Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 11:56 pm BST

PDB ID	:	4UHI
Title	:	HUMAN STEROL 14-ALPHA DEMETHYLASE (CYP51) IN COMPLEX WITH VFV IN C121 SPACE GROUP
Authors	:	Hargrove, T.Y.; Wawrzak, Z.; I Lepesheva, G.
Deposited on	:	2015-03-24
Resolution	:	2.04 Å(reported)

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

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

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

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

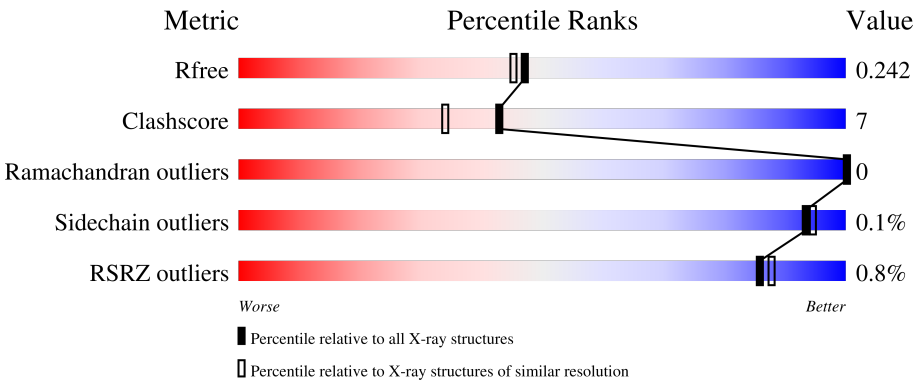
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	443	.% 89% 10%
1	B	443	90% 9%
1	C	443	.% 90% 10%
1	D	443	2% 89% 10%

2 Entry composition (i)

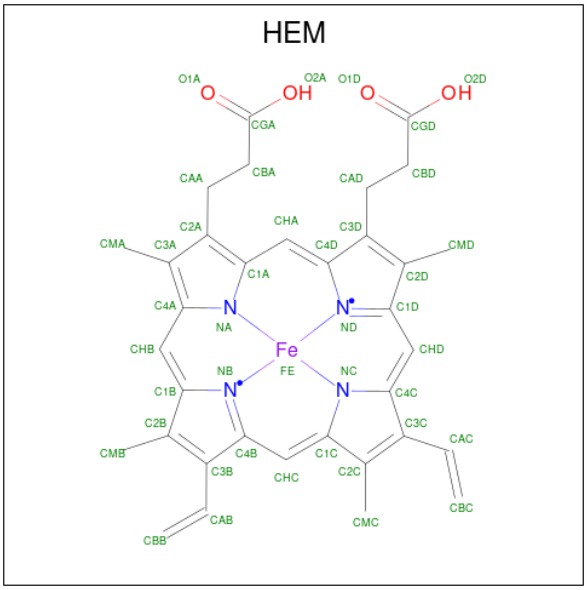
There are 4 unique types of molecules in this entry. The entry contains 15422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STEROL 14-ALPHA DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3567	2296	607	648	16	0	0	0
1	B	442	3567	2296	607	648	16	0	0	0
1	C	442	3567	2296	607	648	16	0	0	0
1	D	442	3567	2296	607	648	16	0	0	0

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



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

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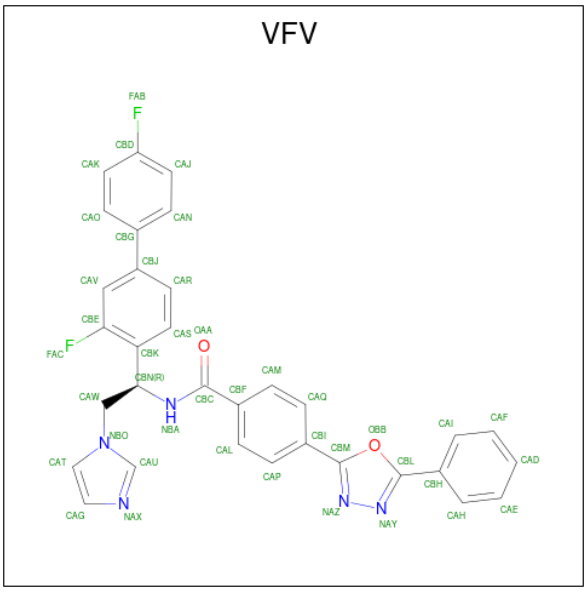
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is N-[(1R)-1-(3,4'-difluorobiphenyl-4-yl)-2-(1H-imidazol-1-yl)ethyl]-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide (three-letter code: VFV) (formula: $C_{32}H_{23}F_2N_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	41	32	2	5	2	0	0
			Total	C	F	N	O		
3	A	1	41	32	2	5	2	0	0
			Total	C	F	N	O		
3	B	1	41	32	2	5	2	0	0
			Total	C	F	N	O		
3	B	1	41	32	2	5	2	0	0
			Total	C	F	N	O		
3	C	1	41	32	2	5	2	0	0
			Total	C	F	N	O		
3	C	1	41	32	2	5	2	0	0
			Total	C	F	N	O		
3	D	1	41	32	2	5	2	0	0
			Total	C	F	N	O		
3	D	1	41	32	2	5	2	0	0

- Molecule 4 is water.

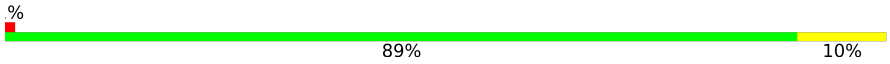
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	222	222	222	0	0
			Total	O		
4	B	180	180	180	0	0
			Total	O		
4	C	131	131	131	0	0
			Total	O		
4	D	121	121	121	0	0

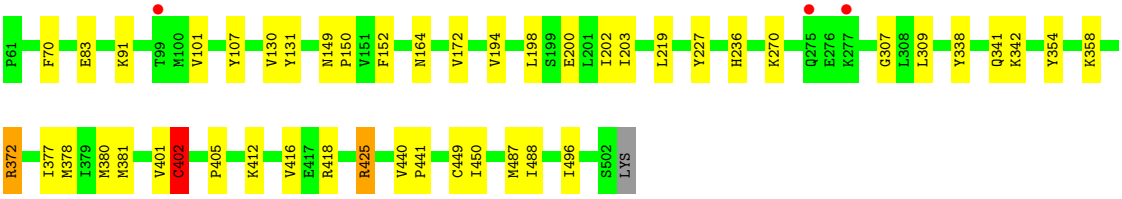
3 Residue-property plots (i)

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: STEROL 14-ALPHA DEMETHYLASE

Chain A:



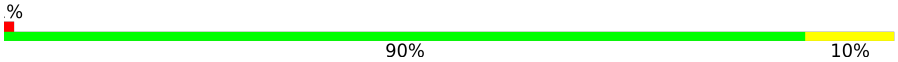


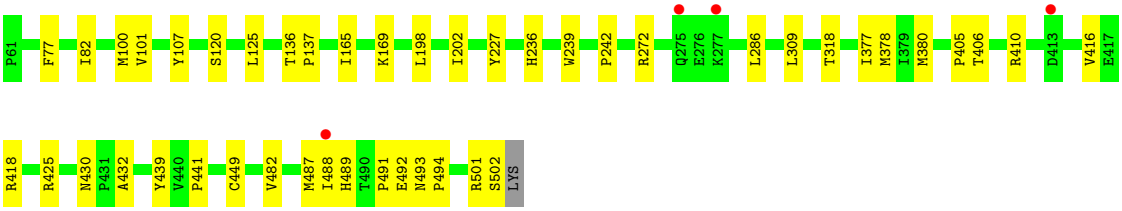
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain B:

• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

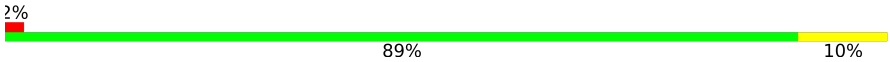
Chain C:

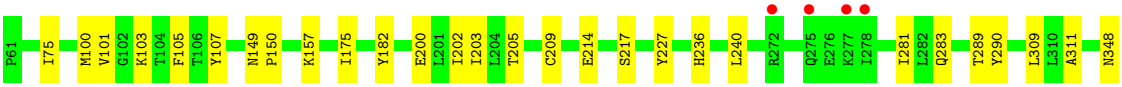


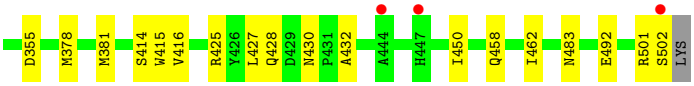


• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain D:






D355
M378
M381
S414
W415
V416
R425
Y426
L427
Q428
D429
N430
P431
A432
A444
H447
I450
Q458
I462
N483
E492
R501
S502
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.66Å 145.87Å 115.99Å 90.00° 127.15° 90.00°	Depositor
Resolution (Å)	50.01 – 2.04 98.85 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-2.04) 98.8 (98.85-2.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.215 , 0.233 0.223 , 0.242	Depositor DCC
R_{free} test set	7026 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15422	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.49	1/3660 (0.0%)	0.56	4/4958 (0.1%)
1	B	0.45	0/3660	0.50	1/4958 (0.0%)
1	C	0.40	0/3660	0.47	0/4958
1	D	0.41	0/3660	0.47	0/4958
All	All	0.44	1/14640 (0.0%)	0.50	5/19832 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	VAL	C-N	-5.56	1.21	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	402	CYS	O-C-N	-9.30	107.83	122.70
1	A	425	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	372	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	372	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	425	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	CYS	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3567	0	3555	53	2
1	B	3567	0	3555	42	0
1	C	3567	0	3555	48	0
1	D	3567	0	3555	38	3
2	A	43	0	30	6	0
2	B	43	0	30	8	0
2	C	43	0	30	7	0
2	D	43	0	30	5	0
3	A	82	0	46	13	0
3	B	82	0	46	2	0
3	C	82	0	46	8	0
3	D	82	0	46	9	0
4	A	222	0	0	14	0
4	B	180	0	0	4	0
4	C	131	0	0	5	0
4	D	121	0	0	6	0
All	All	15422	0	14524	199	3

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 7.

All (199) 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:B:488:ILE:HG22	4:B:2174:HOH:O	1.39	1.18
1:C:77:PHE:HB3	1:C:100:MET:HE2	1.36	1.06
1:B:318:THR:HG21	1:B:488:ILE:HD13	1.34	1.04
1:B:318:THR:HG21	1:B:488:ILE:CD1	1.92	1.00
1:C:487:MET:HE1	4:C:2075:HOH:O	1.70	0.91
1:C:77:PHE:CB	1:C:100:MET:HE2	2.01	0.90
1:B:318:THR:CG2	1:B:488:ILE:HD13	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:TYR:OH	3:C:600:VFV:H12	1.76	0.85
1:B:318:THR:OG1	1:B:488:ILE:HD11	1.79	0.82
1:B:492:GLU:HG3	4:B:2172:HOH:O	1.82	0.79
1:C:101:VAL:HG21	3:C:600:VFV:CAN	2.13	0.78
1:B:289:THR:HG22	1:B:290:TYR:O	1.84	0.76
1:B:318:THR:CG2	1:B:488:ILE:CD1	2.64	0.74
1:C:227:TYR:CE1	1:C:309:LEU:HD23	2.21	0.74
1:C:488:ILE:HD11	3:C:600:VFV:CAD	2.18	0.73
1:A:107:TYR:OH	3:A:600:VFV:H12	1.88	0.73
1:C:318:THR:HG21	1:C:488:ILE:HG21	1.72	0.70
1:D:416:VAL:O	1:D:425:ARG:NH2	2.25	0.70
1:B:416:VAL:O	1:B:425:ARG:NH2	2.25	0.70
2:D:540:HEM:HMC2	2:D:540:HEM:HBC2	1.73	0.69
1:B:372:ARG:NH2	1:B:418:ARG:O	2.21	0.69
1:A:416:VAL:O	1:A:425:ARG:NH2	2.24	0.67
2:D:540:HEM:HBC2	2:D:540:HEM:CMC	2.25	0.67
1:A:194:VAL:CG1	1:A:496:ILE:HG21	2.25	0.67
1:C:77:PHE:CB	1:C:100:MET:CE	2.72	0.66
1:D:107:TYR:OH	3:D:600:VFV:H12	1.96	0.66
1:B:107:TYR:OH	3:B:600:VFV:H12	1.96	0.66
1:A:194:VAL:CG1	1:A:496:ILE:CG2	2.74	0.65
1:C:488:ILE:HD11	3:C:600:VFV:CAF	2.26	0.65
1:D:381:MET:HE1	4:D:2061:HOH:O	1.97	0.65
1:D:240:LEU:HD11	3:D:600:VFV:H3	1.80	0.64
1:A:194:VAL:HG13	1:A:496:ILE:CG2	2.27	0.64
1:C:378:MET:HB3	4:C:2104:HOH:O	1.98	0.64
1:A:307:GLY:HA3	3:A:580:VFV:CAJ	2.28	0.63
1:D:227:TYR:CE1	1:D:309:LEU:HD23	2.33	0.63
1:A:91:LYS:HD3	4:A:2015:HOH:O	1.99	0.63
1:A:372:ARG:NH2	1:A:418:ARG:O	2.23	0.62
1:B:501:ARG:O	1:B:502:SER:C	2.37	0.61
1:A:381:MET:HG3	1:A:402:CYS:SG	2.41	0.60
1:A:101:VAL:HG12	4:A:2020:HOH:O	2.00	0.60
1:A:358:LYS:HD2	1:A:358:LYS:N	2.16	0.60
1:B:227:TYR:CZ	1:B:309:LEU:HD23	2.37	0.60
1:B:225:GLN:HB3	4:B:2081:HOH:O	1.99	0.60
1:D:227:TYR:CZ	1:D:309:LEU:HD23	2.36	0.60
1:A:101:VAL:HG12	1:A:101:VAL:O	2.02	0.59
1:A:194:VAL:HG13	1:A:496:ILE:HG22	1.84	0.59
1:A:307:GLY:HA3	3:A:580:VFV:CAN	2.33	0.59
2:D:540:HEM:HBB2	2:D:540:HEM:HMB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:HEM:HMB2	2:B:540:HEM:HBB2	1.85	0.58
1:A:412:LYS:HG3	4:A:2181:HOH:O	2.03	0.58
1:B:227:TYR:CE1	1:B:309:LEU:HD23	2.38	0.58
1:C:318:THR:HG21	1:C:488:ILE:CG2	2.32	0.58
1:A:101:VAL:HG21	3:A:600:VFV:H4	1.86	0.58
1:A:227:TYR:CE1	1:A:309:LEU:HD23	2.38	0.58
1:D:289:THR:HG22	1:D:290:TYR:O	2.04	0.57
1:C:416:VAL:O	1:C:425:ARG:NH2	2.38	0.57
1:C:101:VAL:O	1:C:101:VAL:HG12	2.05	0.56
1:A:377:ILE:HD12	2:A:540:HEM:CHB	2.35	0.56
1:C:482:VAL:CG1	1:C:489:HIS:HB3	2.35	0.56
1:A:381:MET:HE1	4:A:2117:HOH:O	2.05	0.56
1:D:103:LYS:CE	4:D:2019:HOH:O	2.53	0.56
1:D:348:ASN:HB3	4:D:2079:HOH:O	2.06	0.56
1:A:194:VAL:HG11	1:A:496:ILE:HG21	1.86	0.56
1:C:82:ILE:HD11	1:C:406:THR:HG21	1.88	0.56
1:D:103:LYS:HE3	4:D:2019:HOH:O	2.06	0.56
1:C:120:SER:OG	1:C:125:LEU:HD12	2.04	0.56
1:B:380:MET:HE2	1:B:405:PRO:HD3	1.88	0.55
2:B:540:HEM:CMC	2:B:540:HEM:HBC2	2.37	0.55
1:C:377:ILE:HD12	2:C:540:HEM:C4A	2.42	0.55
1:A:378:MET:CE	4:A:2170:HOH:O	2.55	0.55
2:C:540:HEM:CMC	2:C:540:HEM:HBC2	2.36	0.55
1:C:449:CYS:HA	2:C:540:HEM:C4D	2.42	0.55
1:A:236:HIS:HD2	1:A:487:MET:CE	2.21	0.54
2:A:540:HEM:HBB2	2:A:540:HEM:HMB2	1.88	0.54
1:A:378:MET:HE3	4:A:2170:HOH:O	2.07	0.54
2:B:540:HEM:HBC2	2:B:540:HEM:HMC2	1.89	0.54
1:C:227:TYR:CZ	1:C:309:LEU:CD2	2.91	0.53
1:D:348:ASN:ND2	4:D:2080:HOH:O	2.40	0.53
1:B:377:ILE:HD12	2:B:540:HEM:CHB	2.38	0.53
1:C:227:TYR:CZ	1:C:309:LEU:HD23	2.44	0.53
1:A:307:GLY:C	3:A:580:VFV:H4	2.29	0.53
1:B:380:MET:CE	1:B:405:PRO:HD3	2.37	0.53
1:C:77:PHE:CG	1:C:100:MET:HE2	2.43	0.53
1:A:378:MET:HB3	4:A:2169:HOH:O	2.08	0.53
1:B:67:PRO:O	1:B:69:PRO:HD3	2.09	0.53
1:B:379:ILE:HD12	3:B:600:VFV:H12	1.91	0.53
1:A:70:PHE:CZ	1:A:101:VAL:HG13	2.43	0.53
1:C:492:GLU:HG3	4:C:2123:HOH:O	2.08	0.52
1:C:77:PHE:CG	1:C:100:MET:CE	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:MET:HE1	1:C:405:PRO:HG3	1.91	0.52
1:B:378:MET:HG2	1:B:406:THR:OG1	2.10	0.51
1:A:236:HIS:HD2	1:A:487:MET:HE1	1.76	0.51
1:C:482:VAL:HG13	1:C:489:HIS:HB3	1.93	0.51
2:B:540:HEM:HBB2	2:B:540:HEM:CMB	2.41	0.51
2:C:540:HEM:HBC2	2:C:540:HEM:HMC2	1.93	0.51
4:A:2062:HOH:O	1:D:75:ILE:HD12	2.11	0.50
1:B:380:MET:HE1	1:B:405:PRO:HG3	1.92	0.50
1:B:318:THR:CG2	1:B:488:ILE:HD11	2.42	0.50
1:B:380:MET:HG2	2:B:540:HEM:CGA	2.41	0.50
1:B:378:MET:SD	1:B:378:MET:O	2.69	0.50
1:A:130:VAL:HG23	1:A:131:TYR:CD1	2.47	0.49
1:D:105:PHE:CE1	3:D:600:VFV:H13	2.47	0.49
1:D:483:ASN:HB2	1:D:492:GLU:HG2	1.94	0.49
1:C:100:MET:SD	3:C:600:VFV:H9	2.52	0.49
1:D:501:ARG:O	1:D:502:SER:C	2.51	0.49
1:D:101:VAL:HG21	3:D:600:VFV:H5	1.94	0.49
2:A:540:HEM:HBB2	2:A:540:HEM:CMB	2.43	0.48
1:D:101:VAL:CG2	3:D:600:VFV:H5	2.44	0.48
1:C:236:HIS:CE1	3:C:600:VFV:H6	2.49	0.48
2:D:540:HEM:HBB2	2:D:540:HEM:CMB	2.43	0.48
1:B:449:CYS:HA	2:B:540:HEM:C4D	2.49	0.47
2:A:540:HEM:HBC2	2:A:540:HEM:CMC	2.44	0.47
1:A:227:TYR:CZ	1:A:309:LEU:HD23	2.49	0.47
1:A:152:PHE:HE1	3:A:580:VFV:H2	1.80	0.47
1:B:488:ILE:HG23	1:B:488:ILE:O	2.15	0.47
1:D:240:LEU:CD1	3:D:600:VFV:H3	2.45	0.47
1:C:501:ARG:O	1:C:502:SER:C	2.53	0.46
1:D:430:ASN:OD1	1:D:432:ALA:HB3	2.14	0.46
1:A:152:PHE:CE1	3:A:580:VFV:H2	2.51	0.46
1:C:493:ASN:N	1:C:494:PRO:HD3	2.31	0.46
1:A:378:MET:CG	4:A:2170:HOH:O	2.63	0.46
1:A:338:TYR:CE2	1:A:342:LYS:HE2	2.51	0.46
1:D:209:CYS:O	1:D:281:ILE:HD12	2.16	0.46
1:D:214:GLU:O	1:D:217:SER:OG	2.32	0.46
2:D:540:HEM:HMC2	2:D:540:HEM:CBC	2.46	0.45
1:B:318:THR:CB	1:B:488:ILE:HD11	2.46	0.45
1:D:236:HIS:CE1	3:D:600:VFV:H6	2.50	0.45
1:A:307:GLY:CA	3:A:580:VFV:CAN	2.94	0.45
1:D:100:MET:SD	3:D:600:VFV:H9	2.56	0.45
1:D:427:LEU:O	1:D:428:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:TYR:CZ	1:C:441:PRO:HG3	2.52	0.45
1:D:311:ALA:HB2	3:D:580:VFV:CAV	2.47	0.45
1:A:236:HIS:CE1	3:A:600:VFV:H6	2.52	0.45
1:A:449:CYS:HA	2:A:540:HEM:C4D	2.52	0.45
1:B:159:LEU:HD22	1:B:308:LEU:HD21	1.98	0.45
1:B:410:ARG:HG2	1:B:418:ARG:NH1	2.32	0.45
2:C:540:HEM:HMB2	2:C:540:HEM:HBB2	1.98	0.45
1:C:491:PRO:HG2	1:C:494:PRO:HB3	1.98	0.44
1:D:378:MET:O	1:D:378:MET:HG2	2.16	0.44
1:C:136:THR:HB	1:C:137:PRO:HD3	1.99	0.44
1:C:227:TYR:CD1	1:C:309:LEU:HD23	2.52	0.44
1:D:227:TYR:CZ	1:D:309:LEU:CD2	2.99	0.44
1:A:378:MET:HG3	4:A:2170:HOH:O	2.17	0.44
1:B:484:TYR:HD1	1:B:489:HIS:CE1	2.35	0.44
1:C:165:ILE:CG2	1:C:169:LYS:HE2	2.47	0.44
1:D:202:ILE:HD11	1:D:462:ILE:CD1	2.47	0.44
1:A:488:ILE:HG23	1:A:488:ILE:O	2.17	0.44
1:A:270:LYS:HD2	4:A:2131:HOH:O	2.18	0.44
1:A:338:TYR:O	1:A:341:GLN:HB2	2.17	0.44
1:D:502:SER:O	1:D:502:SER:OG	2.35	0.43
1:D:149:ASN:HB3	1:D:150:PRO:HD3	2.00	0.43
1:A:307:GLY:CA	3:A:580:VFV:H4	2.48	0.43
1:C:380:MET:CE	1:C:405:PRO:HG3	2.48	0.43
1:B:68:ILE:HG23	1:C:242:PRO:HG3	1.99	0.43
1:D:175:ILE:HD13	1:D:458:GLN:HA	2.00	0.43
1:C:430:ASN:OD1	1:C:432:ALA:HB3	2.19	0.43
1:A:101:VAL:CG1	4:A:2020:HOH:O	2.63	0.42
1:B:440:VAL:N	1:B:441:PRO:CD	2.82	0.42
3:A:580:VFV:H4	3:A:580:VFV:H5	1.79	0.42
2:A:540:HEM:HBC2	2:A:540:HEM:HMC2	2.00	0.42
3:A:600:VFV:H15	4:A:2222:HOH:O	2.20	0.42
1:D:182:TYR:OH	1:D:200:GLU:OE1	2.28	0.42
1:A:307:GLY:O	3:A:580:VFV:H4	2.19	0.42
1:D:450:ILE:C	1:D:450:ILE:HD12	2.40	0.42
1:C:82:ILE:CD1	1:C:406:THR:HG21	2.49	0.42
1:D:283:GLN:HG2	4:D:2067:HOH:O	2.18	0.42
1:A:172:VAL:HG21	1:A:354:TYR:HA	2.02	0.42
1:A:378:MET:CG	1:A:378:MET:O	2.67	0.42
1:B:488:ILE:CG2	4:B:2174:HOH:O	2.24	0.42
1:A:380:MET:HE2	1:A:405:PRO:HD3	2.01	0.42
1:D:200:GLU:O	1:D:203:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:THR:HB	1:B:137:PRO:HD3	2.01	0.41
1:C:198:LEU:O	1:C:202:ILE:HG12	2.20	0.41
1:C:410:ARG:HG2	1:C:418:ARG:NH1	2.35	0.41
1:D:202:ILE:HA	1:D:205:THR:OG1	2.20	0.41
2:C:540:HEM:HBB2	2:C:540:HEM:CMB	2.51	0.41
1:B:289:THR:HG21	1:B:293:GLY:HA2	2.02	0.41
1:B:483:ASN:HB2	1:B:492:GLU:HG2	2.03	0.41
1:A:149:ASN:N	1:A:150:PRO:CD	2.83	0.41
1:C:380:MET:HG2	2:C:540:HEM:CGA	2.50	0.41
1:D:101:VAL:HG12	1:D:101:VAL:O	2.20	0.41
1:B:324:GLY:HA2	1:B:463:TRP:CH2	2.56	0.41
1:C:410:ARG:HG2	1:C:410:ARG:O	2.20	0.41
1:A:91:LYS:CD	4:A:2015:HOH:O	2.61	0.41
1:A:200:GLU:O	1:A:203:ILE:HG22	2.21	0.41
1:B:369:GLU:OE1	1:B:372:ARG:HD3	2.20	0.41
1:C:82:ILE:CD1	4:C:2124:HOH:O	2.68	0.41
1:B:121:LYS:HB3	1:B:123:GLU:OE1	2.21	0.41
1:B:380:MET:HE3	1:B:380:MET:HB2	1.98	0.41
1:A:440:VAL:N	1:A:441:PRO:CD	2.84	0.40
1:A:450:ILE:H	1:A:450:ILE:HG13	1.77	0.40
1:C:101:VAL:HG21	3:C:600:VFV:H4	1.99	0.40
1:C:272:ARG:NH2	4:C:2091:HOH:O	2.54	0.40
1:C:272:ARG:HE	1:C:286:LEU:HD22	1.86	0.40
1:D:157:LYS:HD3	1:D:157:LYS:HA	1.92	0.40
1:B:451:GLY:HA3	2:B:540:HEM:C2C	2.57	0.40
1:C:239:TRP:CD1	3:C:580:VFV:CAH	3.04	0.40
1:A:164:ASN:OD1	1:A:164:ASN:C	2.60	0.40
1:A:198:LEU:O	1:A:202:ILE:HG12	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:OE2	1:D:414:SER:C[2_555]	1.83	0.37
1:A:83:GLU:OE2	1:D:415:TRP:N[2_555]	1.86	0.34
1:D:355:ASP:OD2	1:D:355:ASP:OD2[2_554]	1.93	0.27

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	440/443 (99%)	433 (98%)	7 (2%)	0	100	100
1	B	440/443 (99%)	430 (98%)	10 (2%)	0	100	100
1	C	440/443 (99%)	431 (98%)	9 (2%)	0	100	100
1	D	440/443 (99%)	432 (98%)	8 (2%)	0	100	100
All	All	1760/1772 (99%)	1726 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	387/388 (100%)	386 (100%)	1 (0%)	92	93
1	B	387/388 (100%)	386 (100%)	1 (0%)	92	93
1	C	387/388 (100%)	387 (100%)	0	100	100
1	D	387/388 (100%)	387 (100%)	0	100	100
All	All	1548/1552 (100%)	1546 (100%)	2 (0%)	93	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	LEU
1	B	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	HIS
1	A	269	GLN
1	A	493	ASN
1	B	489	HIS
1	B	493	ASN
1	D	236	HIS
1	D	269	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	D	540	3,1	41,50,50	1.29	6 (14%)	45,82,82	1.91	13 (28%)
2	HEM	B	540	3,1	41,50,50	1.27	5 (12%)	45,82,82	1.82	10 (22%)
3	VFV	C	580	2	38,46,46	1.86	6 (15%)	57,64,64	1.14	5 (8%)
3	VFV	D	580	2	38,46,46	1.76	4 (10%)	57,64,64	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	C	540	3,1	41,50,50	1.35	6 (14%)	45,82,82	1.90	11 (24%)
2	HEM	A	540	3,1	41,50,50	1.36	6 (14%)	45,82,82	1.95	12 (26%)
3	VFV	A	600	-	38,46,46	2.86	6 (15%)	57,64,64	1.07	5 (8%)
3	VFV	A	580	2	38,46,46	2.07	8 (21%)	57,64,64	1.15	7 (12%)
3	VFV	B	600	-	38,46,46	1.81	6 (15%)	57,64,64	1.02	5 (8%)
3	VFV	D	600	-	38,46,46	2.14	6 (15%)	57,64,64	1.11	5 (8%)
3	VFV	C	600	-	38,46,46	2.23	6 (15%)	57,64,64	1.07	4 (7%)
3	VFV	B	580	2	38,46,46	2.07	6 (15%)	57,64,64	1.18	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	540	3,1	-	0/12/54/54	-
2	HEM	B	540	3,1	-	0/12/54/54	-
3	VFV	C	580	2	-	0/24/28/28	0/6/6/6
3	VFV	D	580	2	-	0/24/28/28	0/6/6/6
2	HEM	C	540	3,1	-	2/12/54/54	-
2	HEM	A	540	3,1	-	1/12/54/54	-
3	VFV	A	600	-	-	0/24/28/28	0/6/6/6
3	VFV	A	580	2	-	0/24/28/28	0/6/6/6
3	VFV	B	600	-	-	1/24/28/28	0/6/6/6
3	VFV	D	600	-	-	4/24/28/28	0/6/6/6
3	VFV	C	600	-	-	0/24/28/28	0/6/6/6
3	VFV	B	580	2	-	1/24/28/28	0/6/6/6

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	VFV	NAY-NAZ	-12.36	1.13	1.37
3	A	600	VFV	CBK-CBN	-9.32	1.37	1.52
3	D	600	VFV	CBK-CBN	-7.82	1.40	1.52
3	C	600	VFV	NAY-NAZ	-7.71	1.22	1.37
3	D	580	VFV	CBK-CBN	-7.61	1.40	1.52
3	C	600	VFV	CBK-CBN	-7.20	1.41	1.52
3	C	580	VFV	CBK-CBN	-7.06	1.41	1.52
3	D	600	VFV	NAY-NAZ	-7.02	1.23	1.37
3	B	580	VFV	FAC-CBE	-6.82	1.18	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	VFV	CBK-CBN	-6.81	1.41	1.52
3	B	580	VFV	CBK-CBN	-6.72	1.41	1.52
3	A	580	VFV	CBK-CBN	-6.34	1.42	1.52
3	A	580	VFV	NAY-NAZ	-5.74	1.26	1.37
3	A	600	VFV	CBF-CBC	-5.40	1.38	1.50
3	C	600	VFV	CBF-CBC	-5.37	1.39	1.50
3	D	600	VFV	CBF-CBC	-5.12	1.39	1.50
3	C	580	VFV	CBF-CBC	-4.63	1.40	1.50
3	A	580	VFV	FAC-CBE	-4.62	1.23	1.35
3	B	600	VFV	CBF-CBC	-4.45	1.40	1.50
3	A	580	VFV	CBF-CBC	-4.19	1.41	1.50
3	D	580	VFV	CBF-CBC	-4.16	1.41	1.50
3	B	580	VFV	CBF-CBC	-4.12	1.41	1.50
3	C	580	VFV	NAY-NAZ	-4.09	1.29	1.37
3	D	600	VFV	CBJ-CBG	-4.05	1.39	1.49
2	A	540	HEM	C1B-NB	-4.02	1.33	1.40
3	B	600	VFV	NAY-NAZ	-4.00	1.29	1.37
3	C	600	VFV	FAB-CBD	3.97	1.46	1.36
3	A	580	VFV	CBJ-CBG	-3.75	1.39	1.49
3	B	580	VFV	CBJ-CBG	-3.71	1.39	1.49
3	D	580	VFV	CBJ-CBG	-3.60	1.40	1.49
3	B	600	VFV	CBJ-CBG	-3.59	1.40	1.49
2	C	540	HEM	C1B-NB	-3.46	1.34	1.40
2	B	540	HEM	C1B-NB	-3.36	1.34	1.40
3	C	600	VFV	CBJ-CBG	-3.26	1.40	1.49
2	D	540	HEM	C1B-NB	-3.26	1.34	1.40
3	C	580	VFV	CBJ-CBG	-3.24	1.41	1.49
3	D	580	VFV	NAY-NAZ	-3.23	1.31	1.37
3	B	580	VFV	FAB-CBD	-3.21	1.28	1.36
3	A	600	VFV	CBJ-CBG	-3.16	1.41	1.49
2	C	540	HEM	C4B-NB	-3.09	1.32	1.38
3	C	580	VFV	FAC-CBE	3.01	1.43	1.35
2	B	540	HEM	C4B-NB	-2.93	1.32	1.38
2	C	540	HEM	C4D-ND	-2.89	1.35	1.40
2	A	540	HEM	C1D-ND	-2.77	1.33	1.38
3	A	580	VFV	CAW-NBO	-2.75	1.45	1.48
3	A	580	VFV	FAB-CBD	-2.74	1.29	1.36
2	D	540	HEM	C4B-NB	-2.73	1.33	1.38
3	B	600	VFV	FAC-CBE	2.58	1.42	1.35
2	D	540	HEM	C4D-ND	-2.55	1.35	1.40
3	B	580	VFV	CAT-NBO	-2.54	1.33	1.37
3	B	600	VFV	CAT-NBO	-2.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	VFV	CAT-NBO	-2.48	1.33	1.37
3	A	600	VFV	FAC-CBE	-2.48	1.29	1.35
3	A	580	VFV	CAT-NBO	-2.46	1.33	1.37
2	C	540	HEM	C1D-ND	-2.43	1.33	1.38
3	D	600	VFV	CAT-NBO	-2.39	1.33	1.37
2	A	540	HEM	C1A-CHA	-2.37	1.34	1.41
3	C	600	VFV	CAT-NBO	-2.36	1.33	1.37
3	D	600	VFV	CAW-NBO	-2.35	1.45	1.48
2	C	540	HEM	CHB-C1B	2.35	1.41	1.35
2	C	540	HEM	FE-NB	2.31	2.08	1.96
3	C	580	VFV	CAT-NBO	-2.28	1.33	1.37
2	D	540	HEM	FE-NB	2.27	2.08	1.96
2	B	540	HEM	FE-NB	2.23	2.07	1.96
2	A	540	HEM	C4B-NB	-2.20	1.34	1.38
2	A	540	HEM	CHB-C1B	2.17	1.40	1.35
2	B	540	HEM	C1D-ND	-2.09	1.34	1.38
2	A	540	HEM	C2C-C1C	-2.07	1.37	1.42
2	D	540	HEM	C1D-ND	-2.07	1.34	1.38
2	B	540	HEM	C4D-ND	-2.07	1.36	1.40
2	D	540	HEM	CHB-C1B	2.01	1.40	1.35

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	540	HEM	CHC-C4B-NB	5.57	130.48	124.43
2	C	540	HEM	C1B-NB-C4B	5.04	110.27	105.07
2	C	540	HEM	CHC-C4B-NB	4.98	129.85	124.43
2	A	540	HEM	CHC-C4B-NB	4.77	129.62	124.43
2	A	540	HEM	C1B-NB-C4B	4.66	109.89	105.07
2	B	540	HEM	CHC-C4B-NB	4.53	129.36	124.43
2	A	540	HEM	CHA-C4D-ND	4.49	129.93	124.38
2	B	540	HEM	C1B-NB-C4B	4.44	109.66	105.07
2	B	540	HEM	CHD-C1D-ND	4.43	129.24	124.43
2	D	540	HEM	C1B-NB-C4B	4.27	109.48	105.07
2	D	540	HEM	CHD-C1D-ND	4.19	128.98	124.43
2	A	540	HEM	CHD-C1D-ND	4.16	128.95	124.43
2	C	540	HEM	CHD-C1D-ND	3.70	128.45	124.43
3	B	580	VFV	CAW-CBN-NBA	-3.68	104.03	110.45
2	C	540	HEM	CHA-C4D-ND	3.64	128.88	124.38
2	D	540	HEM	CHA-C4D-ND	3.53	128.75	124.38
3	D	600	VFV	CAV-CBE-CBK	-3.52	119.62	123.83
2	A	540	HEM	CHB-C1B-NB	3.44	128.63	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	580	VFV	CAW-CBN-NBA	-3.40	104.52	110.45
2	B	540	HEM	CHA-C4D-ND	3.34	128.51	124.38
2	A	540	HEM	CHA-C4D-C3D	-3.10	119.52	125.33
3	A	580	VFV	CAW-CBN-NBA	-3.08	105.07	110.45
2	B	540	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
3	D	580	VFV	CAV-CBE-CBK	-2.97	120.27	123.83
3	B	600	VFV	CAV-CBE-CBK	-2.92	120.34	123.83
2	C	540	HEM	CHB-C1B-NB	2.88	127.94	124.38
3	B	600	VFV	CAW-CBN-CBK	-2.83	103.21	112.25
2	B	540	HEM	CHB-C1B-NB	2.83	127.88	124.38
2	C	540	HEM	O2D-CGD-CBD	2.81	123.07	114.03
3	C	600	VFV	CAJ-CBD-CAK	-2.74	119.19	122.83
2	D	540	HEM	CHB-C1B-NB	2.72	127.75	124.38
3	C	600	VFV	CAW-CBN-CBK	-2.71	103.59	112.25
3	D	580	VFV	CAS-CBK-CBE	2.70	119.60	116.13
3	C	600	VFV	CAV-CBE-CBK	-2.68	120.61	123.83
3	A	600	VFV	CAS-CBK-CBE	2.68	119.58	116.13
3	D	600	VFV	CAS-CBK-CBE	2.68	119.57	116.13
2	B	540	HEM	O2A-CGA-CBA	2.64	122.53	114.03
2	C	540	HEM	CBA-CAA-C2A	-2.61	108.16	112.62
2	C	540	HEM	CHD-C1D-C2D	-2.59	120.94	124.98
2	C	540	HEM	CHA-C4D-C3D	-2.58	120.48	125.33
3	D	580	VFV	CAW-CBN-NBA	-2.57	105.96	110.45
3	C	580	VFV	CAV-CBE-CBK	-2.54	120.78	123.83
3	D	580	VFV	CAW-NBO-CAU	-2.53	120.78	125.76
3	A	580	VFV	CAJ-CBD-CAK	-2.53	119.46	122.83
3	A	600	VFV	CAV-CBE-CBK	-2.49	120.84	123.83
3	D	600	VFV	CAJ-CBD-CAK	-2.49	119.51	122.83
3	A	580	VFV	CAV-CBE-CBK	-2.48	120.86	123.83
3	D	600	VFV	CAN-CAJ-CBD	2.44	120.88	118.36
2	D	540	HEM	CHD-C1D-C2D	-2.43	121.18	124.98
3	D	580	VFV	CAW-NBO-CAT	2.43	130.92	125.92
2	C	540	HEM	O2A-CGA-CBA	2.42	121.81	114.03
3	A	600	VFV	CAW-CBN-CBK	-2.39	104.62	112.25
2	B	540	HEM	O2D-CGD-CBD	2.39	121.70	114.03
2	A	540	HEM	CMC-C2C-C3C	2.38	129.13	124.68
3	D	600	VFV	CAW-CBN-CBK	-2.37	104.69	112.25
3	B	600	VFV	CAJ-CBD-CAK	-2.35	119.70	122.83
2	B	540	HEM	CHA-C4D-C3D	-2.34	120.94	125.33
2	C	540	HEM	CAD-C3D-C4D	2.33	128.74	124.66
2	D	540	HEM	CHA-C4D-C3D	-2.33	120.94	125.33
2	A	540	HEM	CHD-C1D-C2D	-2.33	121.34	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	600	VFV	CAS-CBK-CBE	2.30	119.08	116.13
3	B	580	VFV	CBK-CBN-NBA	2.28	116.06	111.47
3	B	600	VFV	CAS-CBK-CBE	2.28	119.05	116.13
2	D	540	HEM	CHC-C4B-C3B	-2.26	121.11	124.57
3	A	580	VFV	CAS-CBK-CBE	2.25	119.02	116.13
2	A	540	HEM	CAD-C3D-C4D	2.21	128.53	124.66
3	C	580	VFV	CAS-CBK-CBE	2.21	118.97	116.13
2	D	540	HEM	CAD-C3D-C4D	2.20	128.50	124.66
3	A	580	VFV	FAC-CBE-CBK	2.18	121.76	118.23
3	D	580	VFV	CAJ-CBD-CAK	-2.18	119.93	122.83
3	C	580	VFV	CAJ-CBD-CAK	-2.15	119.97	122.83
2	D	540	HEM	CMC-C2C-C3C	2.15	128.70	124.68
2	D	540	HEM	CAD-CBD-CGD	-2.15	108.97	113.60
2	A	540	HEM	C4B-C3B-C2B	-2.14	105.42	107.11
3	B	600	VFV	CAN-CAJ-CBD	2.13	120.56	118.36
3	A	580	VFV	CBK-CBN-NBA	2.12	115.73	111.47
3	B	580	VFV	CBI-CBM-NAZ	2.11	127.70	124.12
3	A	600	VFV	CAJ-CBD-CAK	-2.11	120.02	122.83
3	C	580	VFV	CBK-CBN-NBA	2.10	115.70	111.47
2	A	540	HEM	O2D-CGD-CBD	2.10	120.77	114.03
2	B	540	HEM	CAD-C3D-C4D	2.08	128.30	124.66
3	B	580	VFV	CAP-CBI-CBM	2.07	123.60	120.44
2	D	540	HEM	CMA-C3A-C4A	-2.07	125.29	128.46
2	D	540	HEM	O2D-CGD-CBD	2.06	120.64	114.03
3	D	580	VFV	CBK-CBN-NBA	2.04	115.58	111.47
3	A	580	VFV	CAO-CAK-CBD	2.04	120.48	118.36
3	A	600	VFV	CAO-CAK-CBD	2.03	120.46	118.36
2	A	540	HEM	C3C-C4C-NC	-2.01	107.14	110.94
3	B	580	VFV	CAV-CBE-CBK	-2.01	121.42	123.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	600	VFV	CAO-CBG-CBJ-CAV
3	B	580	VFV	CAW-CBN-NBA-CBC
3	D	600	VFV	CAN-CBG-CBJ-CAV
3	D	600	VFV	CAO-CBG-CBJ-CAR
3	B	600	VFV	CAW-CBN-NBA-CBC
3	D	600	VFV	CAW-CBN-NBA-CBC
2	C	540	HEM	CAD-CBD-CGD-O2D
2	A	540	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	C	540	HEM	CAA-CBA-CGA-O2A

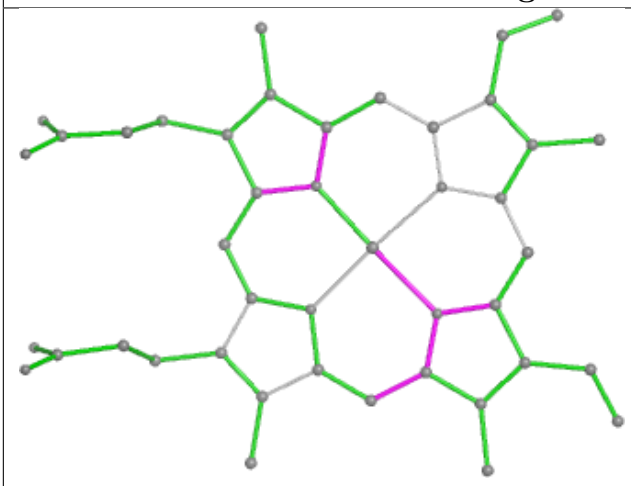
There are no ring outliers.

11 monomers are involved in 58 short contacts:

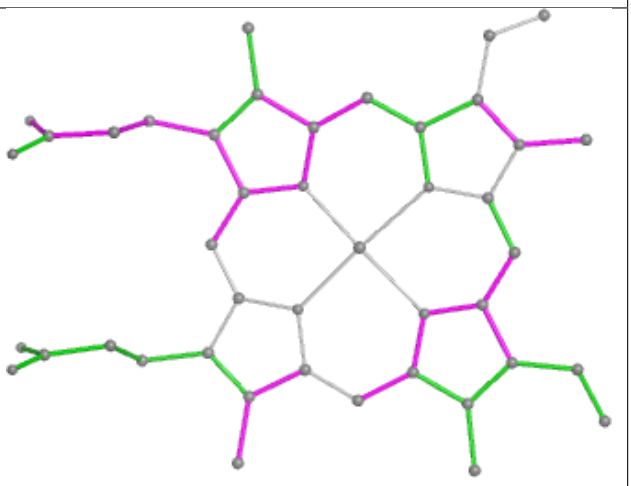
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	540	HEM	5	0
2	B	540	HEM	8	0
3	C	580	VFV	1	0
3	D	580	VFV	1	0
2	C	540	HEM	7	0
2	A	540	HEM	6	0
3	A	600	VFV	4	0
3	A	580	VFV	9	0
3	B	600	VFV	2	0
3	D	600	VFV	8	0
3	C	600	VFV	7	0

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

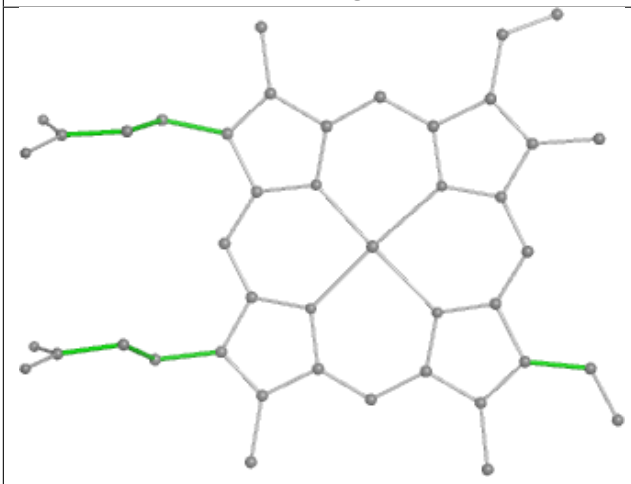
Ligand HEM D 540



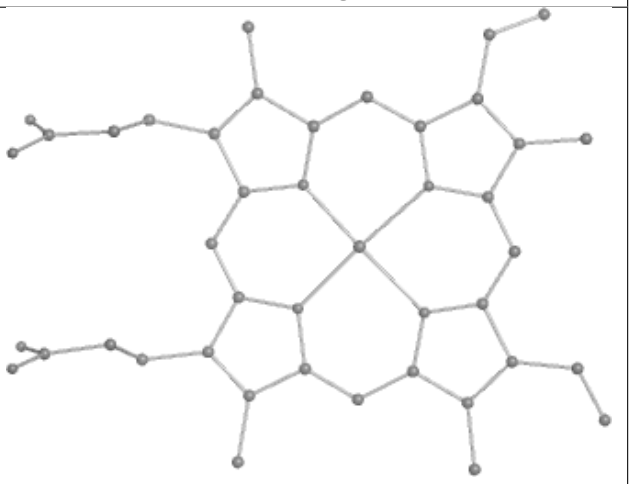
Bond lengths



Bond angles

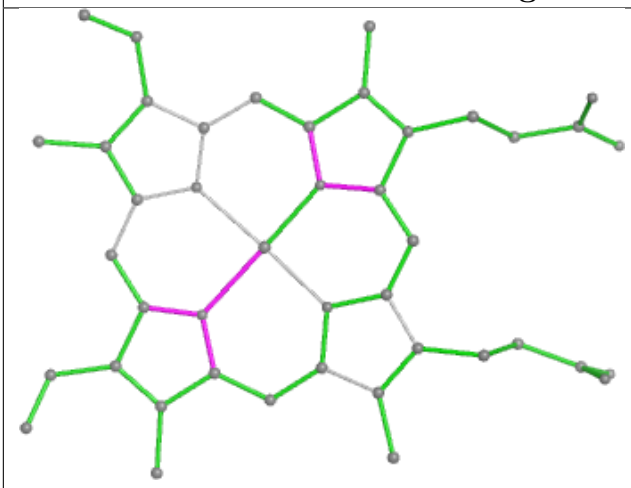


Torsions



Rings

Ligand HEM B 540



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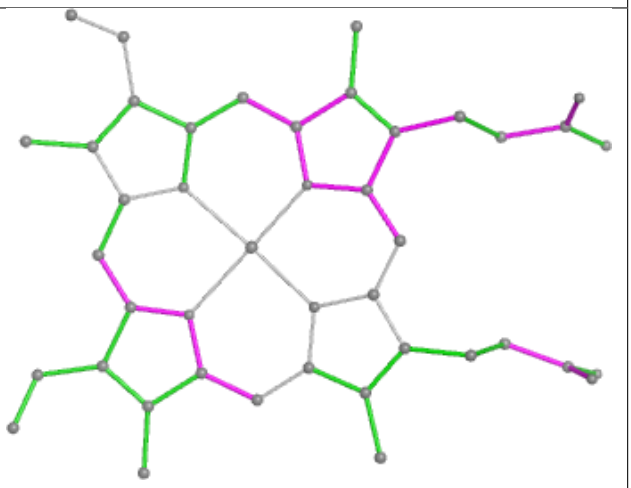

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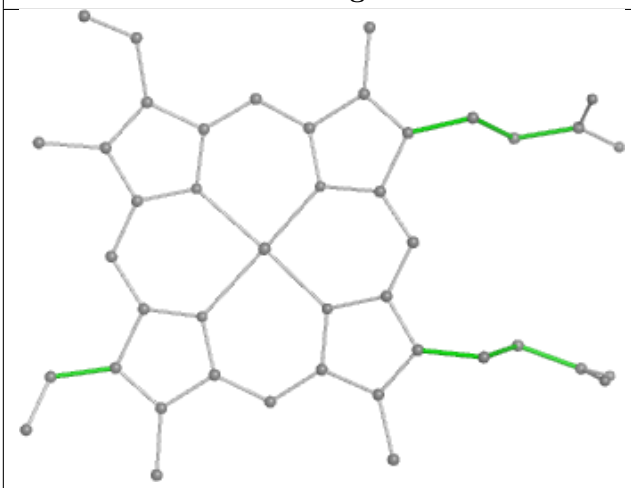

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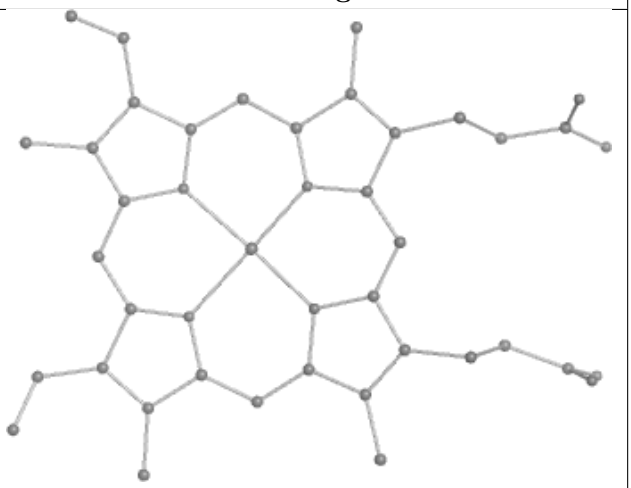
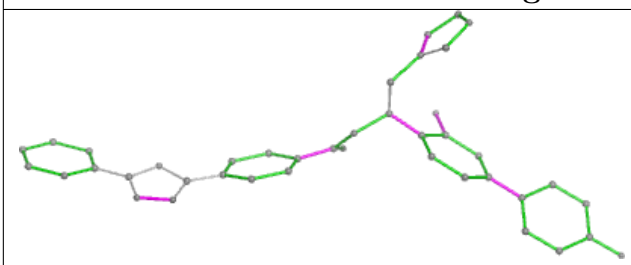


Rings

Ligand VFV C 580



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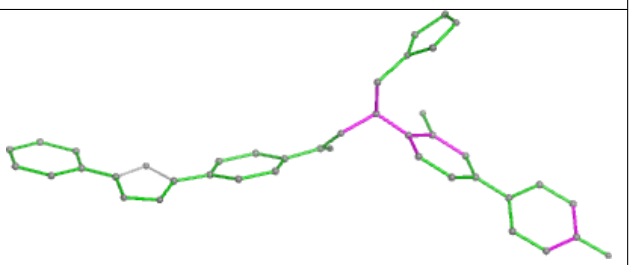

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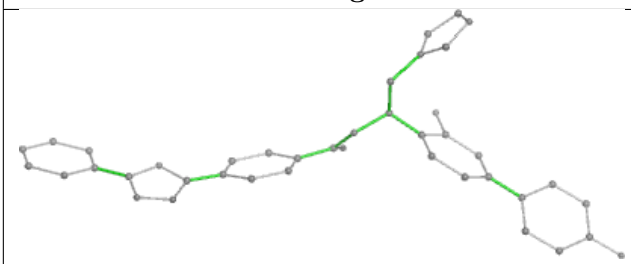

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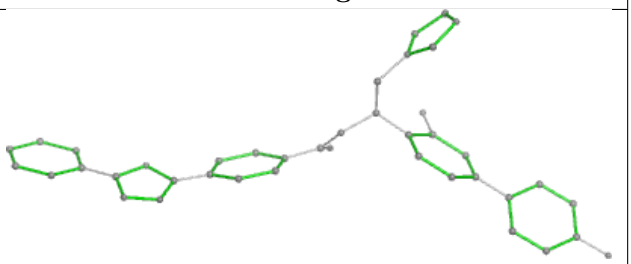
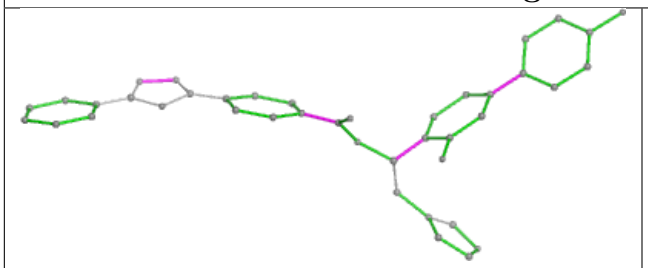


Rings

Ligand VFV D 580



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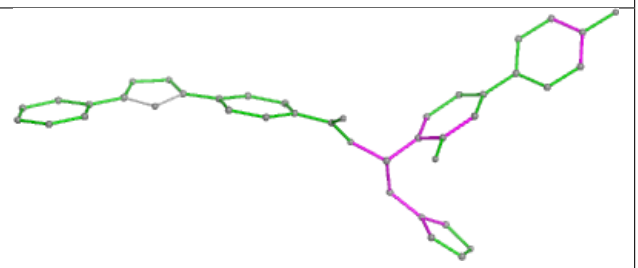

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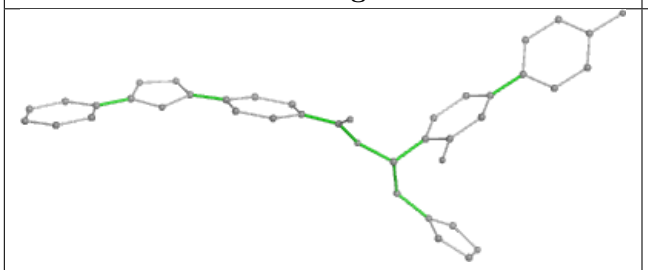

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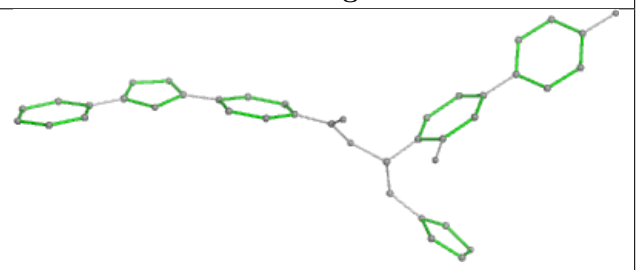
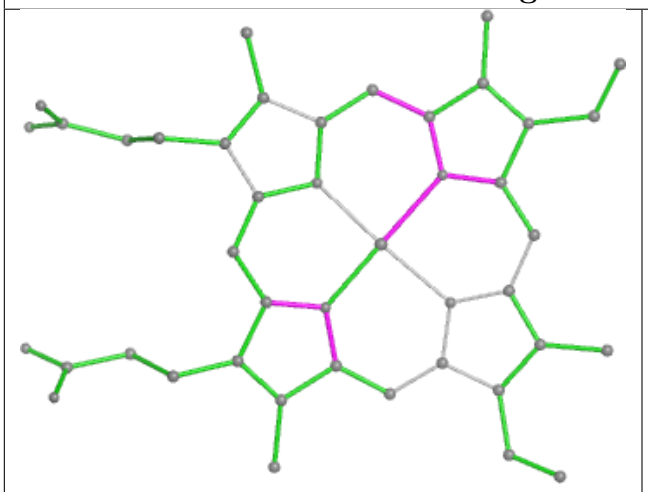


Rings

Ligand HEM C 540



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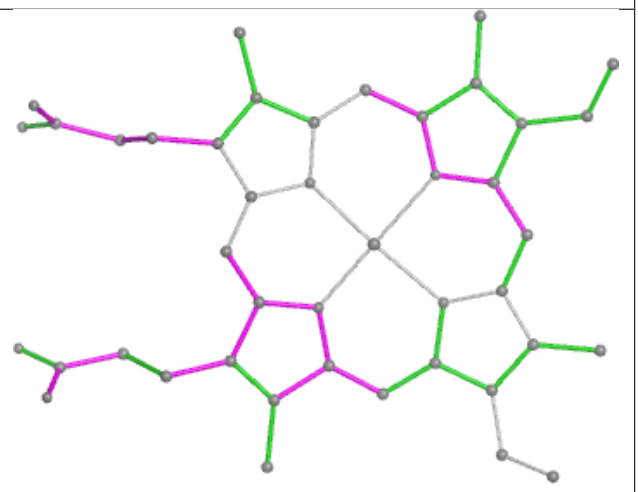

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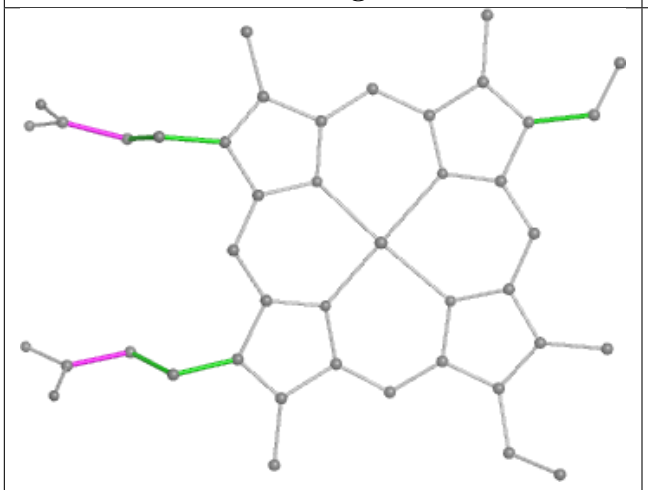

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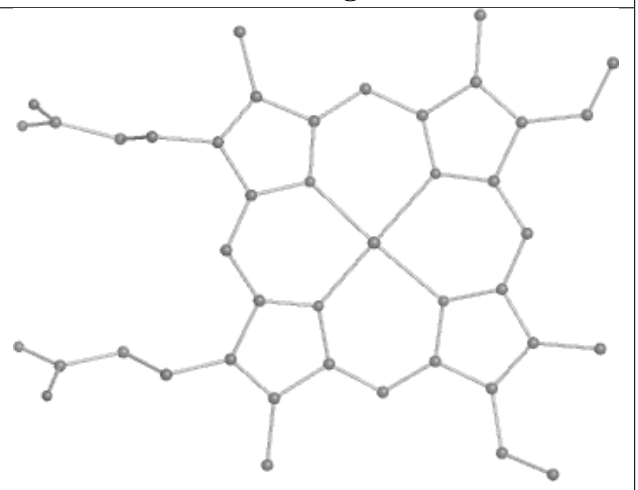

Rings

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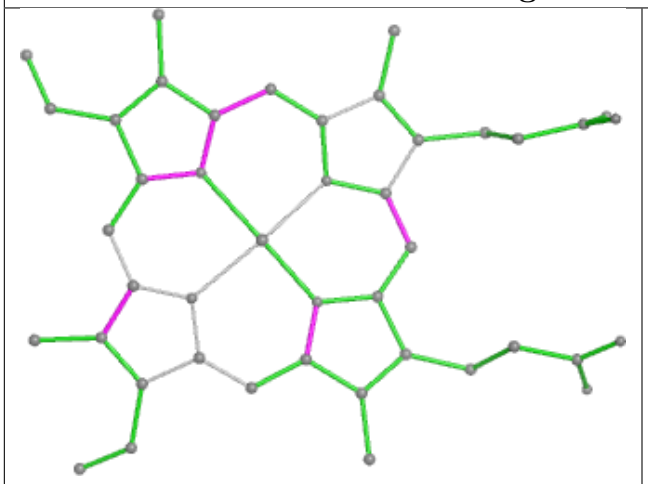

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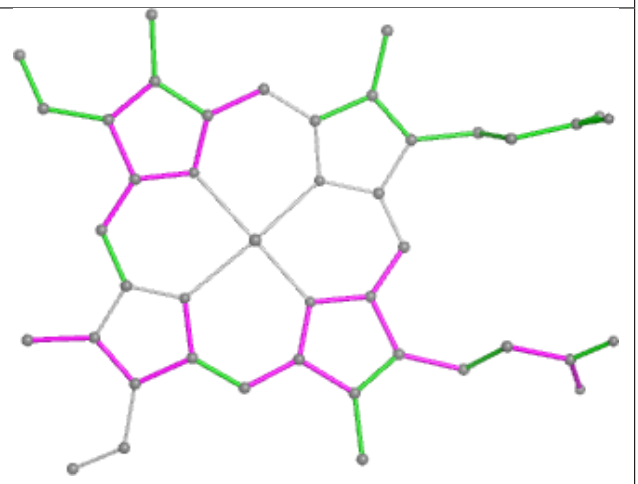

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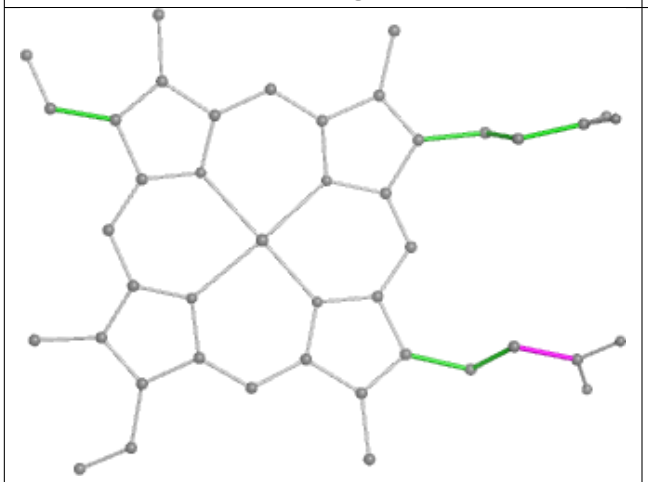

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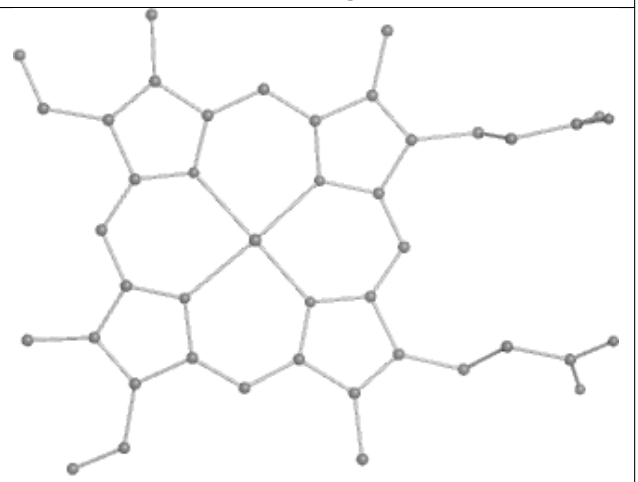
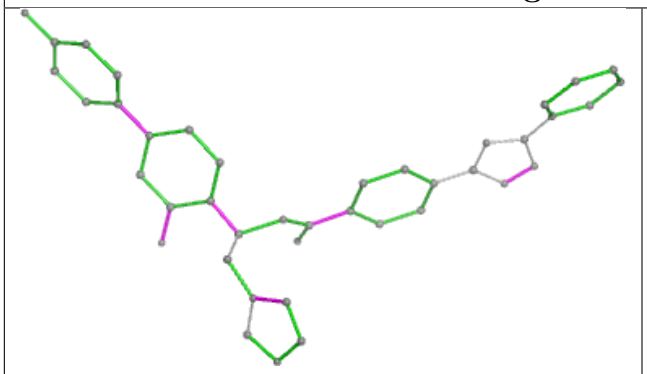


Rings

Ligand VFV A 600



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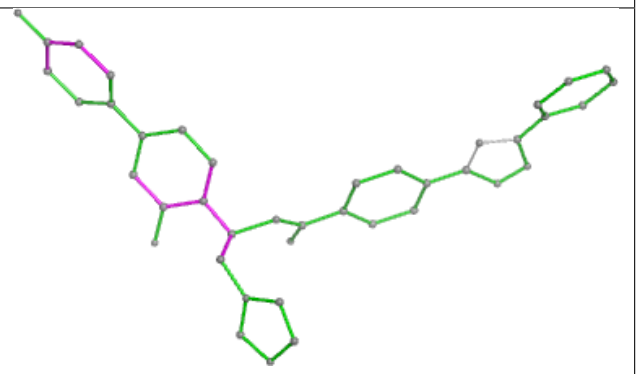

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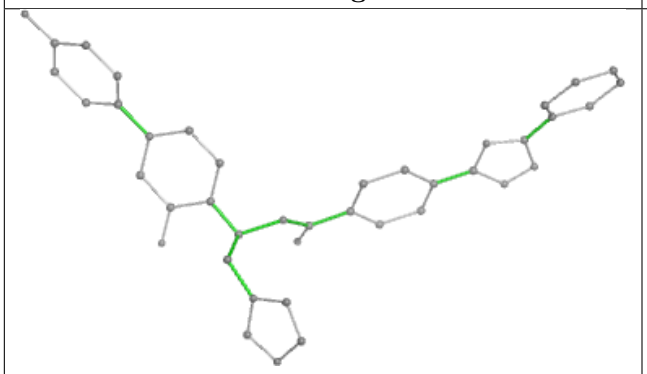

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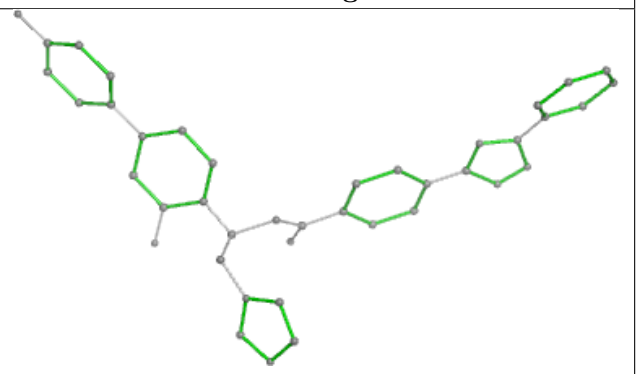
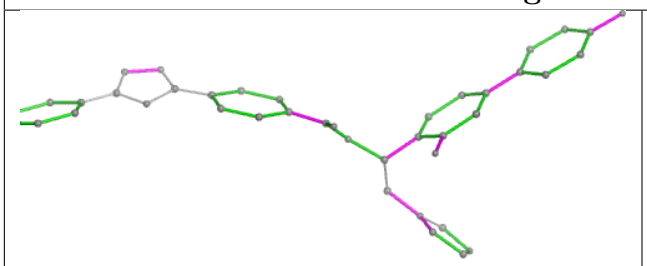
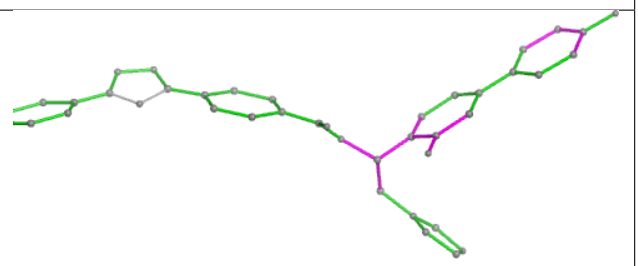


Rings

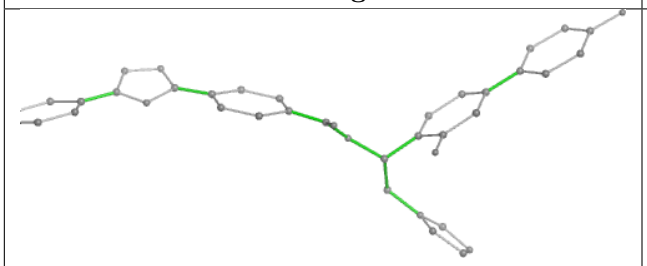
Ligand VFV A 580



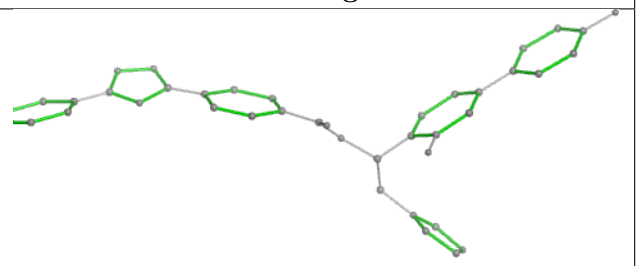
Bond lengths



Bond angles

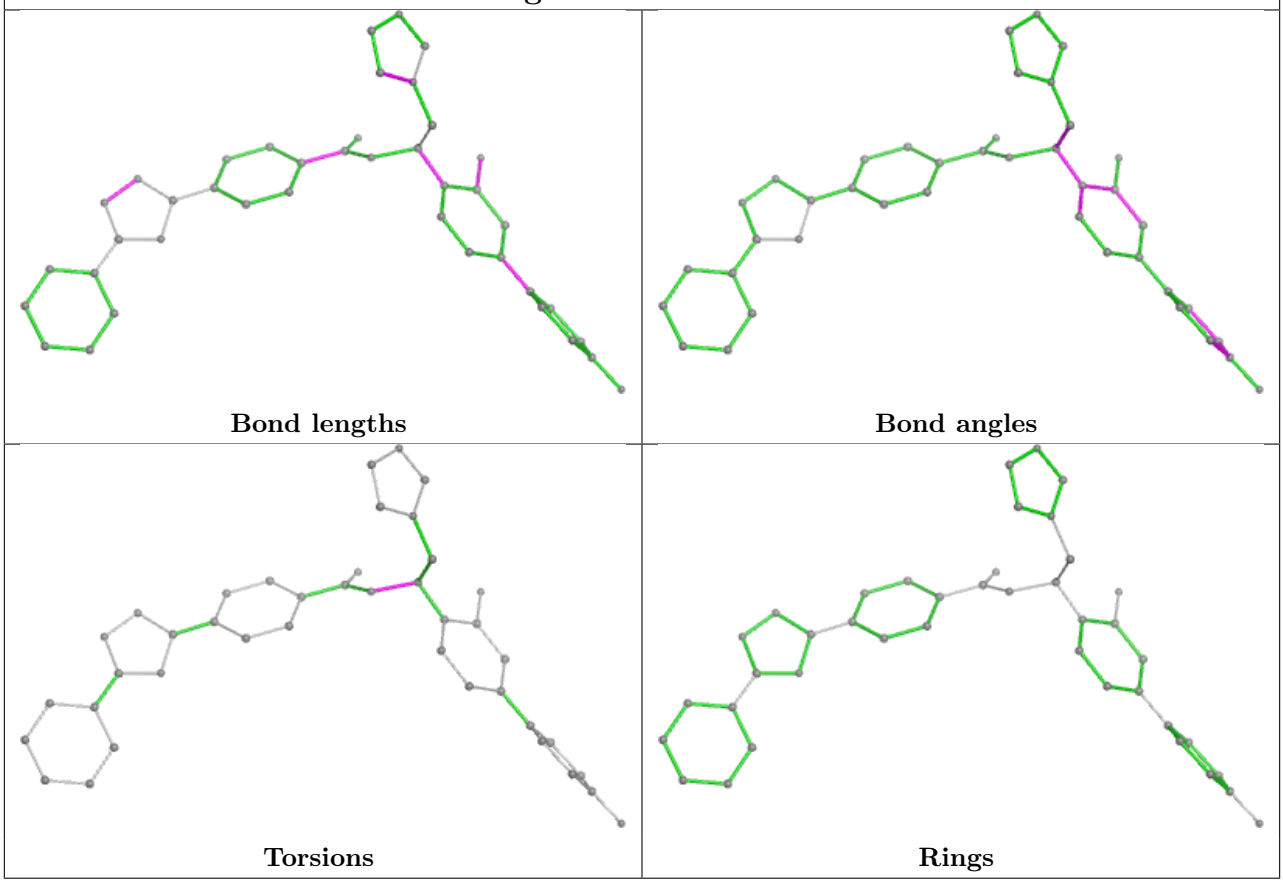


Torsions

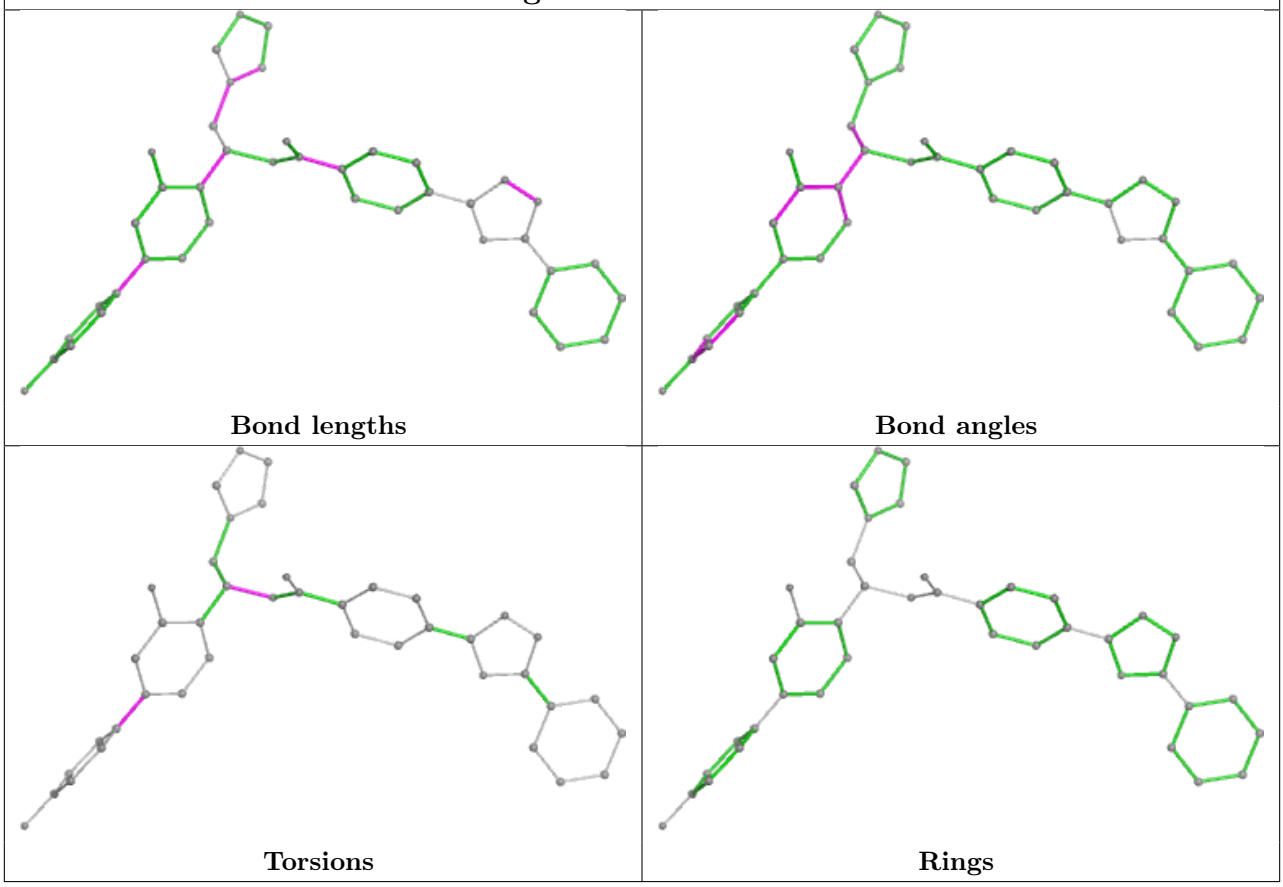


Rings

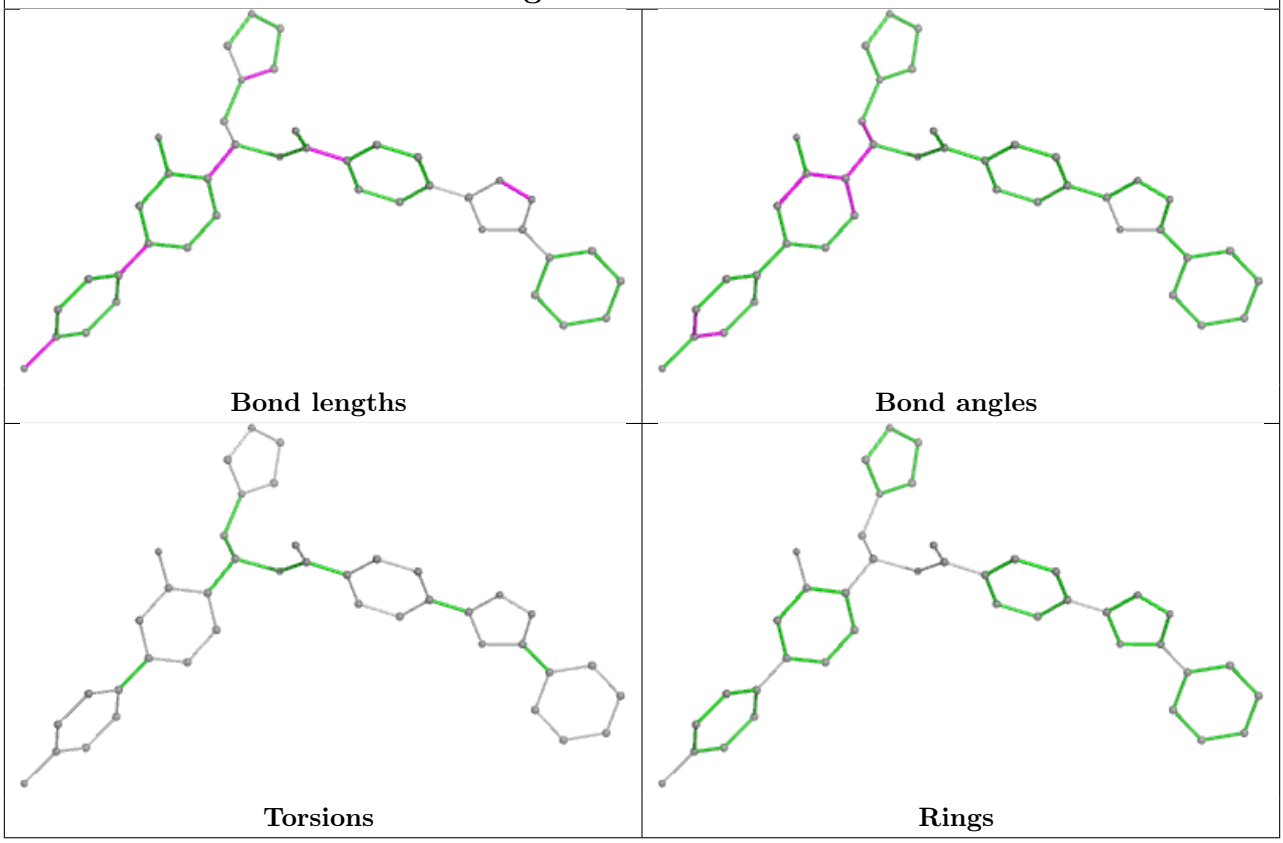
Ligand VFV B 600



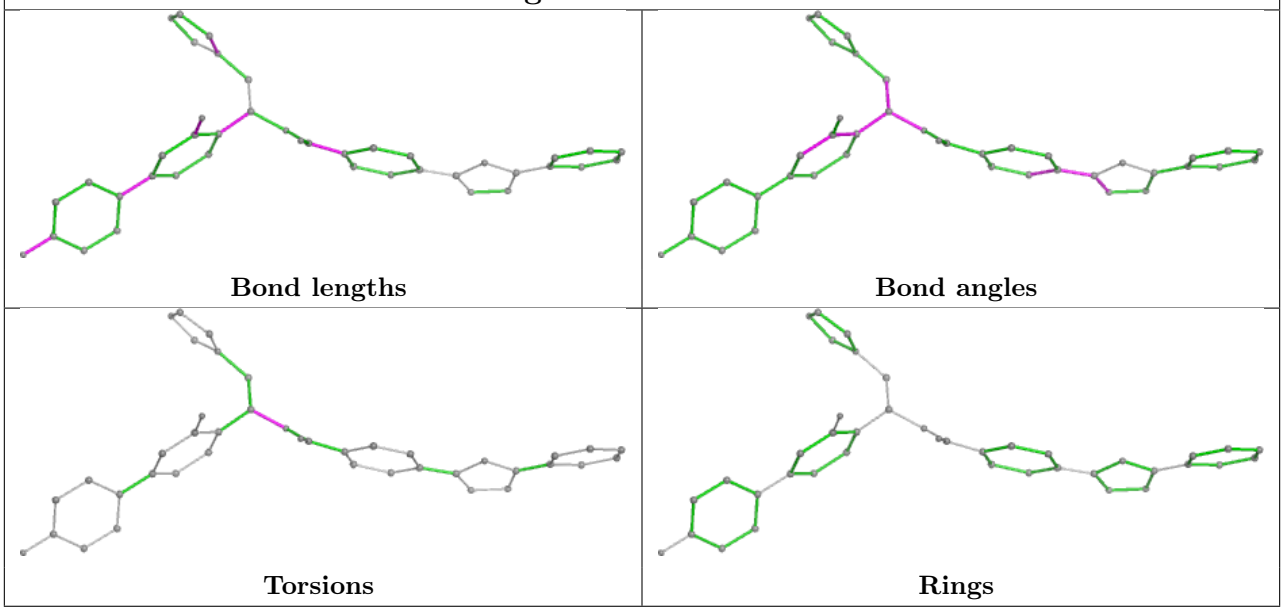
Ligand VFV D 600



Ligand VFV C 600



Ligand VFV B 580



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	442/443 (99%)	-0.25	3 (0%)	87	89	21, 30, 49, 123	0
1	B	442/443 (99%)	-0.25	1 (0%)	95	95	23, 34, 54, 105	0
1	C	442/443 (99%)	-0.14	4 (0%)	84	86	27, 43, 64, 116	0
1	D	442/443 (99%)	0.03	7 (1%)	72	74	25, 43, 72, 143	0
All	All	1768/1772 (99%)	-0.15	15 (0%)	86	88	21, 37, 64, 143	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	GLN	7.5
1	C	277	LYS	4.3
1	D	277	LYS	4.2
1	C	275	GLN	4.2
1	D	278	ILE	3.9
1	D	447	HIS	3.7
1	B	275	GLN	3.3
1	D	502	SER	3.3
1	D	272	ARG	3.2
1	A	99	THR	2.4
1	D	444	ALA	2.4
1	A	277	LYS	2.4
1	C	488	ILE	2.3
1	C	413	ASP	2.1
1	A	275	GLN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

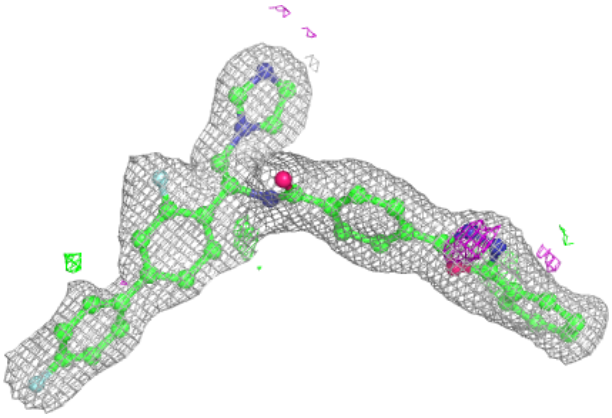
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

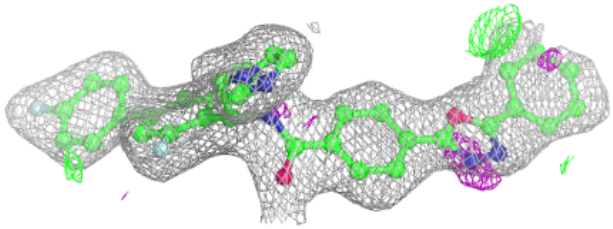
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	VFV	A	600	41/41	0.91	0.13	27,42,53,63	0
3	VFV	C	600	41/41	0.91	0.16	35,48,79,93	0
3	VFV	D	580	41/41	0.93	0.10	28,39,54,60	0
3	VFV	D	600	41/41	0.93	0.12	32,43,54,59	0
3	VFV	C	580	41/41	0.94	0.11	29,37,48,54	0
3	VFV	A	580	41/41	0.94	0.13	25,29,58,65	0
3	VFV	B	580	41/41	0.95	0.11	25,32,36,43	0
3	VFV	B	600	41/41	0.95	0.10	30,36,45,52	0
2	HEM	D	540	43/43	0.97	0.11	26,33,42,54	0
2	HEM	A	540	43/43	0.98	0.11	17,21,27,29	0
2	HEM	B	540	43/43	0.98	0.11	18,23,31,35	0
2	HEM	C	540	43/43	0.98	0.10	26,32,35,37	0

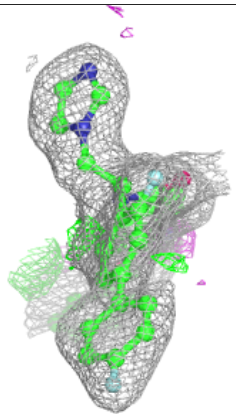
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VFV A 600:

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

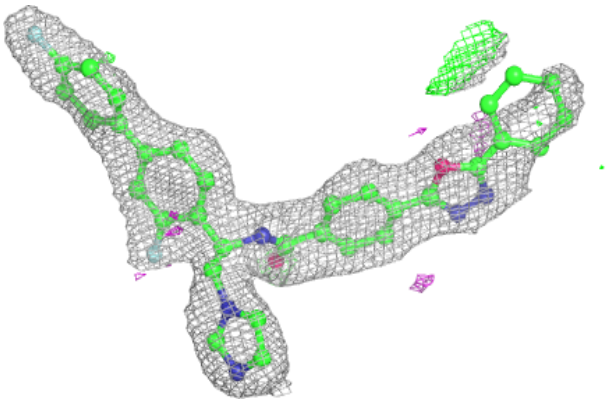


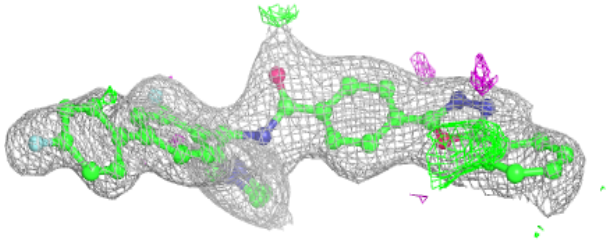


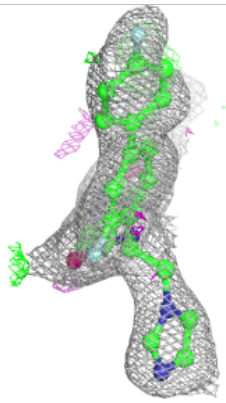


Electron density around VFV C 600:

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

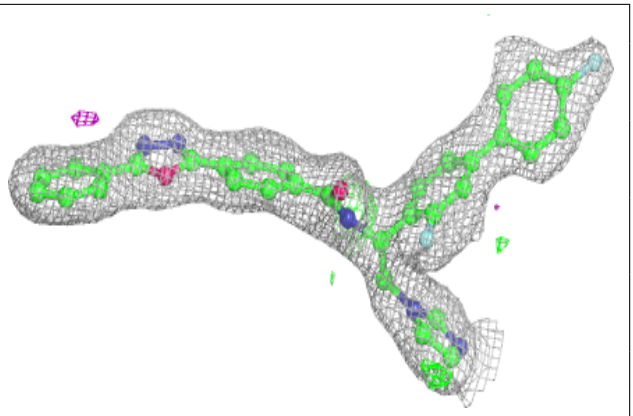


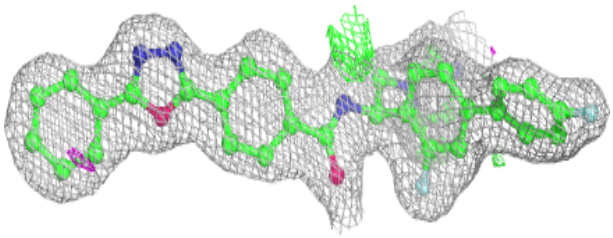


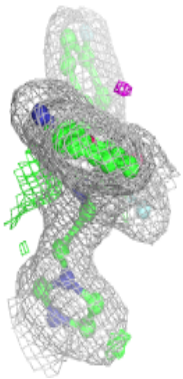


Electron density around VFV D 580:

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

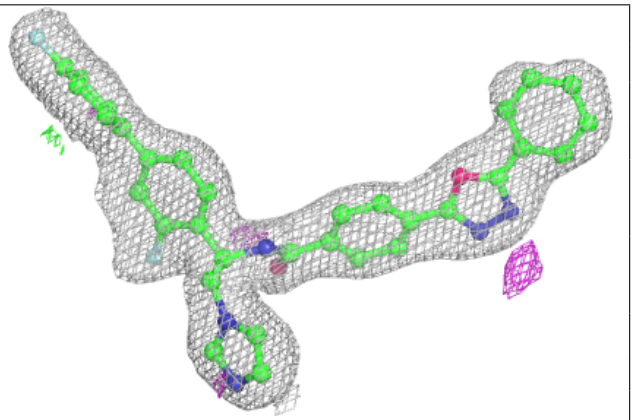


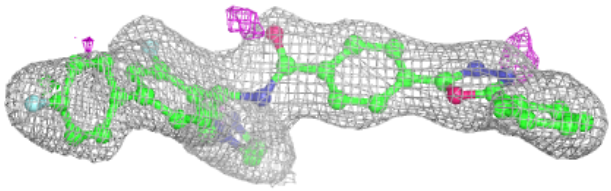


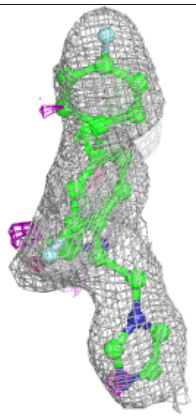


Electron density around VFV D 600:

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

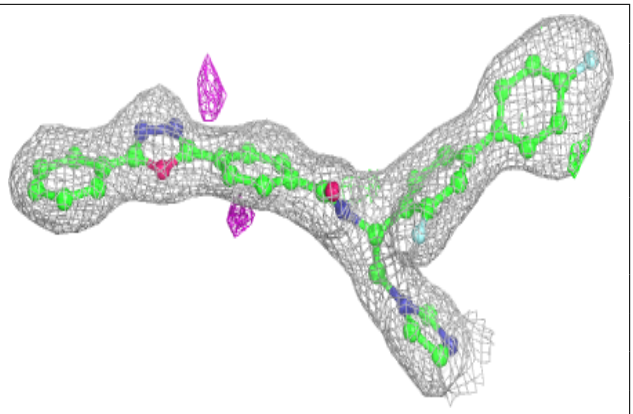


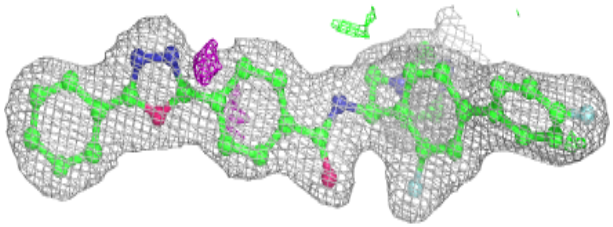


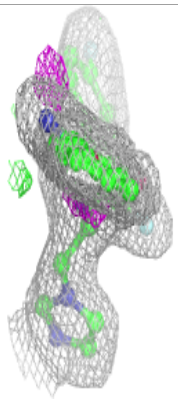


Electron density around VFV C 580:

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

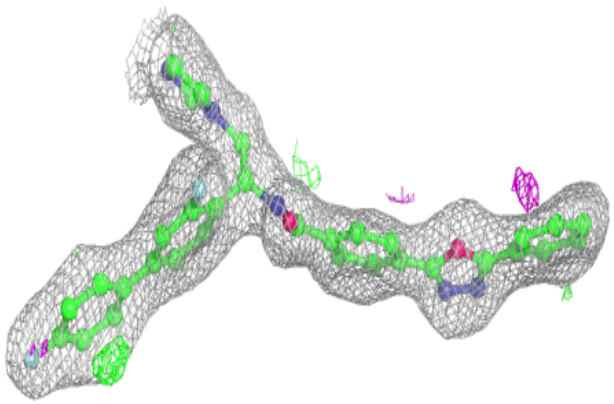


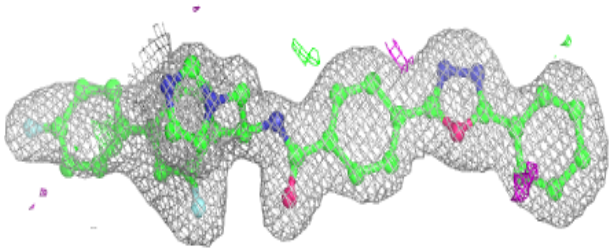


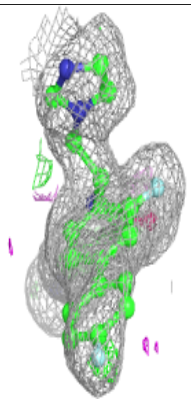


Electron density around VFV A 580:

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







Electron density around VFV B 580:

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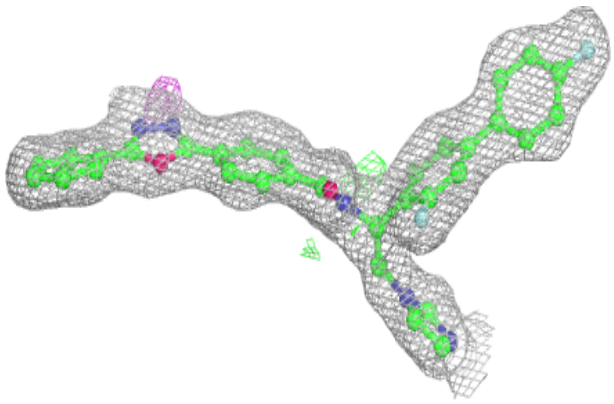
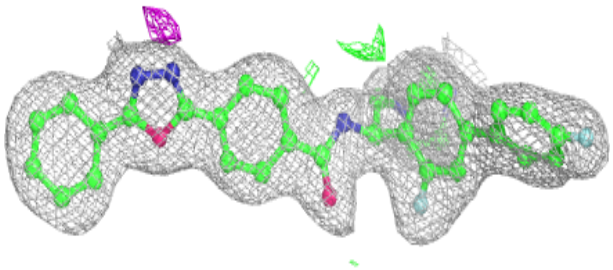
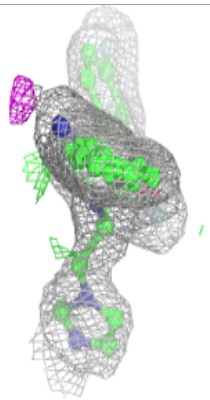
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around VFV B 600:

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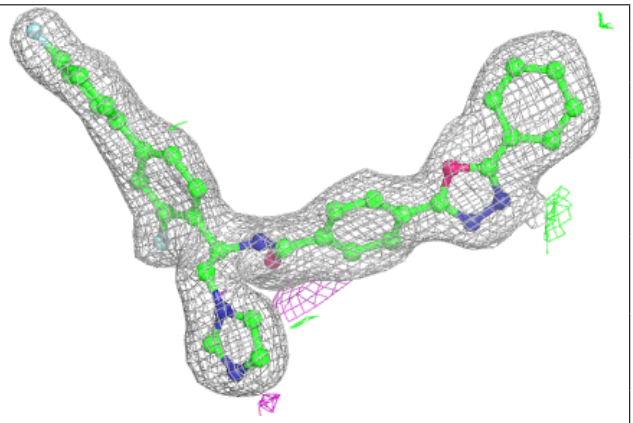
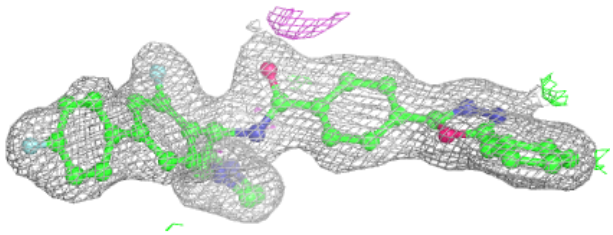
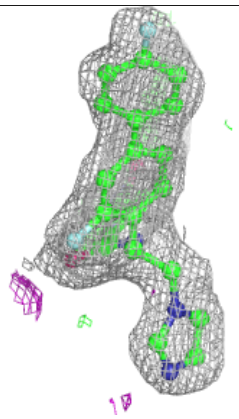
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

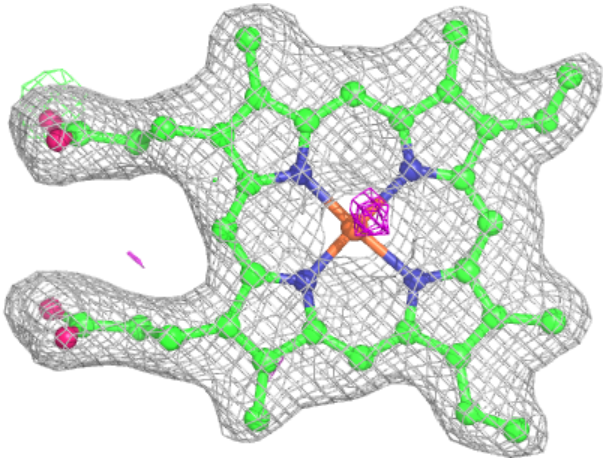


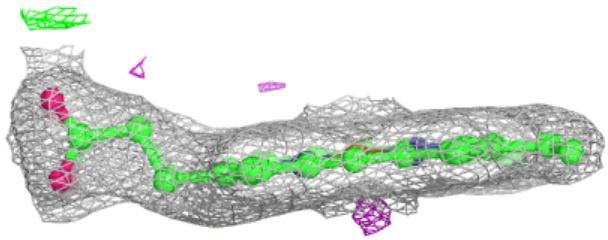


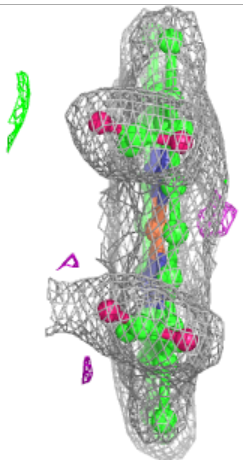


Electron density around HEM D 540:

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

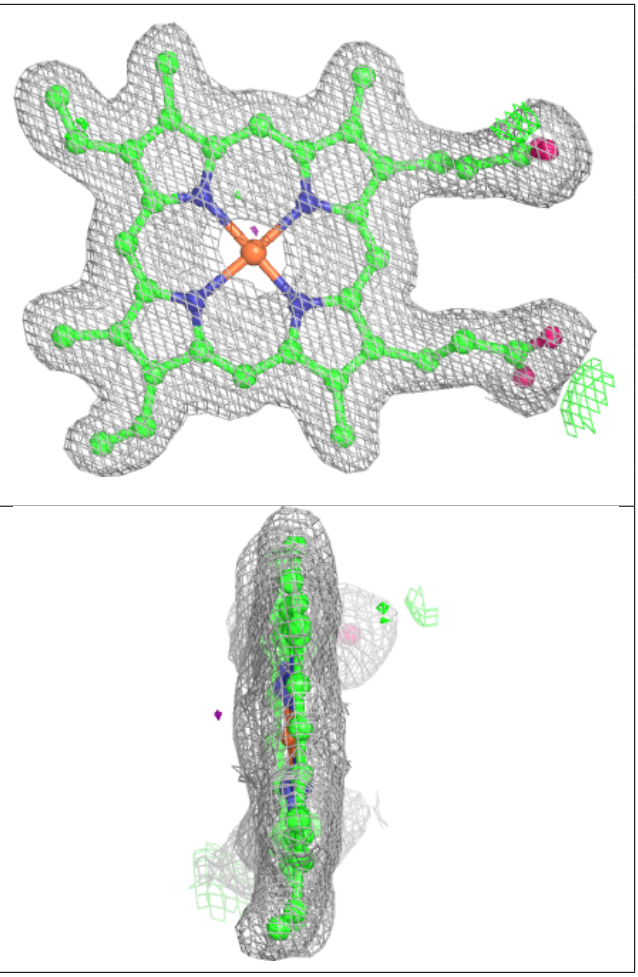






Electron density around HEM A 540:

$2mF_o$-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 540:

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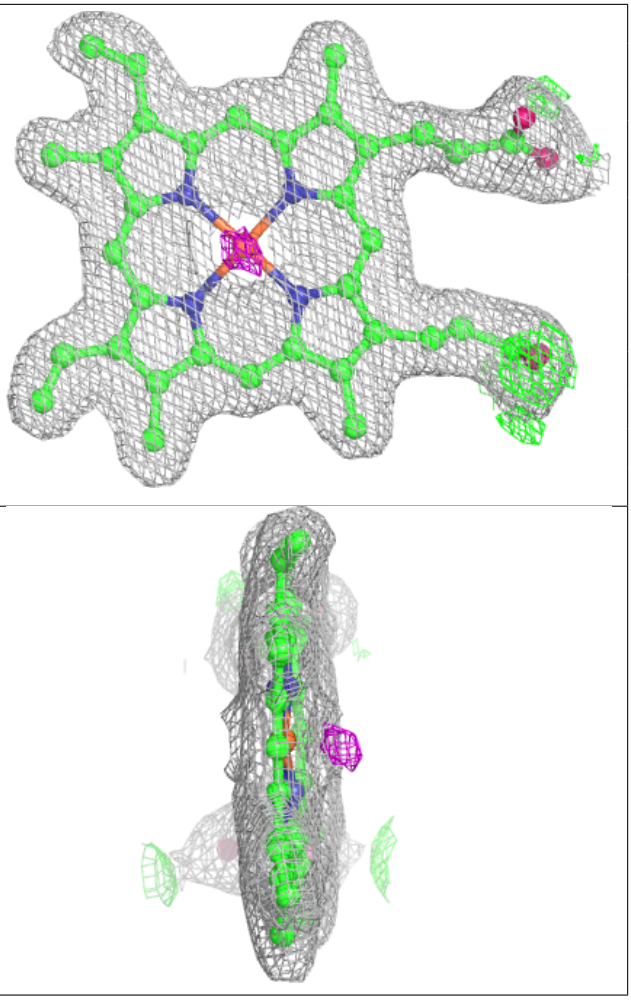
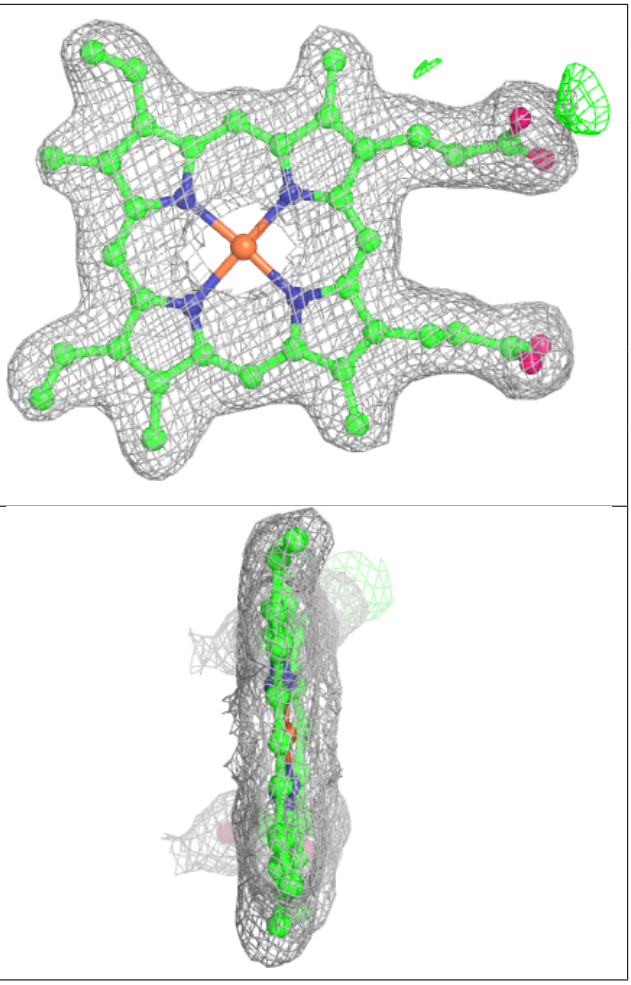
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 540:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.