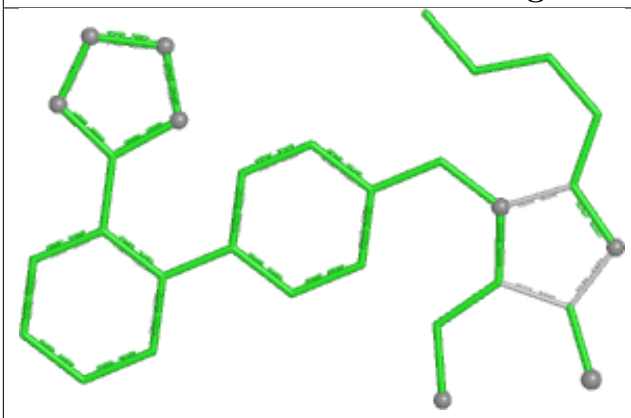


Rings

Ligand LSN B 502



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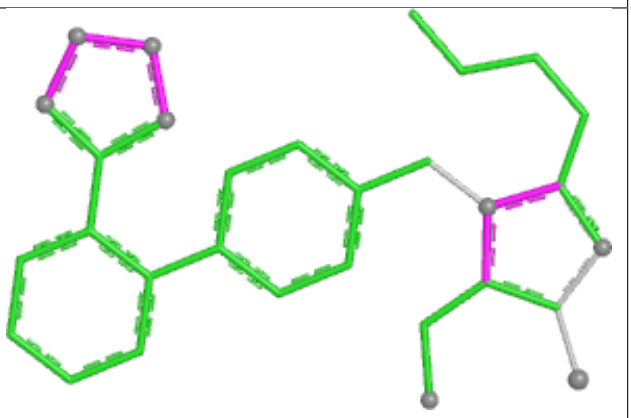
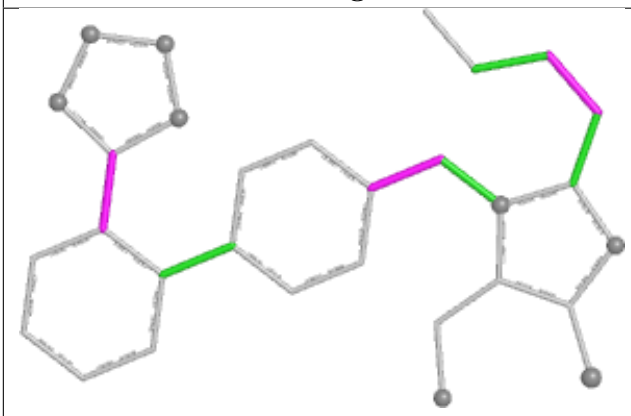


Bond angles



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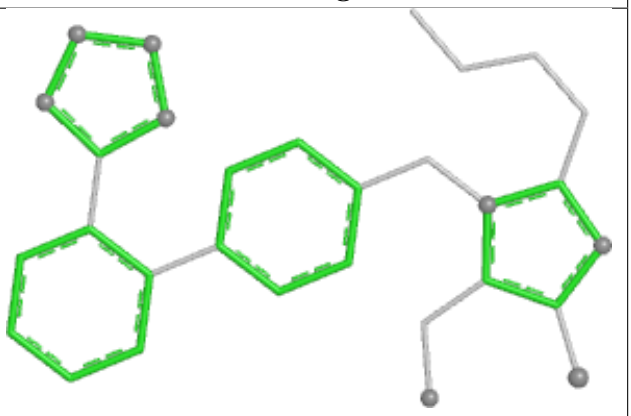
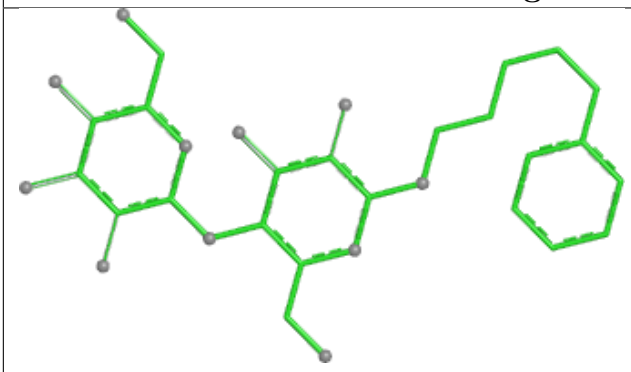


Rings

Ligand CM5 E 501



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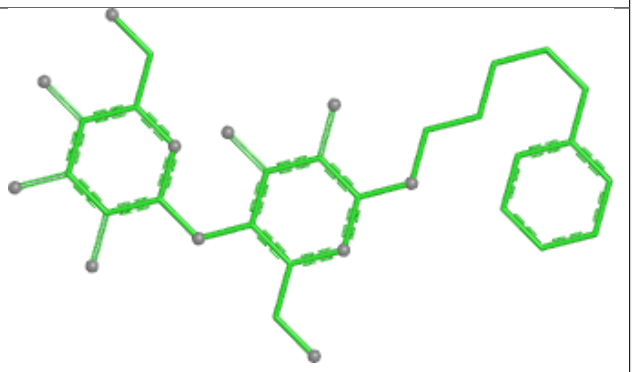

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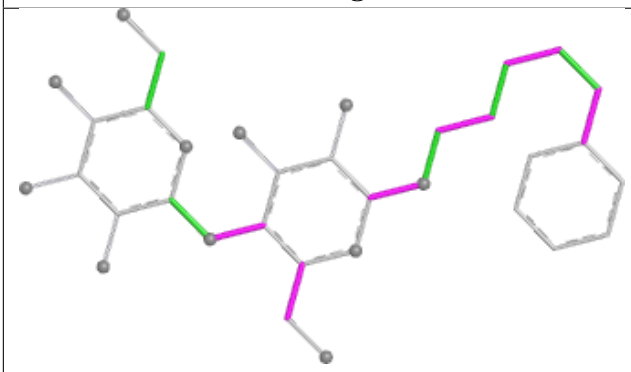
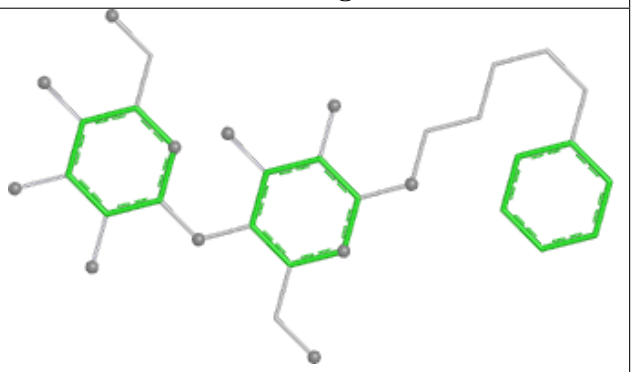


Torsions



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	461/476 (96%)	0.16	0 100 100	26, 73, 107, 152	0
1	B	461/476 (96%)	0.12	1 (0%) 95 91	26, 74, 105, 131	0
1	C	460/476 (96%)	0.14	1 (0%) 95 91	26, 75, 103, 136	0
1	D	461/476 (96%)	0.14	0 100 100	26, 73, 107, 148	0
1	E	460/476 (96%)	0.17	0 100 100	26, 81, 116, 158	0
1	F	460/476 (96%)	0.20	3 (0%) 87 77	26, 81, 118, 184	0
1	G	462/476 (97%)	0.23	4 (0%) 84 71	26, 83, 117, 182	0
1	H	459/476 (96%)	0.17	0 100 100	26, 80, 115, 173	0
All	All	3684/3808 (96%)	0.17	9 (0%) 95 91	26, 77, 113, 184	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	240	MET	2.8
1	G	244	ILE	2.8
1	G	134	PHE	2.6
1	F	244	ILE	2.6
1	G	136	MET	2.1
1	C	320	THR	2.1
1	F	257	MET	2.1
1	F	139	ARG	2.1
1	B	372	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

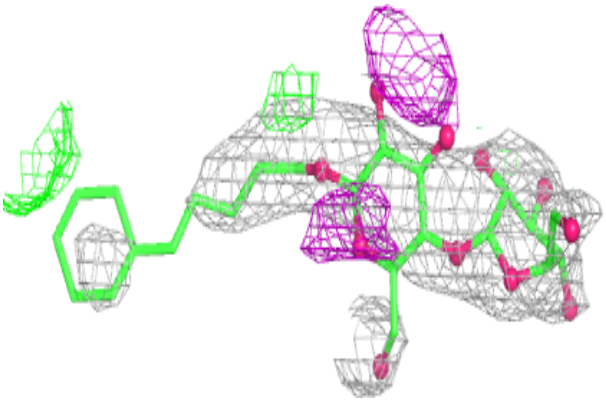
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

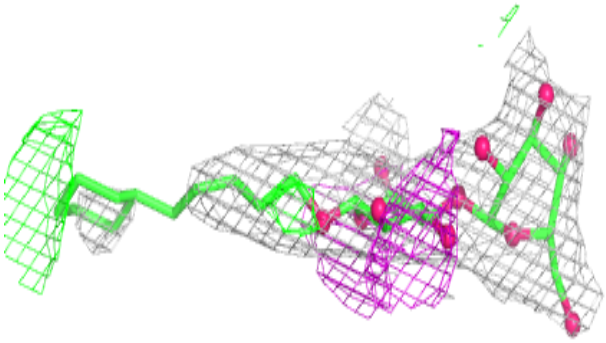
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	G	505	5/5	0.62	0.19	169,180,184,187	0
5	SO4	F	505	5/5	0.70	0.19	174,177,187,193	0
4	CM5	G	501	34/34	0.72	0.43	77,138,158,165	0
4	CM5	H	501	34/34	0.73	0.41	78,128,150,157	0
4	CM5	E	501	34/34	0.76	0.48	83,130,155,167	0
4	CM5	E	504	34/34	0.77	0.46	90,121,138,147	0
4	CM5	F	501	34/34	0.78	0.44	78,134,161,164	0
5	SO4	E	505	5/5	0.80	0.13	163,167,183,183	0
4	CM5	H	504	34/34	0.83	0.36	80,121,150,161	0
4	CM5	F	504	34/34	0.86	0.38	79,120,148,153	0
4	CM5	G	504	34/34	0.88	0.32	88,115,124,130	0
3	LSN	C	502	30/30	0.92	0.51	69,88,117,122	0
3	LSN	F	503	30/30	0.94	0.43	73,88,101,111	0
3	LSN	B	502	30/30	0.94	0.47	69,93,109,111	0
3	LSN	A	502	30/30	0.94	0.40	65,86,112,116	0
3	LSN	D	502	30/30	0.94	0.42	71,88,109,111	0
3	LSN	H	503	30/30	0.95	0.43	70,79,108,111	0
3	LSN	G	503	30/30	0.95	0.42	77,94,110,114	0
3	LSN	E	503	30/30	0.96	0.42	67,76,112,118	0
2	HEM	D	501	43/43	0.99	0.29	51,55,61,69	0
2	HEM	E	502	43/43	0.99	0.26	42,48,62,67	0
2	HEM	F	502	43/43	0.99	0.27	42,55,66,80	0
2	HEM	G	502	43/43	0.99	0.26	45,54,63,73	0
2	HEM	H	502	43/43	0.99	0.29	45,52,63,73	0
2	HEM	A	501	43/43	0.99	0.27	47,52,62,76	0
2	HEM	B	501	43/43	0.99	0.27	42,49,60,67	0
2	HEM	C	501	43/43	0.99	0.27	40,48,59,67	0

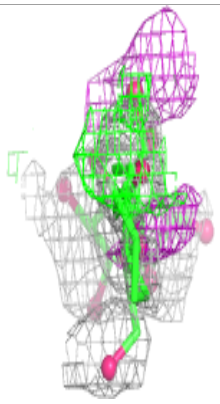
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CM5 G 501:

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

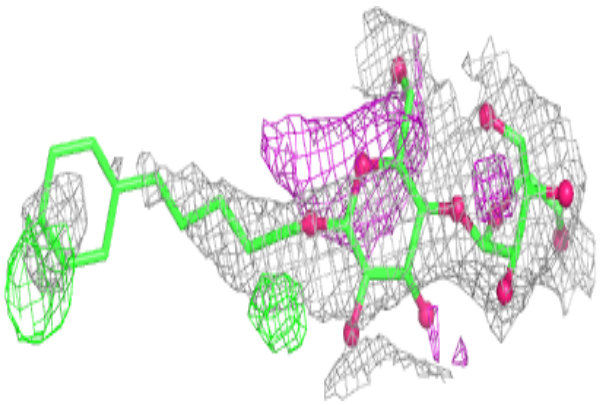


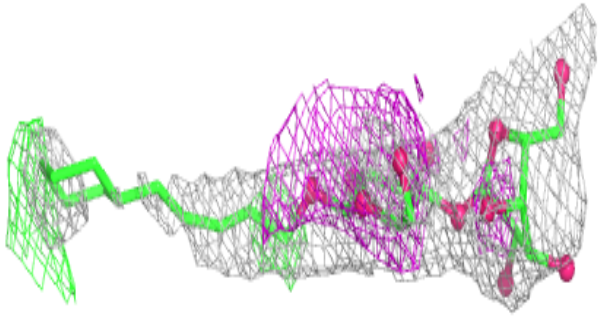


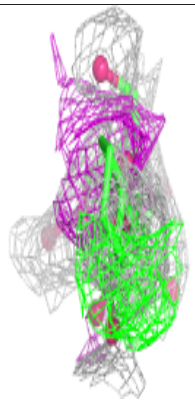


Electron density around CM5 H 501:

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

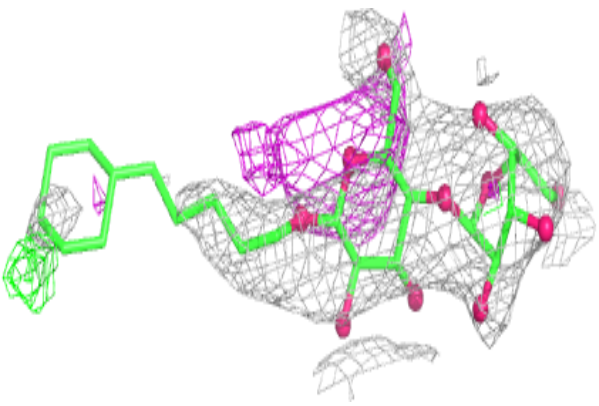


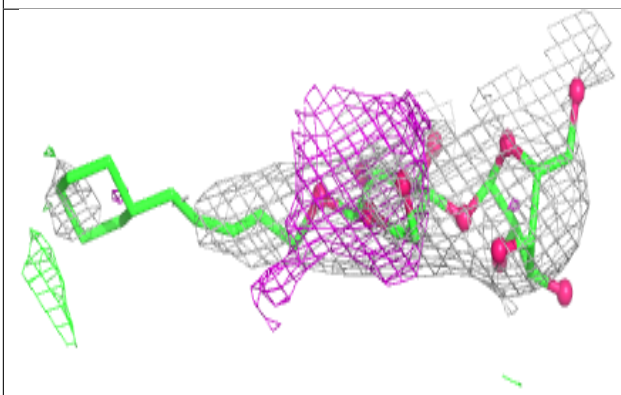


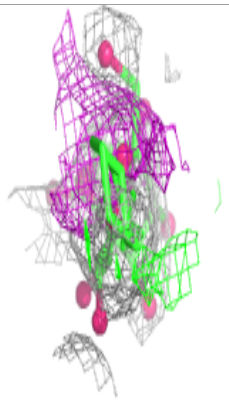


Electron density around CM5 E 501:

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

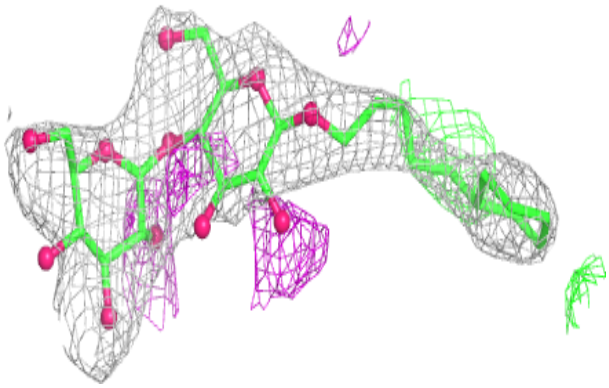


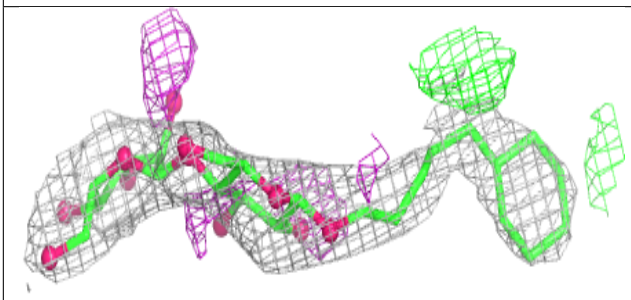


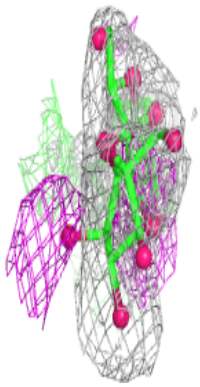


Electron density around CM5 E 504:

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

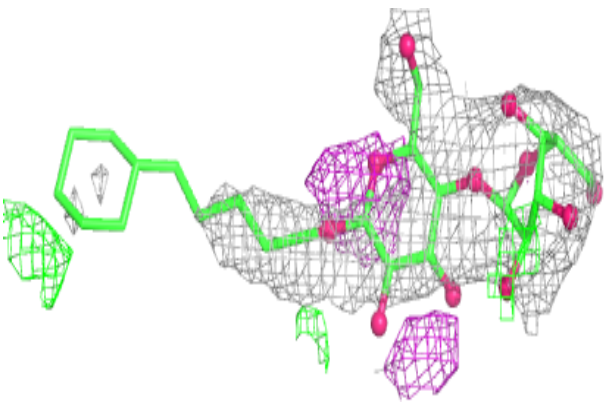


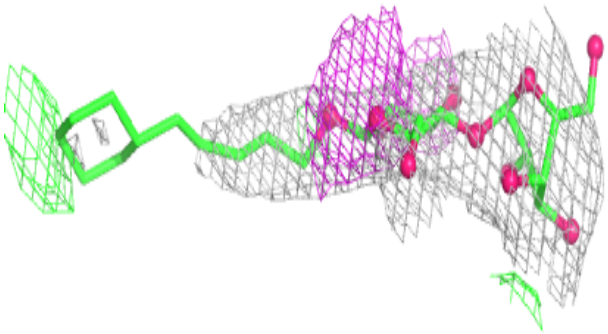


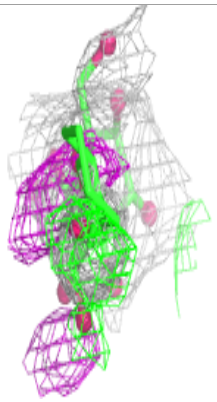


Electron density around CM5 F 501:

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

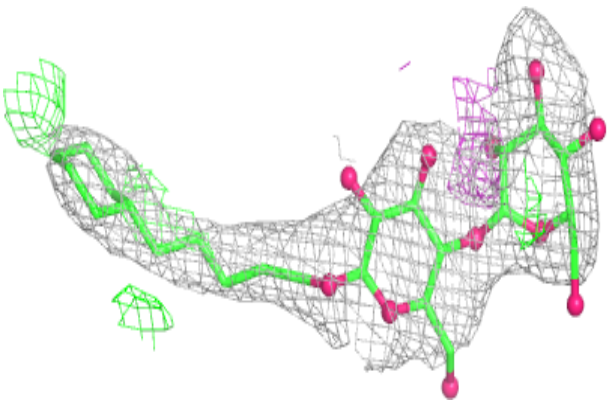


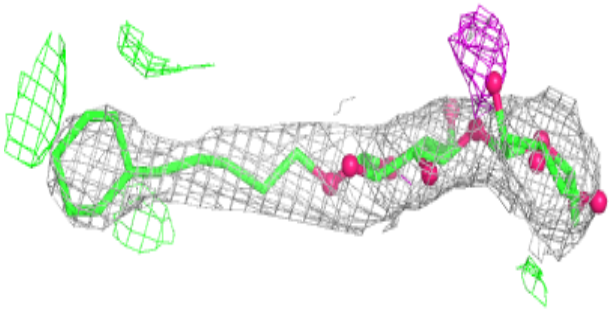


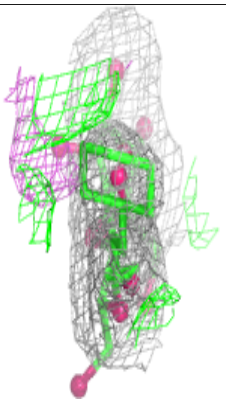


Electron density around CM5 H 504:

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

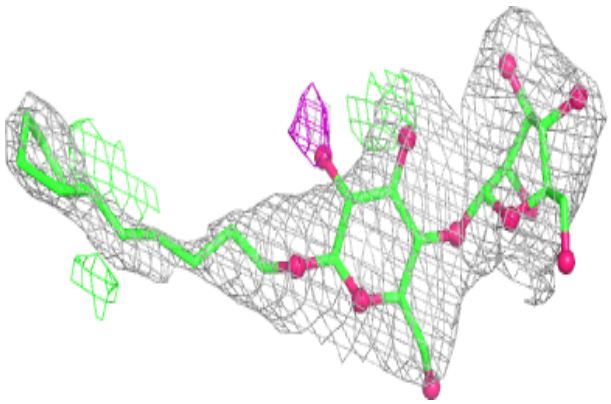


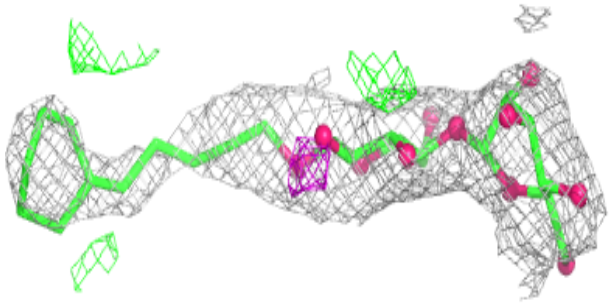


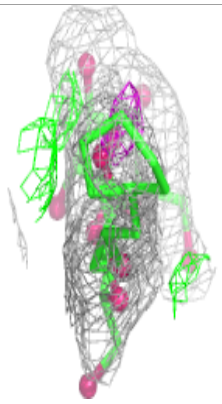


Electron density around CM5 F 504:

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

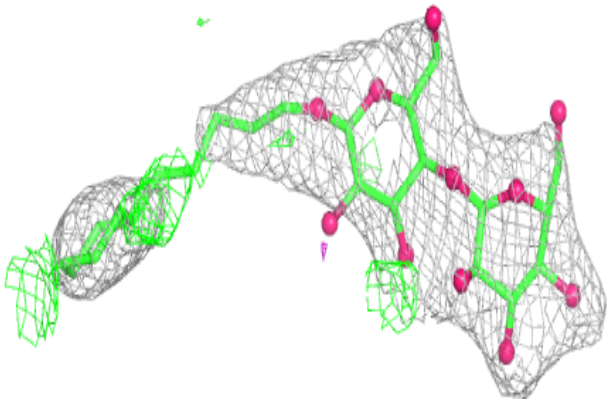


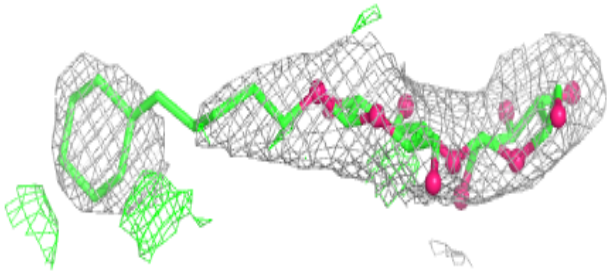


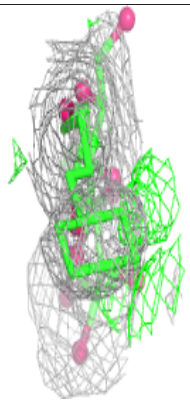


Electron density around CM5 G 504:

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

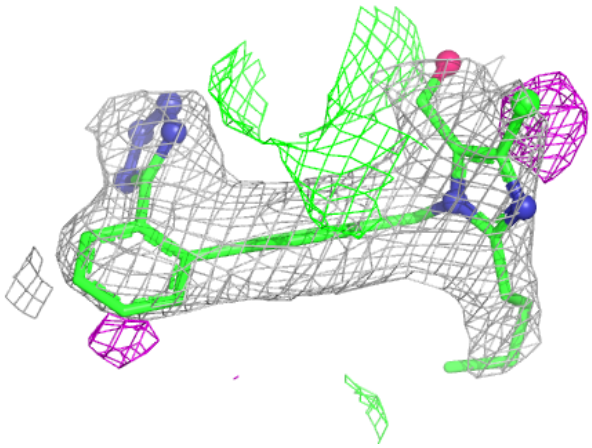


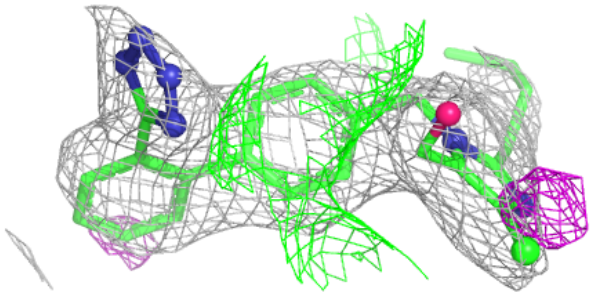


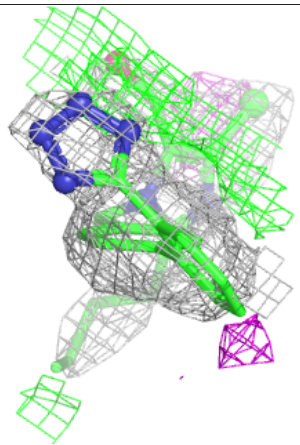


Electron density around LSN C 502:

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

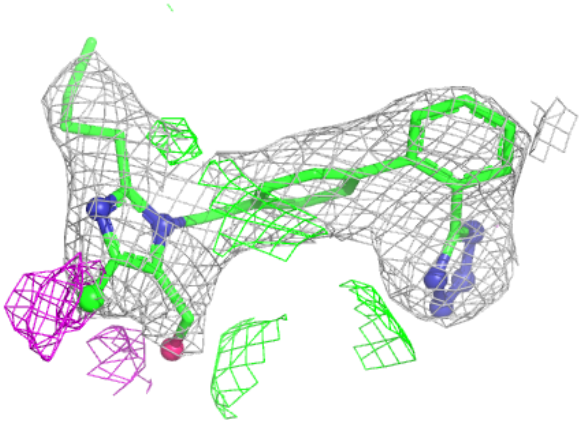


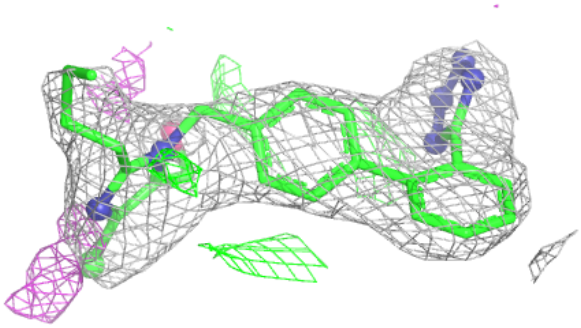


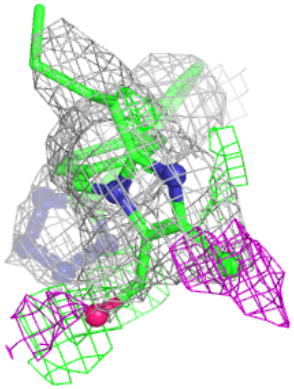


Electron density around LSN F 503:

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

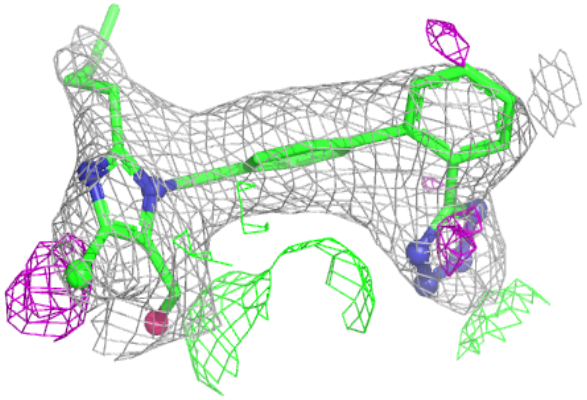


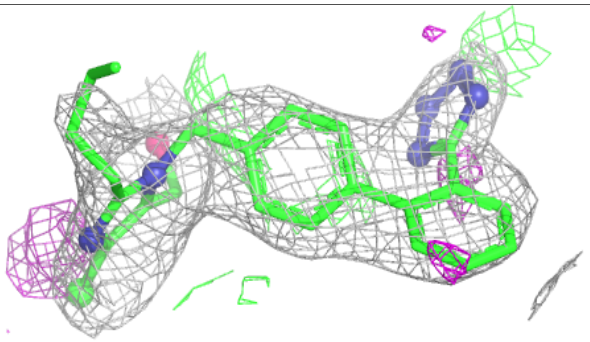


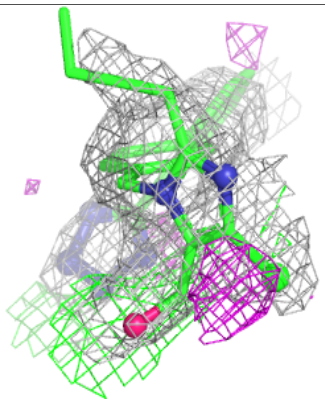


Electron density around LSN B 502:

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

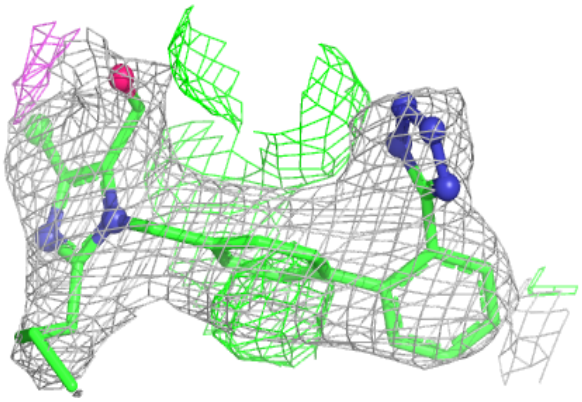


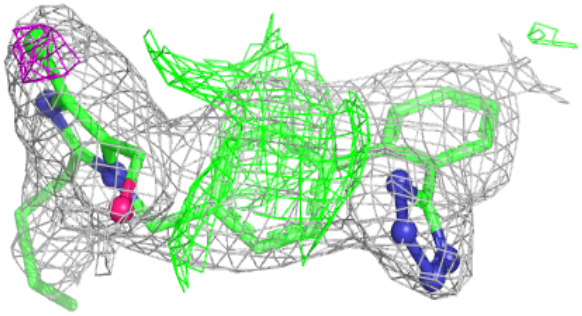


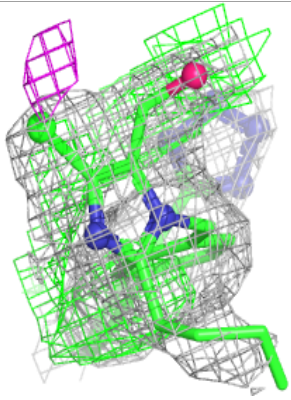


Electron density around LSN A 502:

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

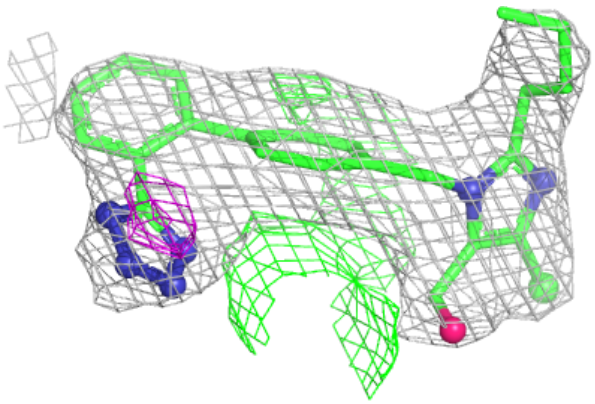


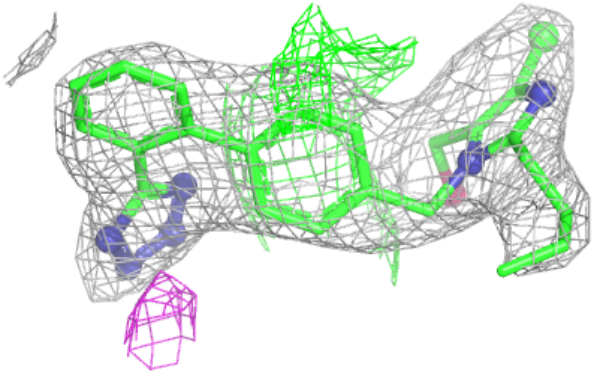


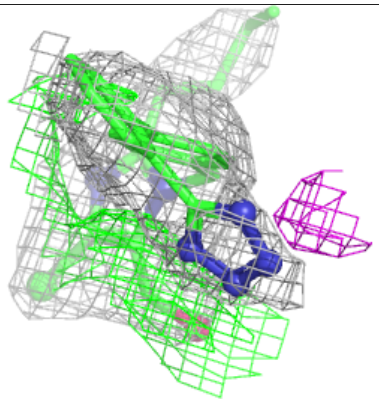


Electron density around LSN D 502:

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

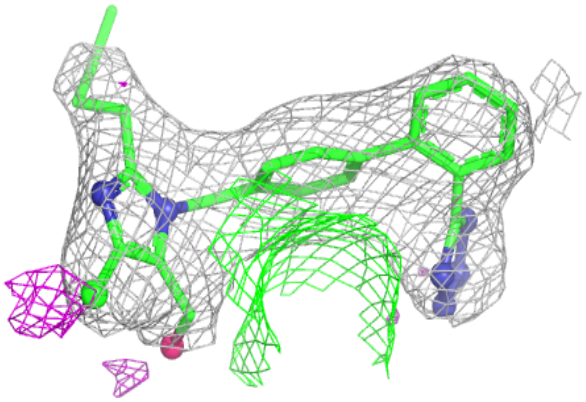


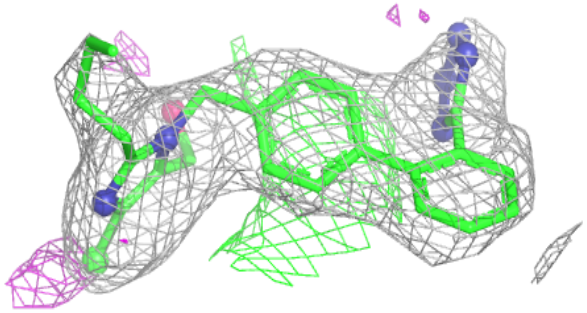


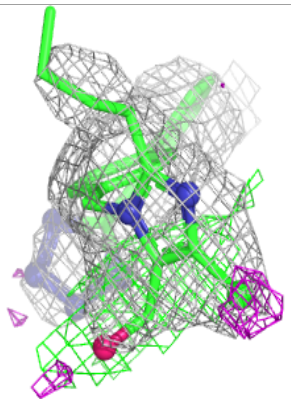


Electron density around LSN H 503:

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

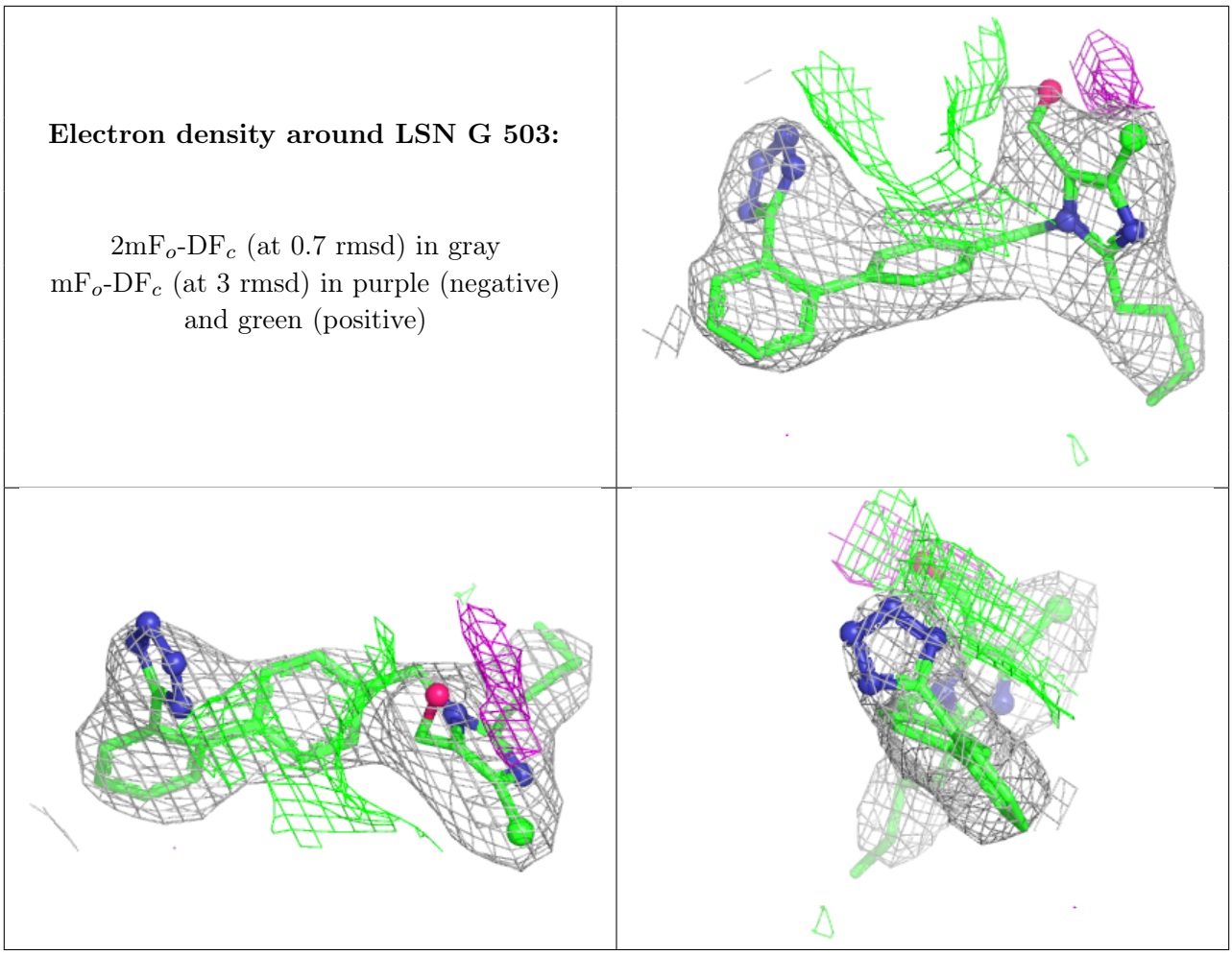






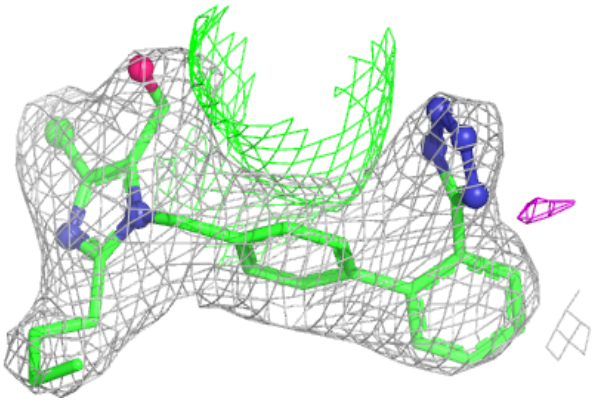
Electron density around LSN G 503:

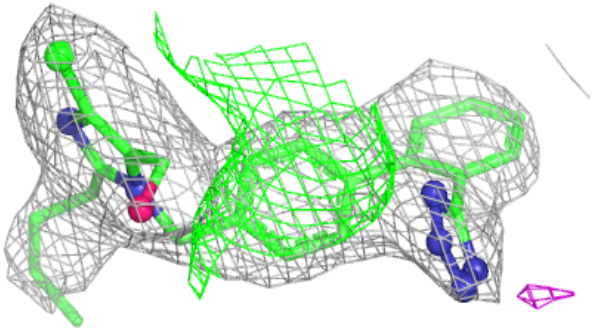
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

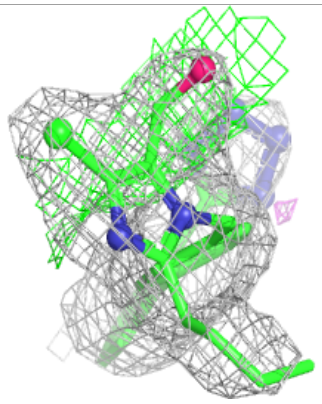


Electron density around LSN E 503:

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

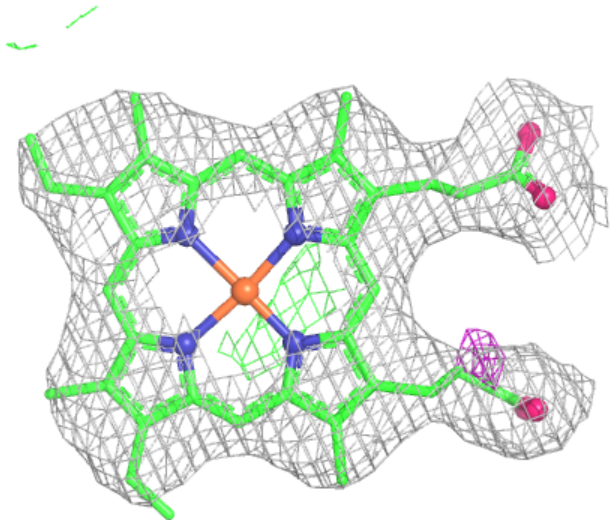


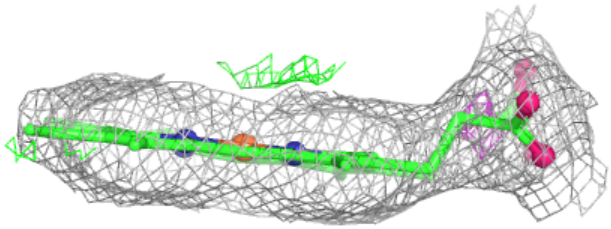


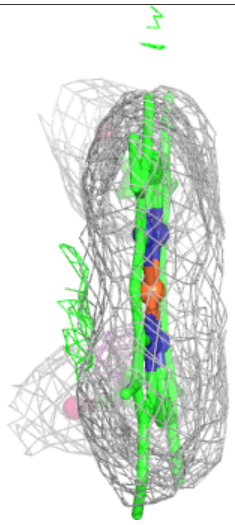


Electron density around HEM D 501:

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

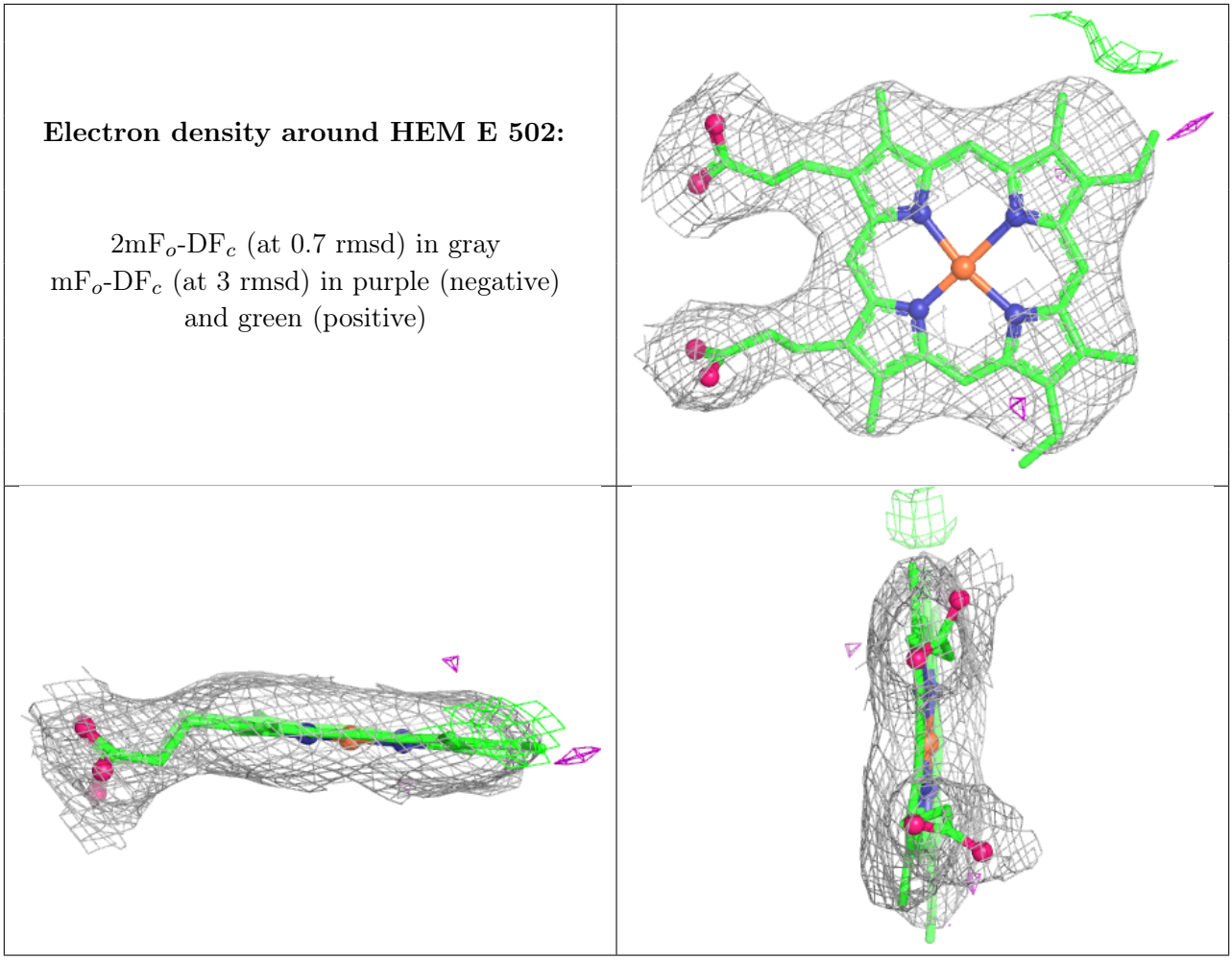






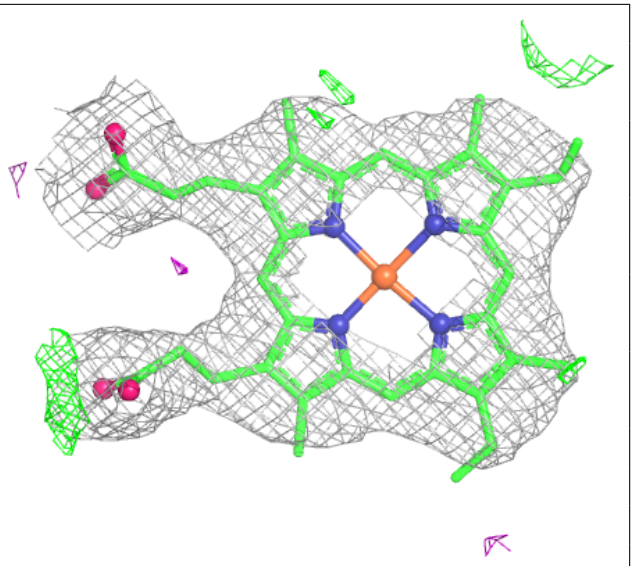
Electron density around HEM E 502:

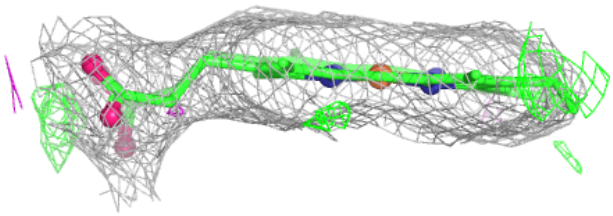
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

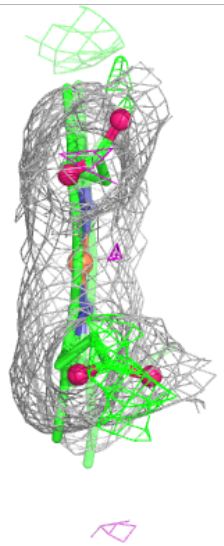


Electron density around HEM F 502:

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

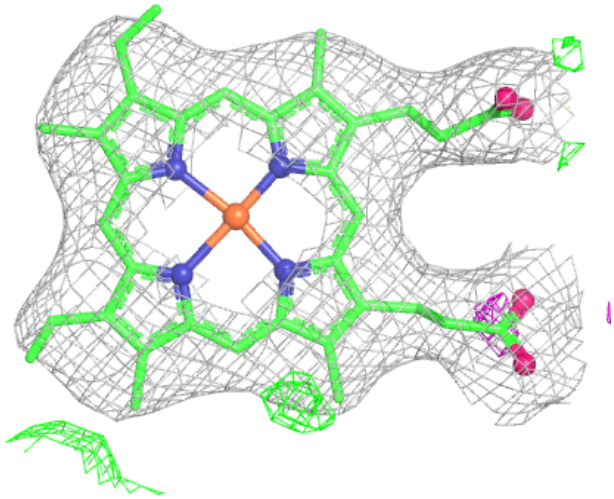


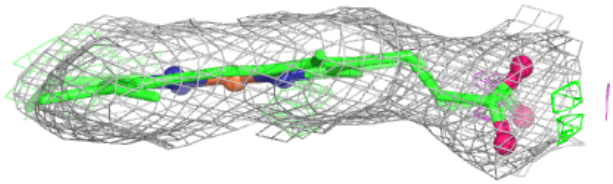


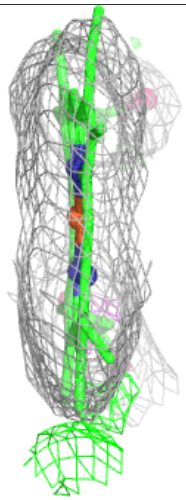


Electron density around HEM G 502:

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

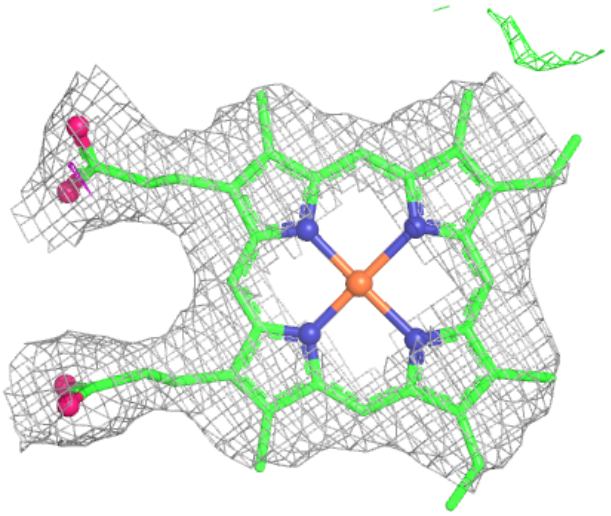


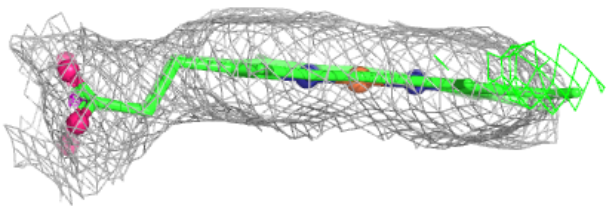


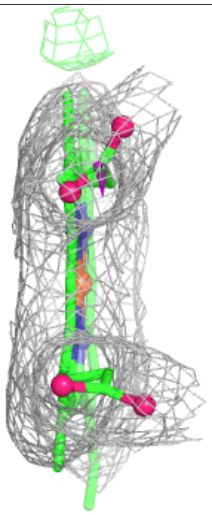


Electron density around HEM H 502:

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

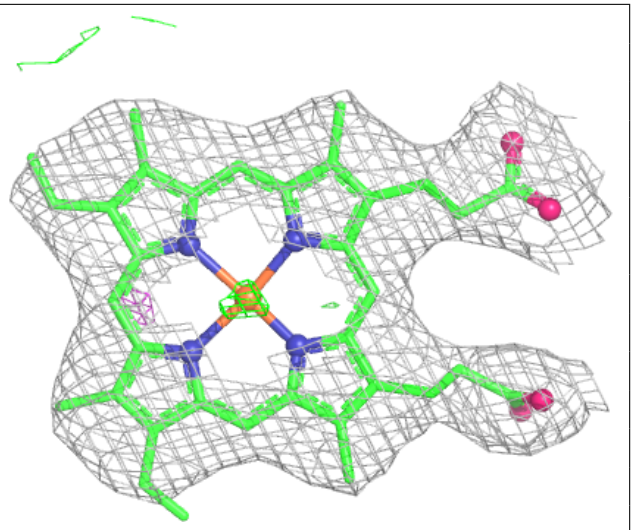


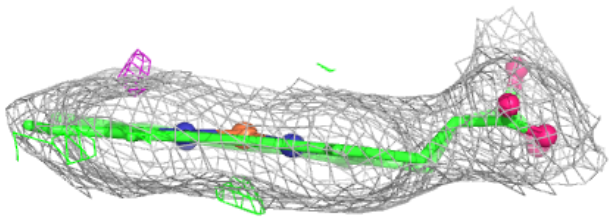


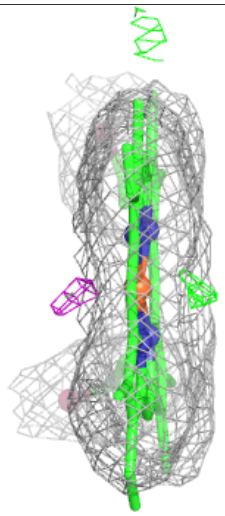


Electron density around HEM A 501:

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

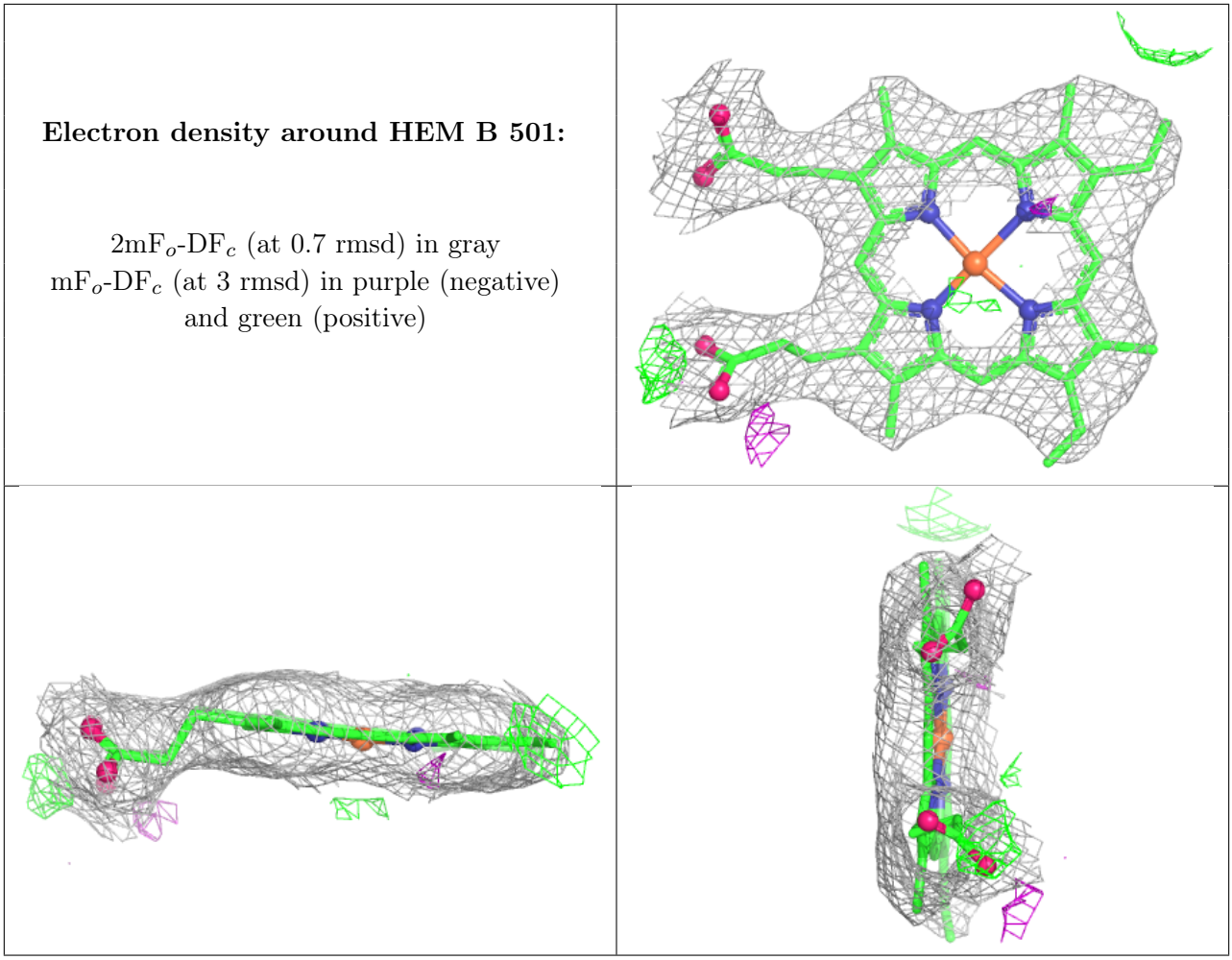






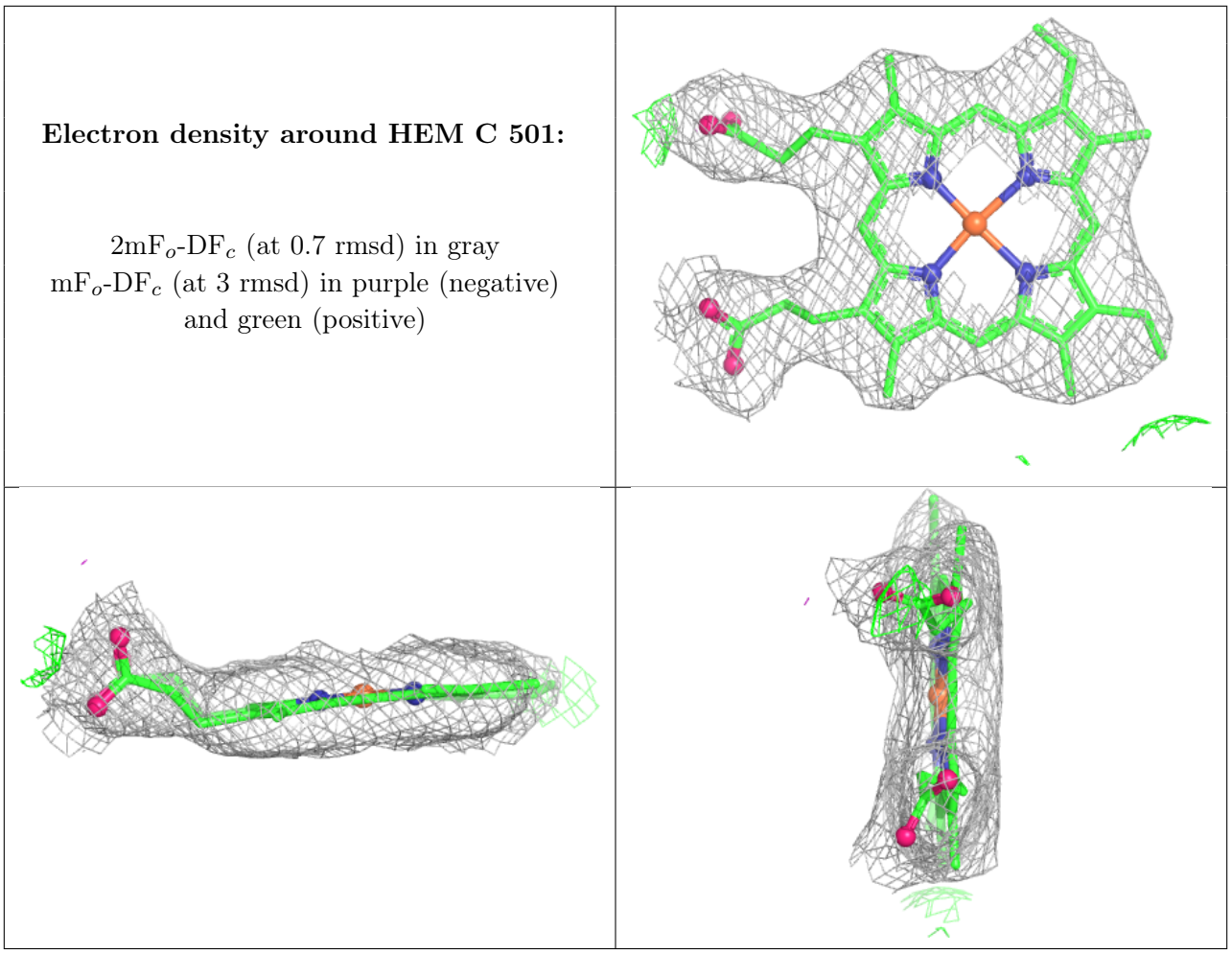
Electron density around HEM B 501:

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



Electron density around HEM C 501:

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



6.5 Other polymers

There are no such residues in this entry.