Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2024 – 03:24 am GMT

PDB ID	:	4UHL
Title	:	HUMAN STEROL 14-ALPHA DEMETHYLASE (CYP51) IN COMPLEX WITH VFV IN P1 SPACE GROUP
Authors	:	Hargrove, T.Y.; Wawrzak, Z.; I Lepesheva, G.
Deposited on	:	2015-03-24
Resolution	:	2.50 Å(reported)

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

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

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

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

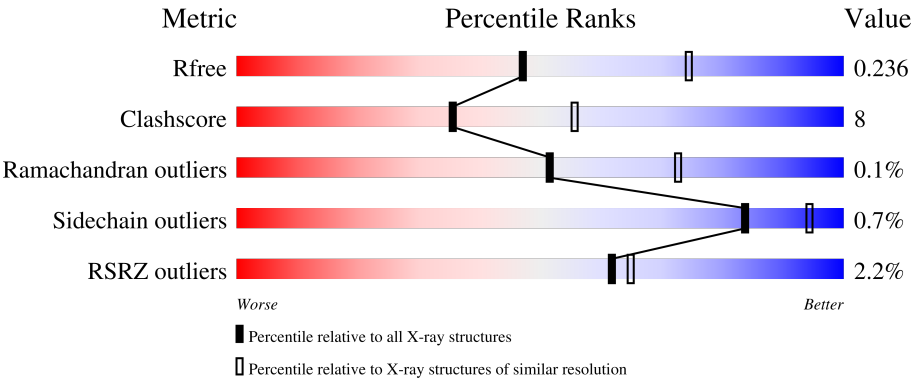
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	446	86% 13%
1	B	446	85% 14%
1	C	446	85% 15%
1	D	446	89% 10%
1	E	446	3% 85% 14%

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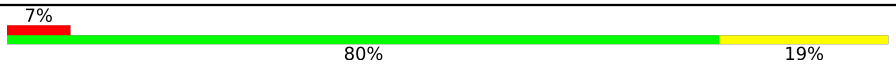
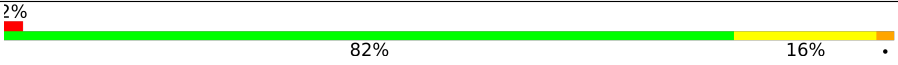
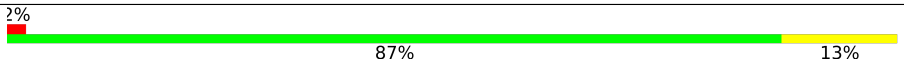
Mol	Chain	Length	Quality of chain
1	F	446	
1	G	446	
1	H	446	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30632 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
1	A	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	B	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	C	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	D	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	E	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	F	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	G	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	H	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLY	-	expression tag	UNP Q16850
A	59	LYS	-	expression tag	UNP Q16850
A	60	LEU	-	expression tag	UNP Q16850
B	58	GLY	-	expression tag	UNP Q16850
B	59	LYS	-	expression tag	UNP Q16850
B	60	LEU	-	expression tag	UNP Q16850
C	58	GLY	-	expression tag	UNP Q16850
C	59	LYS	-	expression tag	UNP Q16850
C	60	LEU	-	expression tag	UNP Q16850
D	58	GLY	-	expression tag	UNP Q16850
D	59	LYS	-	expression tag	UNP Q16850
D	60	LEU	-	expression tag	UNP Q16850
E	58	GLY	-	expression tag	UNP Q16850

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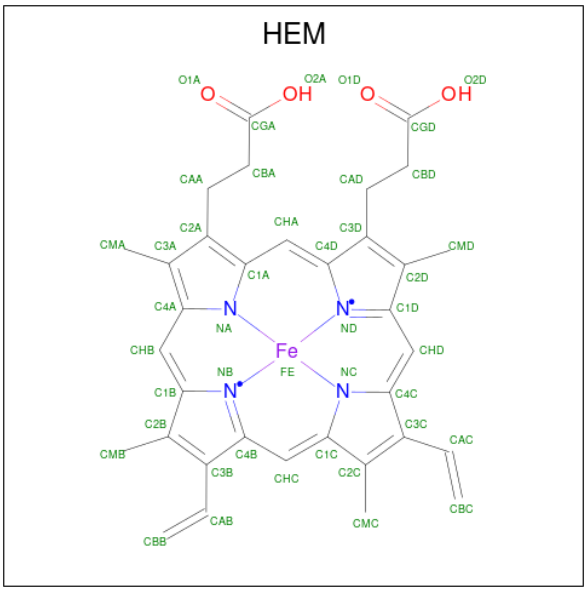
Chain	Residue	Modelled	Actual	Comment	Reference
E	59	LYS	-	expression tag	UNP Q16850
E	60	LEU	-	expression tag	UNP Q16850
F	58	GLY	-	expression tag	UNP Q16850
F	59	LYS	-	expression tag	UNP Q16850
F	60	LEU	-	expression tag	UNP Q16850
G	58	GLY	-	expression tag	UNP Q16850
G	59	LYS	-	expression tag	UNP Q16850
G	60	LEU	-	expression tag	UNP Q16850
H	58	GLY	-	expression tag	UNP Q16850
H	59	LYS	-	expression tag	UNP Q16850
H	60	LEU	-	expression tag	UNP Q16850

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



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

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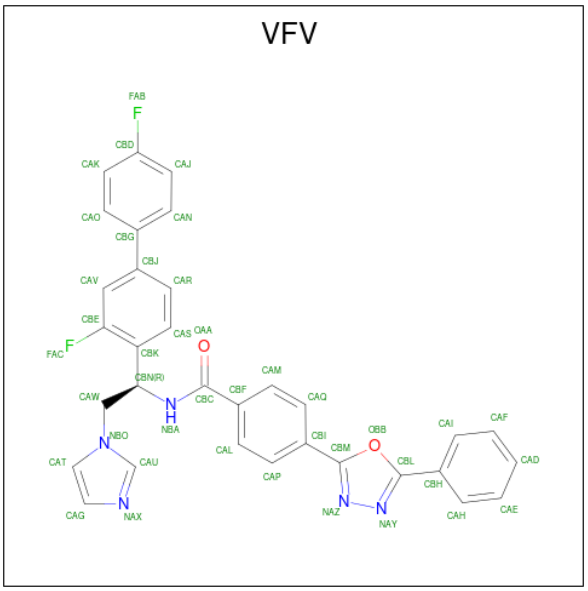
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 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
3	A	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	A	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	B	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	B	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	C	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	C	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	D	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	D	1	Total	C	F	N	O	0	0
			41	32	2	5	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	E	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	F	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	F	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	G	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	G	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	H	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	H	1	Total	C	F	N	O	0	0
			41	32	2	5	2		

- Molecule 4 is water.

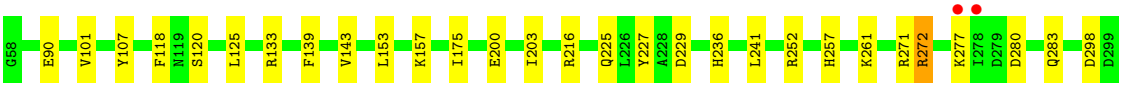
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	152	Total	O	0	0
			152	152		
4	C	141	Total	O	0	0
			141	141		
4	D	144	Total	O	0	0
			144	144		
4	E	113	Total	O	0	0
			113	113		
4	F	62	Total	O	0	0
			62	62		
4	G	114	Total	O	0	0
			114	114		
4	H	82	Total	O	0	0
			82	82		

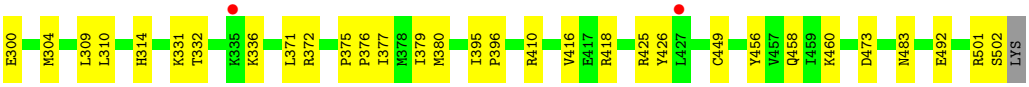
3 Residue-property plots (i)

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

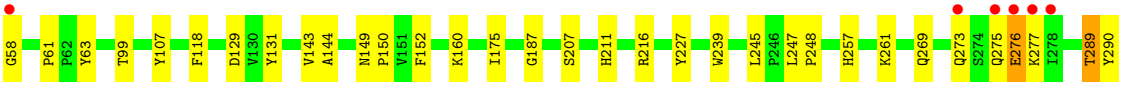
Chain A:

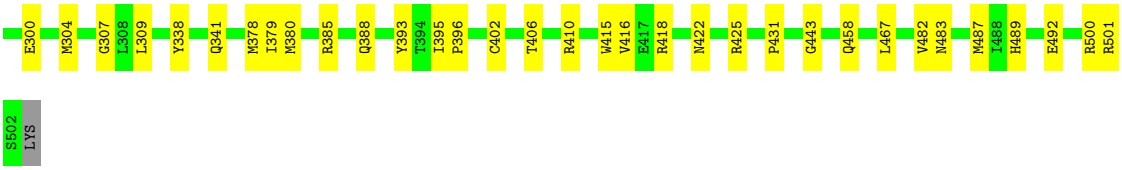




• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

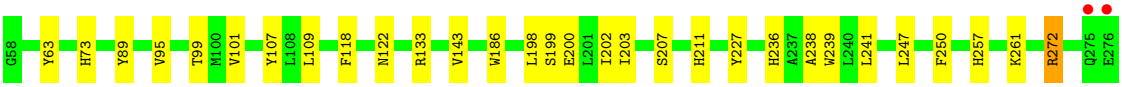
Chain B:

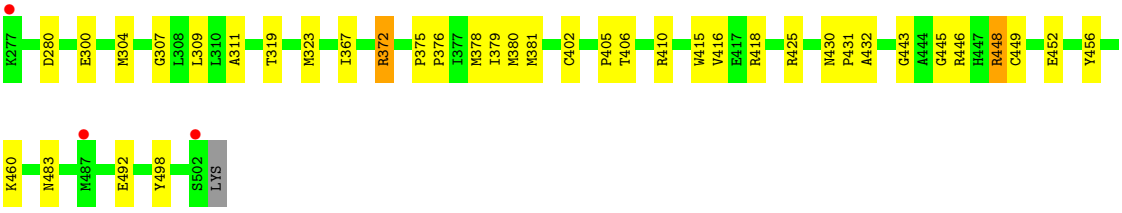




• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

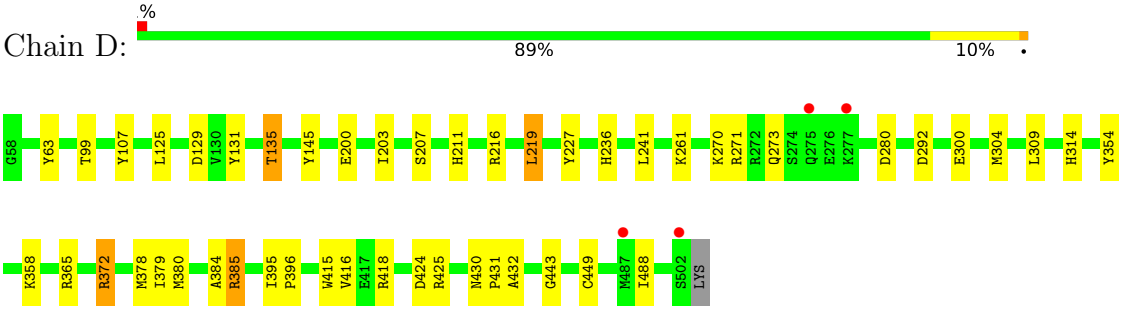
Chain C:





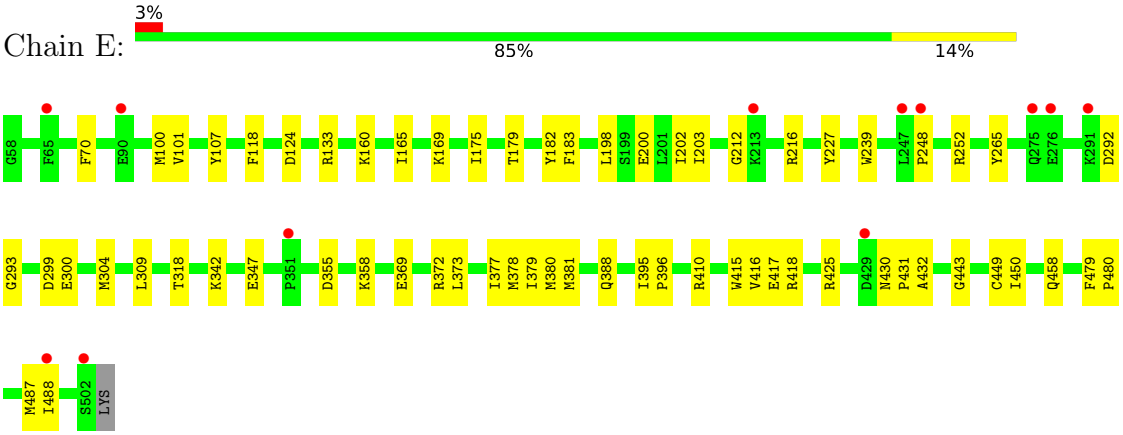
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain D:



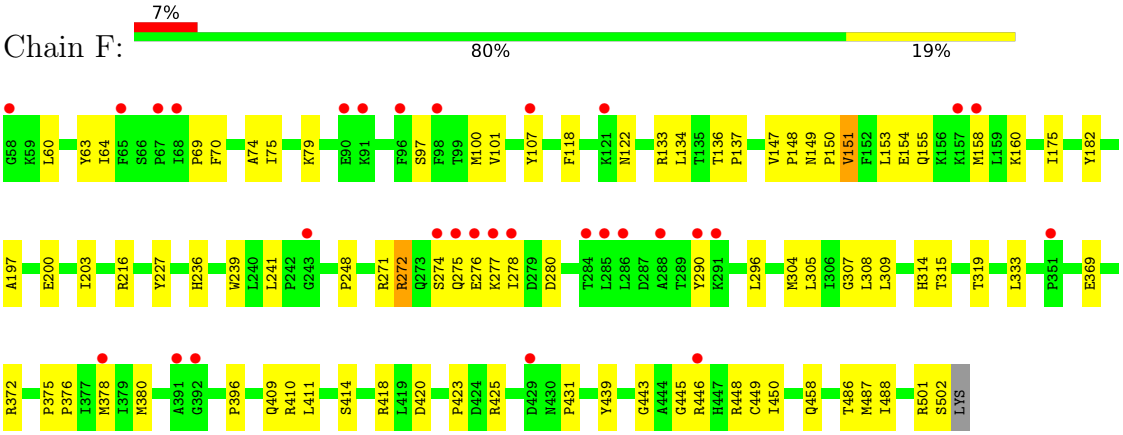
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain E:



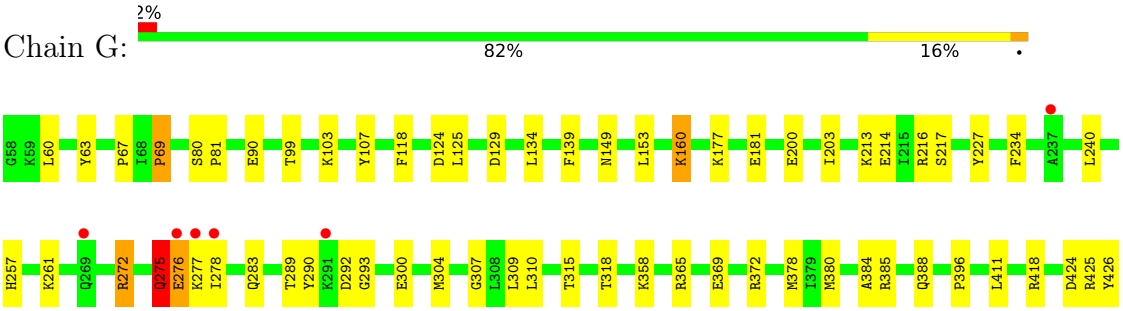
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain F:



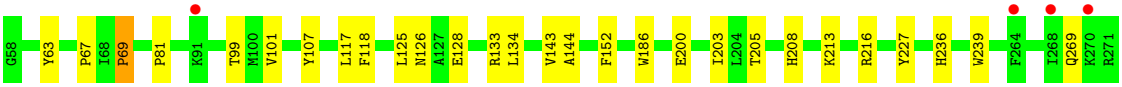
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

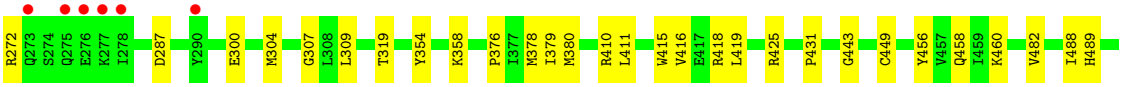
Chain G:



• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	111.21Å 111.50Å 118.48Å 64.09° 75.07° 62.42°	Depositor
Resolution (Å)	54.27 – 2.50 54.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (54.27-2.50) 98.5 (54.27-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.190 , 0.237 0.192 , 0.236	Depositor DCC
R_{free} test set	7786 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	30632	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: 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	0.26	0/3681	0.46	1/4986 (0.0%)
1	B	0.26	0/3681	0.45	0/4986
1	C	0.28	0/3681	0.46	0/4986
1	D	0.25	0/3681	0.44	0/4986
1	E	0.25	0/3681	0.44	0/4986
1	F	0.25	0/3681	0.44	0/4986
1	G	0.27	0/3681	0.48	4/4986 (0.1%)
1	H	0.26	0/3681	0.43	0/4986
All	All	0.26	0/29448	0.45	5/39888 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	G	488	ILE	N-CA-C	-6.45	93.59	111.00
1	G	276	GLU	N-CA-C	-6.07	94.62	111.00
1	G	275	GLN	N-CA-C	5.41	125.60	111.00
1	G	487	MET	CA-CB-CG	-5.03	104.75	113.30

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	3588	0	3581	41	0
1	B	3588	0	3581	51	0
1	C	3588	0	3581	64	0
1	D	3588	0	3581	40	0
1	E	3588	0	3581	53	0
1	F	3588	0	3581	81	0
1	G	3588	0	3581	76	0
1	H	3588	0	3581	45	0
2	A	43	0	30	7	0
2	B	43	0	30	2	0
2	C	43	0	30	7	0
2	D	43	0	30	4	0
2	E	43	0	30	9	0
2	F	43	0	30	7	0
2	G	43	0	30	5	0
2	H	43	0	30	8	0
3	A	82	0	46	5	0
3	B	82	0	46	7	0
3	C	82	0	46	17	0
3	D	82	0	46	5	0
3	E	82	0	46	5	0
3	F	82	0	46	17	0
3	G	82	0	46	5	0
3	H	82	0	46	12	0
4	A	120	0	0	4	0
4	B	152	0	0	3	0
4	C	141	0	0	6	0
4	D	144	0	0	2	0
4	E	113	0	0	6	0
4	F	62	0	0	3	0
4	G	114	0	0	4	0
4	H	82	0	0	2	0
All	All	30632	0	29256	477	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 8.

All (477) 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:C:107:TYR:OH	3:C:600:VFV:H12	1.38	1.19
1:F:155:GLN:HG2	1:F:304:MET:CE	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:TYR:OH	3:G:600:VFV:H12	1.67	0.95
1:G:272:ARG:HH11	1:G:272:ARG:HG2	1.32	0.93
1:F:101:VAL:HG21	3:F:600:VFV:CAN	2.00	0.92
1:C:236:HIS:HD2	3:C:600:VFV:CAO	1.84	0.91
1:F:101:VAL:HG21	3:F:600:VFV:H4	1.52	0.89
1:F:487:MET:HE3	3:F:600:VFV:H19	1.55	0.89
1:F:101:VAL:HG12	1:F:101:VAL:O	1.74	0.86
1:F:487:MET:CE	3:F:600:VFV:H19	2.05	0.86
1:E:183:PHE:HB2	4:E:2046:HOH:O	1.75	0.84
2:F:540:HEM:HBC2	2:F:540:HEM:HMC2	1.60	0.84
1:H:488:ILE:HG13	3:H:600:VFV:H20	1.61	0.83
1:F:236:HIS:HD2	3:F:600:VFV:CAO	1.92	0.83
1:F:236:HIS:CD2	3:F:600:VFV:H1	2.14	0.83
1:C:236:HIS:CD2	3:C:600:VFV:CAO	2.63	0.82
1:F:236:HIS:HD2	3:F:600:VFV:H1	1.43	0.81
1:C:323:MET:HE1	1:C:367:ILE:HG12	1.62	0.81
1:B:107:TYR:OH	3:B:600:VFV:H12	1.81	0.80
1:F:272:ARG:HG2	1:F:272:ARG:HH11	1.45	0.80
1:E:107:TYR:OH	3:E:600:VFV:H12	1.81	0.80
1:G:216:ARG:HD2	1:G:216:ARG:O	1.83	0.79
1:G:227:TYR:CZ	1:G:309:LEU:HD22	2.18	0.79
2:E:540:HEM:HBB2	2:E:540:HEM:HMB2	1.64	0.79
1:C:101:VAL:HG21	3:C:600:VFV:CAN	2.12	0.79
1:C:272:ARG:HG2	1:C:272:ARG:HH11	1.49	0.78
1:G:149:ASN:OD1	1:G:446:ARG:HD3	1.84	0.78
1:E:416:VAL:HG12	1:E:417:GLU:HG2	1.65	0.77
1:F:372:ARG:NH2	1:F:418:ARG:O	2.18	0.77
1:H:488:ILE:HD11	3:H:600:VFV:H21	1.66	0.76
1:C:272:ARG:HH11	1:C:272:ARG:CG	1.97	0.76
1:C:372:ARG:NH2	1:C:418:ARG:O	2.18	0.75
1:E:216:ARG:HD2	1:E:216:ARG:O	1.86	0.75
1:F:155:GLN:HG2	1:F:304:MET:HE1	1.67	0.75
1:D:372:ARG:NH2	1:D:418:ARG:O	2.19	0.74
1:D:135:THR:HG21	1:D:145:TYR:HD2	1.52	0.74
1:F:272:ARG:HH11	1:F:272:ARG:CG	2.01	0.74
1:F:155:GLN:HG2	1:F:304:MET:HE3	1.68	0.73
1:A:107:TYR:OH	3:A:600:VFV:H12	1.88	0.73
1:D:416:VAL:O	1:D:425:ARG:NH2	2.21	0.73
1:E:300:GLU:O	1:E:304:MET:HG3	1.89	0.73
1:B:276:GLU:N	1:B:276:GLU:OE1	2.23	0.72
1:F:275:GLN:NE2	4:F:2036:HOH:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:VAL:HG21	3:F:600:VFV:CAJ	2.19	0.71
1:F:107:TYR:OH	3:F:600:VFV:H12	1.91	0.71
1:B:487:MET:SD	3:B:580:VFV:H19	2.31	0.70
1:A:416:VAL:O	1:A:425:ARG:NH2	2.23	0.70
1:C:300:GLU:O	1:C:304:MET:HG3	1.92	0.70
1:B:467:LEU:O	1:B:501:ARG:NE	2.25	0.69
1:H:63:TYR:OH	1:H:99:THR:HG23	1.92	0.69
1:G:372:ARG:NH2	1:G:418:ARG:O	2.26	0.69
2:E:540:HEM:HBB2	2:E:540:HEM:CMB	2.24	0.68
1:H:107:TYR:OH	3:H:600:VFV:H12	1.93	0.68
1:A:272:ARG:NH1	1:A:298:ASP:OD1	2.26	0.68
1:F:101:VAL:O	1:F:101:VAL:CG1	2.42	0.68
1:F:133:ARG:NH2	1:F:239:TRP:O	2.27	0.68
1:F:153:LEU:HD11	1:F:446:ARG:HD3	1.75	0.68
1:G:275:GLN:O	1:G:277:LYS:N	2.27	0.67
1:G:227:TYR:CE1	1:G:309:LEU:CD2	2.77	0.67
1:B:415:TRP:CE2	1:B:431:PRO:HG2	2.30	0.67
1:B:129:ASP:OD2	1:B:385:ARG:HD3	1.95	0.67
1:F:376:PRO:HG2	2:F:540:HEM:HMB2	1.75	0.67
1:D:379:ILE:HD12	3:D:600:VFV:H12	1.76	0.67
1:A:200:GLU:O	1:A:203:ILE:HG22	1.95	0.67
2:H:540:HEM:CMC	2:H:540:HEM:HBC2	2.25	0.66
1:F:155:GLN:CG	1:F:304:MET:CE	2.73	0.66
1:C:107:TYR:OH	3:C:600:VFV:CAG	2.30	0.65
1:D:107:TYR:OH	3:D:600:VFV:H12	1.96	0.65
1:D:415:TRP:CE2	1:D:431:PRO:HG2	2.31	0.65
1:D:300:GLU:O	1:D:304:MET:HG3	1.96	0.65
1:C:236:HIS:CD2	3:C:600:VFV:H1	2.30	0.65
1:B:275:GLN:HG2	1:B:277:LYS:NZ	2.11	0.65
1:E:179:THR:O	4:E:2046:HOH:O	2.14	0.65
2:F:540:HEM:HBC2	2:F:540:HEM:CMC	2.27	0.65
1:G:272:ARG:HH11	1:G:272:ARG:CG	2.08	0.65
1:D:261:LYS:NZ	4:D:2034:HOH:O	2.30	0.64
1:E:416:VAL:O	1:E:417:GLU:HG3	1.98	0.64
1:H:488:ILE:CG1	3:H:600:VFV:H20	2.27	0.64
2:G:540:HEM:HMB2	2:G:540:HEM:HBB2	1.79	0.64
1:E:252:ARG:HE	1:G:485:THR:HG21	1.63	0.64
1:G:234:PHE:O	1:G:487:MET:CE	2.46	0.63
1:B:245:LEU:HD11	1:G:69:PRO:HG2	1.79	0.63
1:A:216:ARG:HD2	1:A:216:ARG:O	1.99	0.62
1:D:365:ARG:NH1	1:D:424:ASP:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:THR:HG23	1:B:290:TYR:O	2.00	0.62
1:E:355:ASP:O	1:E:358:LYS:HG2	2.00	0.61
1:G:378:MET:O	1:G:378:MET:HG2	2.00	0.61
1:G:277:LYS:O	1:G:277:LYS:HG2	2.00	0.61
1:H:216:ARG:HD2	1:H:216:ARG:O	2.01	0.61
1:C:63:TYR:OH	1:C:99:THR:HG23	2.01	0.60
1:G:470:TYR:O	1:G:501:ARG:NH2	2.30	0.60
1:B:388:GLN:NE2	4:B:2121:HOH:O	2.24	0.60
2:C:540:HEM:HBB2	2:C:540:HEM:HMB2	1.83	0.60
1:G:63:TYR:OH	1:G:99:THR:HG23	2.02	0.60
1:H:133:ARG:NH2	1:H:239:TRP:O	2.29	0.60
1:G:227:TYR:CE1	1:G:309:LEU:HD23	2.37	0.60
1:C:101:VAL:HG12	1:C:101:VAL:O	2.02	0.60
2:G:540:HEM:HBB2	2:G:540:HEM:CMB	2.30	0.60
1:C:415:TRP:CE2	1:C:431:PRO:HG2	2.37	0.60
1:D:314:HIS:HB3	1:D:488:ILE:HD12	1.84	0.60
1:E:415:TRP:CE2	1:E:431:PRO:HG2	2.37	0.59
1:H:101:VAL:HG12	1:H:101:VAL:O	2.01	0.59
1:C:378:MET:O	1:C:378:MET:HG2	2.01	0.59
1:E:372:ARG:NH2	1:E:418:ARG:O	2.29	0.58
2:H:540:HEM:HBC2	2:H:540:HEM:HMC2	1.85	0.58
1:E:248:PRO:HB3	1:G:485:THR:HG23	1.85	0.58
1:G:283:GLN:OE1	1:G:283:GLN:HA	2.03	0.58
1:G:234:PHE:O	1:G:487:MET:SD	2.61	0.58
2:B:540:HEM:CMB	2:B:540:HEM:HBB2	2.34	0.58
2:A:540:HEM:HMB2	2:A:540:HEM:HBB2	1.85	0.58
1:B:300:GLU:O	1:B:304:MET:HG3	2.02	0.58
1:C:378:MET:HG3	1:C:406:THR:OG1	2.04	0.58
1:B:378:MET:HG2	1:B:378:MET:O	2.03	0.57
1:D:378:MET:O	1:D:378:MET:HG2	2.04	0.57
1:B:275:GLN:C	1:B:276:GLU:OE1	2.43	0.57
1:F:305:LEU:HD23	1:F:308:LEU:HD12	1.87	0.57
1:B:275:GLN:HG2	1:B:277:LYS:HZ2	1.69	0.57
1:E:378:MET:O	1:E:378:MET:HG2	2.03	0.57
1:B:307:GLY:HA3	3:B:580:VFV:CAJ	2.35	0.57
1:C:107:TYR:CZ	3:C:600:VFV:H12	2.35	0.57
1:G:139:PHE:HE1	1:G:310:LEU:HD12	1.69	0.57
1:E:380:MET:HE1	1:E:443:GLY:HA2	1.87	0.57
1:G:227:TYR:CE1	1:G:309:LEU:HD22	2.39	0.57
1:H:488:ILE:HD11	3:H:600:VFV:CAD	2.33	0.57
1:A:410:ARG:HG2	1:A:418:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:CYS:HA	2:F:540:HEM:C4D	2.39	0.56
1:G:227:TYR:CD1	1:G:309:LEU:HD23	2.39	0.56
2:C:540:HEM:HBB2	2:C:540:HEM:CMB	2.35	0.56
1:D:63:TYR:OH	1:D:99:THR:HG23	2.05	0.56
1:G:358:LYS:HD2	4:G:2080:HOH:O	2.05	0.56
1:H:118:PHE:HE1	1:H:380:MET:HE1	1.70	0.56
1:B:487:MET:SD	3:B:580:VFV:CAI	2.93	0.56
1:F:216:ARG:HD2	1:F:216:ARG:O	2.05	0.56
1:G:483:ASN:ND2	1:G:486:THR:HG23	2.20	0.56
2:H:540:HEM:CMB	2:H:540:HEM:HBB2	2.36	0.56
1:B:422:ASN:HB3	1:B:425:ARG:HH11	1.70	0.56
1:C:207:SER:O	1:C:211:HIS:HB2	2.05	0.56
1:G:471:GLU:HA	1:G:501:ARG:NH2	2.21	0.56
1:B:416:VAL:O	1:B:425:ARG:NH2	2.39	0.56
1:C:379:ILE:HD11	1:C:402:CYS:HB3	1.88	0.56
1:D:273:GLN:HA	1:D:273:GLN:NE2	2.21	0.55
1:E:381:MET:HE1	4:E:2060:HOH:O	2.06	0.55
1:C:430:ASN:OD1	1:C:432:ALA:HB3	2.07	0.55
1:B:118:PHE:HE1	1:B:380:MET:HE1	1.71	0.55
1:H:236:HIS:HD2	3:H:600:VFV:CAO	2.20	0.55
1:G:300:GLU:O	1:G:304:MET:HG3	2.07	0.55
2:C:540:HEM:HBC2	2:C:540:HEM:CMC	2.37	0.55
1:C:272:ARG:HG2	1:C:272:ARG:NH1	2.16	0.55
1:B:63:TYR:OH	1:B:99:THR:HG23	2.08	0.54
1:G:278:ILE:O	1:G:283:GLN:HG2	2.07	0.54
2:D:540:HEM:HBD2	2:D:540:HEM:HHA	1.89	0.54
1:E:379:ILE:HD12	3:E:600:VFV:H12	1.90	0.54
2:E:540:HEM:HBC2	2:E:540:HEM:CMC	2.37	0.54
1:H:378:MET:O	1:H:378:MET:HG2	2.08	0.54
1:B:277:LYS:H	1:B:277:LYS:HD2	1.73	0.54
1:H:488:ILE:CG1	3:H:600:VFV:CAF	2.86	0.54
1:A:139:PHE:HE1	1:A:310:LEU:HD12	1.72	0.54
1:H:307:GLY:HA3	3:H:580:VFV:CAN	2.38	0.54
1:F:236:HIS:CD2	3:F:600:VFV:CAO	2.79	0.54
1:H:411:LEU:HG	4:H:2012:HOH:O	2.08	0.54
1:F:122:ASN:CG	1:F:149:ASN:HD22	2.12	0.54
1:G:227:TYR:CZ	1:G:309:LEU:CD2	2.89	0.54
1:A:227:TYR:CE1	1:A:309:LEU:HD22	2.44	0.53
1:B:257:HIS:CE1	1:B:261:LYS:HE3	2.43	0.53
1:C:307:GLY:HA3	3:C:580:VFV:CAJ	2.37	0.53
1:E:198:LEU:O	1:E:202:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:487:MET:HE2	3:F:600:VFV:H19	1.89	0.53
1:G:501:ARG:O	1:G:502:SER:C	2.46	0.53
2:F:540:HEM:CMB	2:F:540:HEM:HBB2	2.39	0.53
2:H:540:HEM:HBB2	2:H:540:HEM:HMB2	1.89	0.53
1:F:60:LEU:HD22	1:F:396:PRO:HG3	1.89	0.53
1:F:445:GLY:O	1:F:448:ARG:HG2	2.08	0.53
1:B:379:ILE:HD11	1:B:402:CYS:HB3	1.91	0.53
1:C:449:CYS:HA	2:C:540:HEM:C4D	2.43	0.53
1:C:381:MET:HE1	4:C:2077:HOH:O	2.08	0.53
1:B:378:MET:HG3	1:B:406:THR:OG1	2.09	0.52
1:G:430:ASN:HD22	1:G:432:ALA:H	1.57	0.52
1:B:483:ASN:HB2	1:B:492:GLU:HG3	1.91	0.52
1:E:410:ARG:HG2	1:E:418:ARG:NH1	2.23	0.52
1:G:160:LYS:NZ	4:G:2053:HOH:O	2.43	0.52
1:A:271:ARG:NH1	1:A:280:ASP:OD1	2.41	0.52
1:C:261:LYS:NZ	4:C:2046:HOH:O	2.41	0.52
2:G:540:HEM:HBC2	2:G:540:HEM:CMC	2.39	0.52
1:D:273:GLN:HA	1:D:273:GLN:HE21	1.75	0.52
1:A:449:CYS:HA	2:A:540:HEM:C4D	2.45	0.52
1:C:257:HIS:CE1	1:C:261:LYS:HE3	2.44	0.52
1:F:160:LYS:HG2	1:F:450:ILE:HB	1.91	0.52
1:E:198:LEU:O	1:E:202:ILE:CG1	2.58	0.52
1:B:482:VAL:HG13	1:B:489:HIS:HB3	1.91	0.52
1:C:227:TYR:CE1	1:C:309:LEU:HD22	2.45	0.52
1:E:70:PHE:CZ	1:E:101:VAL:HG13	2.45	0.52
1:D:216:ARG:HD2	1:D:216:ARG:O	2.10	0.52
1:H:380:MET:HE1	1:H:443:GLY:HA2	1.92	0.52
1:C:236:HIS:HD2	3:C:600:VFV:CAK	2.22	0.51
1:E:377:ILE:HD12	2:E:540:HEM:CHB	2.40	0.51
1:F:277:LYS:C	1:F:278:ILE:HD13	2.31	0.51
2:A:540:HEM:HBC2	2:A:540:HEM:CMC	2.40	0.51
1:B:410:ARG:HG2	1:B:418:ARG:NH1	2.26	0.51
1:G:272:ARG:HG2	1:G:272:ARG:NH1	2.12	0.51
2:D:540:HEM:HBB2	2:D:540:HEM:HMB2	1.91	0.51
1:F:60:LEU:CD2	1:F:396:PRO:HG3	2.41	0.51
2:A:540:HEM:HBB2	2:A:540:HEM:CMB	2.41	0.51
1:C:380:MET:HE1	1:C:443:GLY:HA2	1.93	0.51
1:E:372:ARG:NH1	1:E:373:LEU:HG	2.26	0.51
1:A:118:PHE:HE1	1:A:380:MET:HE1	1.75	0.51
1:C:239:TRP:CD1	3:C:580:VFV:CAH	2.94	0.51
1:G:369:GLU:OE2	1:G:425:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HH12	1:A:280:ASP:CG	2.14	0.50
1:F:154:GLU:O	1:F:158:MET:HG3	2.11	0.50
1:G:118:PHE:HE1	1:G:380:MET:HE1	1.76	0.50
1:B:269:GLN:O	1:B:273:GLN:HG2	2.10	0.50
2:D:540:HEM:HBB2	2:D:540:HEM:CMB	2.41	0.50
1:E:200:GLU:O	1:E:203:ILE:HG22	2.12	0.50
1:H:134:LEU:HD22	3:H:580:VFV:CBL	2.41	0.50
1:H:287:ASP:O	4:H:2053:HOH:O	2.19	0.50
1:E:182:TYR:OH	4:E:2047:HOH:O	2.18	0.50
1:C:257:HIS:NE2	1:C:261:LYS:HE3	2.26	0.50
1:F:378:MET:O	1:F:378:MET:HG2	2.11	0.50
1:G:449:CYS:HA	2:G:540:HEM:C4D	2.47	0.50
2:B:540:HEM:HBB2	2:B:540:HEM:HMB2	1.94	0.50
1:C:448:ARG:HD3	1:C:449:CYS:O	2.12	0.50
1:G:216:ARG:HD2	1:G:216:ARG:C	2.32	0.50
1:H:354:TYR:CE2	1:H:358:LYS:HD2	2.47	0.49
1:C:133:ARG:NH2	1:C:238:ALA:O	2.45	0.49
1:D:135:THR:HG21	1:D:145:TYR:CD2	2.41	0.49
1:E:377:ILE:HD12	2:E:540:HEM:C4A	2.47	0.49
1:G:289:THR:HG22	1:G:290:TYR:O	2.12	0.49
1:A:483:ASN:HB2	1:A:492:GLU:HG3	1.94	0.49
1:C:416:VAL:O	1:C:425:ARG:NH2	2.45	0.49
1:E:239:TRP:CD1	3:E:580:VFV:CAH	2.95	0.49
1:G:307:GLY:HA3	3:G:580:VFV:CAN	2.42	0.49
1:E:160:LYS:HG2	1:E:450:ILE:HB	1.94	0.49
1:F:414:SER:O	1:F:431:PRO:HG3	2.12	0.49
1:A:272:ARG:NH2	4:A:2078:HOH:O	2.46	0.49
1:D:271:ARG:HH12	1:D:280:ASP:CG	2.15	0.49
1:F:101:VAL:HG21	3:F:600:VFV:H3	1.93	0.49
1:G:292:ASP:OD1	1:G:293:GLY:N	2.46	0.49
1:F:425:ARG:NH1	4:F:2051:HOH:O	2.34	0.49
1:E:252:ARG:HE	1:G:485:THR:CG2	2.26	0.49
1:F:307:GLY:HA3	3:F:580:VFV:CAJ	2.42	0.49
1:E:175:ILE:HD13	1:E:458:GLN:HA	1.94	0.48
2:C:540:HEM:C1A	3:C:580:VFV:H13	2.48	0.48
1:G:153:LEU:HD21	1:G:446:ARG:CG	2.43	0.48
1:E:252:ARG:HH21	1:G:485:THR:HG22	1.78	0.48
1:F:315:THR:HB	2:F:540:HEM:CAB	2.44	0.48
1:F:380:MET:HE1	1:F:443:GLY:CA	2.44	0.48
1:C:101:VAL:HG21	3:C:600:VFV:H4	1.93	0.48
1:B:175:ILE:HD13	1:B:458:GLN:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:PHE:CE1	1:G:310:LEU:HD12	2.48	0.48
1:F:64:ILE:HD12	1:F:97:SER:O	2.14	0.48
1:G:67:PRO:O	1:G:69:PRO:HD3	2.13	0.48
1:G:358:LYS:HB3	1:G:358:LYS:HE3	1.64	0.48
1:H:415:TRP:CE2	1:H:431:PRO:HG2	2.48	0.48
1:F:149:ASN:HB3	1:F:150:PRO:HD3	1.95	0.48
1:H:227:TYR:CZ	1:H:309:LEU:HD22	2.49	0.48
1:H:307:GLY:HA3	3:H:580:VFV:CAJ	2.44	0.48
1:A:261:LYS:NZ	4:A:2043:HOH:O	2.45	0.48
1:C:415:TRP:CD2	1:C:431:PRO:HG2	2.49	0.48
1:E:369:GLU:OE1	1:E:372:ARG:HD3	2.12	0.48
1:B:227:TYR:CE1	1:B:309:LEU:HD22	2.49	0.48
1:B:467:LEU:O	1:B:501:ARG:CD	2.62	0.48
2:E:540:HEM:HMB2	2:E:540:HEM:CBB	2.41	0.48
1:F:70:PHE:CZ	1:F:101:VAL:HG13	2.48	0.48
1:C:445:GLY:O	1:C:448:ARG:HB2	2.14	0.48
1:B:467:LEU:O	1:B:501:ARG:HD2	2.13	0.47
1:C:307:GLY:HA3	3:C:580:VFV:CAN	2.44	0.47
1:D:227:TYR:CZ	1:D:309:LEU:HD22	2.48	0.47
1:G:307:GLY:HA3	3:G:580:VFV:CAJ	2.43	0.47
1:A:133:ARG:NH1	4:A:2037:HOH:O	2.47	0.47
1:F:75:ILE:HG22	1:F:79:LYS:HE2	1.97	0.47
1:G:177:LYS:HE2	1:G:181:GLU:OE2	2.14	0.47
1:H:300:GLU:O	1:H:304:MET:HG3	2.15	0.47
1:H:380:MET:HE3	2:H:540:HEM:HAA1	1.96	0.47
1:H:410:ARG:HG2	1:H:418:ARG:NH1	2.29	0.47
1:C:448:ARG:NH2	1:C:452:GLU:OE1	2.38	0.47
1:D:379:ILE:HD12	3:D:600:VFV:CAG	2.45	0.47
1:E:118:PHE:HE1	1:E:380:MET:HE1	1.79	0.47
1:G:275:GLN:O	1:G:276:GLU:C	2.51	0.47
1:G:125:LEU:HD23	1:G:384:ALA:HA	1.97	0.47
1:G:200:GLU:O	1:G:203:ILE:HG22	2.13	0.47
1:G:272:ARG:CG	1:G:272:ARG:NH1	2.73	0.47
1:H:205:THR:OG1	1:H:458:GLN:NE2	2.48	0.47
1:B:338:TYR:O	1:B:341:GLN:HB2	2.14	0.47
1:A:101:VAL:HG21	3:A:600:VFV:CAN	2.44	0.47
1:A:380:MET:HE3	2:A:540:HEM:HAA1	1.97	0.47
1:C:410:ARG:HG2	1:C:418:ARG:NH1	2.30	0.47
1:D:292:ASP:C	1:D:292:ASP:OD1	2.53	0.47
1:G:129:ASP:OD2	1:G:385:ARG:HD3	2.15	0.47
1:G:213:LYS:O	1:G:217:SER:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:NZ	1:D:270:LYS:HE3	2.29	0.47
1:A:314:HIS:ND1	4:A:2062:HOH:O	2.35	0.47
1:F:271:ARG:HA	1:F:274:SER:OG	2.15	0.47
1:H:236:HIS:CD2	3:H:600:VFV:CAO	2.97	0.47
1:D:385:ARG:NH1	4:D:2022:HOH:O	2.32	0.47
1:H:208:HIS:NE2	1:H:213:LYS:HG2	2.30	0.47
1:A:501:ARG:O	1:A:502:SER:C	2.53	0.46
1:B:207:SER:O	1:B:211:HIS:HB2	2.16	0.46
1:D:354:TYR:CE2	1:D:358:LYS:HD2	2.50	0.46
1:H:118:PHE:HE1	1:H:380:MET:CE	2.28	0.46
1:A:257:HIS:NE2	1:A:261:LYS:HE3	2.30	0.46
1:A:372:ARG:HD3	1:A:426:TYR:OH	2.15	0.46
1:B:415:TRP:CD2	1:B:431:PRO:HG2	2.51	0.46
1:G:257:HIS:NE2	1:G:261:LYS:HE3	2.31	0.46
1:A:300:GLU:O	1:A:304:MET:HG3	2.15	0.46
1:D:380:MET:HE1	1:D:443:GLY:HA2	1.97	0.46
1:E:487:MET:HE3	3:E:580:VFV:H20	1.97	0.46
2:E:540:HEM:HBD2	2:E:540:HEM:HHA	1.97	0.46
1:F:425:ARG:NH2	4:F:2051:HOH:O	2.33	0.46
1:A:236:HIS:CD2	1:F:248:PRO:HG2	2.51	0.46
1:D:200:GLU:O	1:D:203:ILE:HG22	2.16	0.46
1:D:415:TRP:CZ2	1:D:431:PRO:HG2	2.50	0.46
1:E:227:TYR:CZ	1:E:309:LEU:HD22	2.51	0.46
1:F:319:THR:OG1	1:F:376:PRO:HG3	2.15	0.46
1:G:380:MET:HE1	1:G:443:GLY:HA2	1.97	0.46
1:G:318:THR:HG21	1:G:488:ILE:HG12	1.96	0.46
1:B:239:TRP:CD1	3:B:580:VFV:CAH	2.99	0.46
1:B:380:MET:HE1	1:B:443:GLY:HA2	1.98	0.46
1:F:275:GLN:O	1:F:276:GLU:C	2.53	0.46
1:B:61:PRO:HA	1:B:393:TYR:CD1	2.51	0.46
1:E:342:LYS:HB3	1:E:347:GLU:HG2	1.97	0.46
1:F:200:GLU:O	1:F:203:ILE:HG22	2.15	0.46
1:G:99:THR:HA	1:G:103:LYS:O	2.15	0.46
1:D:430:ASN:ND2	1:D:432:ALA:HB3	2.31	0.46
1:G:60:LEU:HD21	1:G:396:PRO:HG3	1.98	0.46
1:G:118:PHE:HE1	1:G:380:MET:CE	2.29	0.46
1:H:81:PRO:HB2	1:H:378:MET:HE3	1.98	0.46
1:F:227:TYR:CE1	1:F:309:LEU:HD22	2.52	0.45
1:H:418:ARG:HG3	1:H:419:LEU:HG	1.97	0.45
1:A:120:SER:OG	1:A:125:LEU:HB2	2.16	0.45
1:F:314:HIS:HB3	1:F:488:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PHE:CE1	1:B:380:MET:HE1	2.50	0.45
1:F:272:ARG:HG2	1:F:272:ARG:NH1	2.17	0.45
3:F:600:VFV:H4	3:F:600:VFV:H5	1.69	0.45
1:A:227:TYR:CD1	1:A:309:LEU:HD22	2.51	0.45
1:D:129:ASP:OD2	1:D:385:ARG:NH1	2.49	0.45
2:C:540:HEM:NA	3:C:580:VFV:CAU	2.80	0.45
1:C:133:ARG:HH22	1:C:239:TRP:C	2.19	0.45
1:F:101:VAL:CG2	3:F:600:VFV:H4	2.37	0.45
1:F:136:THR:HB	1:F:137:PRO:HD3	1.98	0.45
1:H:200:GLU:O	1:H:203:ILE:HG22	2.17	0.45
1:A:332:THR:HG22	1:A:336:LYS:HE2	1.98	0.45
1:B:144:ALA:HA	1:B:152:PHE:CE1	2.51	0.45
1:C:107:TYR:OH	1:C:379:ILE:HD13	2.17	0.45
1:E:100:MET:O	1:E:101:VAL:C	2.55	0.45
1:F:380:MET:HE1	1:F:443:GLY:HA2	1.99	0.45
1:H:416:VAL:O	1:H:425:ARG:NH2	2.50	0.45
1:A:225:GLN:NE2	1:A:229:ASP:OD1	2.46	0.45
1:C:198:LEU:O	1:C:202:ILE:CG1	2.64	0.45
1:E:318:THR:HG21	1:E:488:ILE:HG22	1.98	0.45
1:F:236:HIS:HD2	3:F:600:VFV:CAK	2.28	0.44
1:F:410:ARG:O	1:F:410:ARG:HG2	2.17	0.44
1:H:67:PRO:O	1:H:69:PRO:HD3	2.18	0.44
1:C:101:VAL:HG21	3:C:600:VFV:CAJ	2.48	0.44
1:C:133:ARG:NH2	1:C:239:TRP:O	2.49	0.44
1:F:501:ARG:HG3	1:F:502:SER:N	2.31	0.44
1:E:124:ASP:HB3	1:E:388:GLN:NE2	2.32	0.44
1:C:200:GLU:O	1:C:203:ILE:HG22	2.17	0.44
1:C:186:TRP:O	1:C:498:TYR:OH	2.20	0.44
1:D:236:HIS:HD2	3:D:600:VFV:CAO	2.31	0.44
1:H:379:ILE:HD12	3:H:600:VFV:H12	1.99	0.44
1:H:456:TYR:O	1:H:460:LYS:HB2	2.17	0.44
1:F:278:ILE:HD13	1:F:278:ILE:N	2.32	0.44
1:B:309:LEU:O	1:B:309:LEU:HG	2.18	0.44
1:E:425:ARG:NH2	4:E:2100:HOH:O	2.37	0.44
1:G:365:ARG:NH1	1:G:424:ASP:OD1	2.49	0.44
1:A:252:ARG:HH22	1:F:486:THR:HG23	1.83	0.44
1:F:290:TYR:CE1	1:F:296:LEU:HD23	2.52	0.44
1:C:378:MET:O	1:C:405:PRO:HD2	2.18	0.43
1:B:160:LYS:NZ	4:B:2056:HOH:O	2.51	0.43
1:D:415:TRP:CD2	1:D:431:PRO:HG2	2.53	0.43
2:E:540:HEM:HBC2	2:E:540:HEM:HMC2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:LEU:HD12	3:G:580:VFV:CBL	2.48	0.43
1:F:118:PHE:O	1:F:445:GLY:HA3	2.18	0.43
1:A:379:ILE:HD12	3:A:600:VFV:H12	2.01	0.43
1:C:280:ASP:HB2	4:C:2066:HOH:O	2.17	0.43
1:D:449:CYS:HA	2:D:540:HEM:C4D	2.53	0.43
1:E:252:ARG:NE	1:G:485:THR:HG21	2.31	0.43
1:G:227:TYR:CD1	1:G:309:LEU:CD2	3.01	0.43
1:C:247:LEU:HD12	1:C:250:PHE:CZ	2.54	0.43
1:E:183:PHE:N	4:E:2046:HOH:O	2.33	0.43
1:G:80:SER:HA	1:G:81:PRO:HD3	1.85	0.43
1:F:410:ARG:HG2	1:F:418:ARG:NH1	2.33	0.43
1:B:131:TYR:CD1	3:B:580:VFV:H18	2.54	0.43
1:C:319:THR:OG1	1:C:376:PRO:HG3	2.18	0.43
2:C:540:HEM:HBC2	2:C:540:HEM:HMC2	2.00	0.43
1:A:175:ILE:HD13	1:A:458:GLN:HA	2.01	0.43
1:D:131:TYR:O	1:D:135:THR:HB	2.19	0.43
1:F:227:TYR:CZ	1:F:309:LEU:HD22	2.54	0.43
1:C:456:TYR:O	1:C:460:LYS:HB2	2.19	0.43
1:D:125:LEU:HD23	1:D:384:ALA:HA	2.00	0.43
1:C:118:PHE:HE1	1:C:380:MET:HE1	1.84	0.43
1:C:323:MET:HE2	1:C:323:MET:HB2	1.92	0.43
2:H:540:HEM:CMC	2:H:540:HEM:CBC	2.96	0.43
1:D:207:SER:O	1:D:211:HIS:HB2	2.18	0.42
1:G:124:ASP:HB3	1:G:388:GLN:NE2	2.33	0.42
1:B:307:GLY:HA3	3:B:580:VFV:CAN	2.49	0.42
1:F:409:GLN:HG2	1:F:439:TYR:HA	2.00	0.42
1:G:426:TYR:HA	1:G:430:ASN:OD1	2.19	0.42
1:H:482:VAL:HG13	1:H:489:HIS:HB3	2.00	0.42
2:A:540:HEM:C1A	3:A:580:VFV:H13	2.54	0.42
1:G:315:THR:HB	2:G:540:HEM:CAB	2.49	0.42
1:A:241:LEU:HD21	1:F:241:LEU:HD21	2.01	0.42
1:F:74:ALA:HA	1:F:100:MET:HE3	2.01	0.42
1:H:63:TYR:OH	1:H:99:THR:CG2	2.66	0.42
1:A:371:LEU:HA	1:A:371:LEU:HD23	1.87	0.42
1:B:187:GLY:O	1:B:500:ARG:NH2	2.52	0.42
1:C:446:ARG:HD3	4:C:2052:HOH:O	2.20	0.42
1:D:227:TYR:CE1	1:D:309:LEU:HD22	2.55	0.42
1:C:89:TYR:HB2	1:C:109:LEU:HD12	2.02	0.42
1:C:375:PRO:HA	1:C:376:PRO:HD3	1.92	0.42
3:C:580:VFV:H4	3:C:580:VFV:H5	1.62	0.42
1:D:129:ASP:OD2	1:D:385:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:ASN:ND2	1:G:432:ALA:HB3	2.34	0.42
1:E:449:CYS:HA	2:E:540:HEM:C4D	2.54	0.42
1:A:153:LEU:O	1:A:157:LYS:HG3	2.19	0.42
1:B:58:GLY:N	4:B:2002:HOH:O	2.52	0.42
1:E:239:TRP:CZ3	3:E:600:VFV:H4	2.55	0.42
1:E:265:TYR:OH	1:E:299:ASP:OD1	2.35	0.42
1:G:240:LEU:HD12	1:G:240:LEU:HA	1.86	0.42
1:A:456:TYR:O	1:A:460:LYS:HB2	2.20	0.42
1:C:311:ALA:HB1	3:C:580:VFV:H12	2.02	0.42
1:B:395:ILE:HA	1:B:396:PRO:HD3	1.89	0.41
1:B:149:ASN:HB3	1:B:150:PRO:HD3	2.02	0.41
1:C:241:LEU:HD21	1:D:241:LEU:HD21	2.01	0.41
1:D:395:ILE:HA	1:D:396:PRO:HD3	1.89	0.41
1:F:333:LEU:HD21	1:F:423:PRO:HG2	2.01	0.41
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.93	0.41
1:E:430:ASN:OD1	1:E:432:ALA:HB3	2.20	0.41
1:F:148:PRO:O	1:F:151:VAL:HG13	2.20	0.41
1:F:153:LEU:HD21	1:F:446:ARG:CG	2.50	0.41
1:G:214:GLU:O	1:G:217:SER:OG	2.32	0.41
1:G:411:LEU:HD12	1:G:411:LEU:HA	1.84	0.41
1:E:292:ASP:OD1	1:E:293:GLY:N	2.53	0.41
1:F:147:VAL:HG21	1:F:151:VAL:HG22	2.03	0.41
1:G:488:ILE:O	1:G:488:ILE:HG23	2.20	0.41
1:H:269:GLN:HA	1:H:272:ARG:HB2	2.03	0.41
1:H:319:THR:OG1	1:H:376:PRO:HG3	2.21	0.41
1:C:95:VAL:O	4:C:2020:HOH:O	2.22	0.41
1:E:133:ARG:NH2	1:E:239:TRP:O	2.54	0.41
1:H:117:LEU:HA	1:H:125:LEU:HD12	2.03	0.41
3:A:600:VFV:H1	3:A:600:VFV:H6	1.80	0.41
1:E:165:ILE:HG22	1:E:169:LYS:HE3	2.02	0.41
1:G:90:GLU:HG2	4:G:2025:HOH:O	2.21	0.41
1:G:307:GLY:C	3:G:580:VFV:H4	2.41	0.41
1:B:216:ARG:O	1:B:216:ARG:NH1	2.41	0.41
1:E:395:ILE:HA	1:E:396:PRO:HD3	1.95	0.41
1:F:182:TYR:OH	1:F:197:ALA:HA	2.20	0.41
1:H:126:ASN:ND2	1:H:128:GLU:OE1	2.43	0.41
1:H:186:TRP:O	1:H:498:TYR:OH	2.20	0.41
1:A:271:ARG:HD3	1:A:283:GLN:OE1	2.20	0.41
1:A:375:PRO:HA	1:A:376:PRO:HD3	1.86	0.41
1:F:375:PRO:HA	1:F:376:PRO:HD3	1.93	0.41
1:B:247:LEU:HA	1:B:248:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:HIS:HA	4:C:2010:HOH:O	2.20	0.41
1:C:483:ASN:HB2	1:C:492:GLU:HG3	2.03	0.41
1:D:379:ILE:CD1	3:D:600:VFV:H12	2.48	0.41
1:F:271:ARG:NH1	1:F:280:ASP:OD1	2.39	0.41
2:H:540:HEM:HMC2	2:H:540:HEM:CBC	2.49	0.41
1:A:331:LYS:HZ2	1:A:473:ASP:CG	2.24	0.40
1:B:276:GLU:N	1:B:276:GLU:CD	2.74	0.40
1:C:133:ARG:HH22	1:C:239:TRP:HA	1.86	0.40
1:E:227:TYR:CE1	1:E:309:LEU:HD22	2.56	0.40
1:F:63:TYR:HA	1:F:97:SER:O	2.20	0.40
1:F:134:LEU:HD21	1:F:239:TRP:HA	2.04	0.40
1:F:449:CYS:HB2	2:F:540:HEM:NA	2.36	0.40
1:C:122:ASN:H	1:C:446:ARG:NH1	2.19	0.40
1:E:212:GLY:O	1:E:216:ARG:HB3	2.21	0.40
1:E:416:VAL:C	1:E:417:GLU:HG3	2.41	0.40
1:F:369:GLU:OE2	1:F:372:ARG:NH1	2.54	0.40
3:F:600:VFV:H1	3:F:600:VFV:H6	1.81	0.40
1:H:144:ALA:HA	1:H:152:PHE:CE1	2.57	0.40
1:H:449:CYS:HA	2:H:540:HEM:C4D	2.56	0.40
1:A:377:ILE:HD12	2:A:540:HEM:CHB	2.51	0.40
1:A:395:ILE:HA	1:A:396:PRO:HD3	1.90	0.40
1:E:479:PHE:HA	1:E:480:PRO:HD3	1.99	0.40
1:F:175:ILE:HD13	1:F:458:GLN:HA	2.03	0.40
1:G:261:LYS:NZ	4:G:2045:HOH:O	2.54	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	443/446 (99%)	431 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	443/446 (99%)	434 (98%)	9 (2%)	0	100	100
1	C	443/446 (99%)	434 (98%)	9 (2%)	0	100	100
1	D	443/446 (99%)	434 (98%)	9 (2%)	0	100	100
1	E	443/446 (99%)	431 (97%)	12 (3%)	0	100	100
1	F	443/446 (99%)	431 (97%)	11 (2%)	1 (0%)	47	68
1	G	443/446 (99%)	432 (98%)	10 (2%)	1 (0%)	47	68
1	H	443/446 (99%)	428 (97%)	14 (3%)	1 (0%)	47	68
All	All	3544/3568 (99%)	3455 (98%)	86 (2%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	69	PRO
1	F	69	PRO
1	G	69	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	389/390 (100%)	387 (100%)	2 (0%)	88	96
1	B	389/390 (100%)	386 (99%)	3 (1%)	81	93
1	C	389/390 (100%)	384 (99%)	5 (1%)	69	87
1	D	389/390 (100%)	385 (99%)	4 (1%)	76	90
1	E	389/390 (100%)	389 (100%)	0	100	100
1	F	389/390 (100%)	385 (99%)	4 (1%)	76	90
1	G	389/390 (100%)	385 (99%)	4 (1%)	76	90
1	H	389/390 (100%)	388 (100%)	1 (0%)	92	97
All	All	3112/3120 (100%)	3089 (99%)	23 (1%)	84	94

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	143	VAL
1	B	143	VAL
1	B	276	GLU
1	B	289	THR
1	C	143	VAL
1	C	199	SER
1	C	272	ARG
1	C	372	ARG
1	C	448	ARG
1	D	135	THR
1	D	219	LEU
1	D	372	ARG
1	D	385	ARG
1	F	151	VAL
1	F	272	ARG
1	F	411	LEU
1	F	420	ASP
1	G	160	LYS
1	G	272	ARG
1	G	275	GLN
1	G	430	ASN
1	H	143	VAL

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

Mol	Chain	Res	Type
1	C	236	HIS
1	D	236	HIS
1	D	273	GLN
1	D	430	ASN
1	F	149	ASN
1	F	236	HIS
1	G	430	ASN
1	H	236	HIS
1	H	458	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)

24 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	VFV	B	580	2	38,46,46	1.86	6 (15%)	57,64,64	1.16	5 (8%)
2	HEM	F	540	3,1	41,50,50	1.33	7 (17%)	45,82,82	1.97	10 (22%)
2	HEM	E	540	3,1	41,50,50	1.34	5 (12%)	45,82,82	1.84	8 (17%)
3	VFV	E	580	2	38,46,46	2.15	7 (18%)	57,64,64	1.14	5 (8%)
3	VFV	E	600	-	38,46,46	2.28	5 (13%)	57,64,64	1.19	4 (7%)
3	VFV	A	580	2	38,46,46	2.00	6 (15%)	57,64,64	1.08	3 (5%)
3	VFV	G	580	2	38,46,46	1.93	7 (18%)	57,64,64	1.14	4 (7%)
3	VFV	F	580	2	38,46,46	2.03	6 (15%)	57,64,64	1.17	5 (8%)
3	VFV	D	580	2	38,46,46	2.00	5 (13%)	57,64,64	1.14	4 (7%)
3	VFV	A	600	-	38,46,46	2.52	5 (13%)	57,64,64	1.34	8 (14%)
3	VFV	D	600	-	38,46,46	2.38	6 (15%)	57,64,64	1.12	4 (7%)
3	VFV	B	600	-	38,46,46	2.46	5 (13%)	57,64,64	1.01	3 (5%)
2	HEM	D	540	3,1	41,50,50	1.35	6 (14%)	45,82,82	1.88	9 (20%)
3	VFV	C	600	-	38,46,46	2.55	7 (18%)	57,64,64	1.32	7 (12%)
2	HEM	C	540	3,1	41,50,50	1.34	6 (14%)	45,82,82	1.96	8 (17%)
2	HEM	A	540	3,1	41,50,50	1.32	6 (14%)	45,82,82	1.89	10 (22%)
3	VFV	G	600	-	38,46,46	2.48	8 (21%)	57,64,64	1.23	3 (5%)
3	VFV	C	580	2	38,46,46	1.94	5 (13%)	57,64,64	1.18	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	H	540	3,1	41,50,50	1.36	6 (14%)	45,82,82	1.94	10 (22%)
2	HEM	G	540	3,1	41,50,50	1.38	4 (9%)	45,82,82	1.85	8 (17%)
3	VFV	F	600	-	38,46,46	2.62	6 (15%)	57,64,64	1.32	6 (10%)
3	VFV	H	580	2	38,46,46	1.89	6 (15%)	57,64,64	1.17	6 (10%)
2	HEM	B	540	3,1	41,50,50	1.33	7 (17%)	45,82,82	1.97	9 (20%)
3	VFV	H	600	-	38,46,46	2.91	8 (21%)	57,64,64	1.12	4 (7%)

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	VFV	B	580	2	-	0/24/28/28	0/6/6/6
2	HEM	F	540	3,1	-	2/12/54/54	-
2	HEM	E	540	3,1	-	3/12/54/54	-
3	VFV	E	580	2	-	0/24/28/28	0/6/6/6
3	VFV	E	600	-	-	0/24/28/28	0/6/6/6
3	VFV	A	580	2	-	1/24/28/28	0/6/6/6
3	VFV	G	580	2	-	1/24/28/28	0/6/6/6
3	VFV	F	580	2	-	1/24/28/28	0/6/6/6
3	VFV	D	580	2	-	0/24/28/28	0/6/6/6
3	VFV	A	600	-	-	0/24/28/28	0/6/6/6
3	VFV	D	600	-	-	0/24/28/28	0/6/6/6
3	VFV	B	600	-	-	0/24/28/28	0/6/6/6
2	HEM	D	540	3,1	-	5/12/54/54	-
3	VFV	C	600	-	-	0/24/28/28	0/6/6/6
2	HEM	C	540	3,1	-	0/12/54/54	-
2	HEM	A	540	3,1	-	0/12/54/54	-
3	VFV	G	600	-	-	0/24/28/28	0/6/6/6
3	VFV	C	580	2	-	2/24/28/28	0/6/6/6
2	HEM	H	540	3,1	-	2/12/54/54	-
2	HEM	G	540	3,1	-	2/12/54/54	-
3	VFV	F	600	-	-	0/24/28/28	0/6/6/6
3	VFV	H	580	2	-	0/24/28/28	0/6/6/6
2	HEM	B	540	3,1	-	0/12/54/54	-
3	VFV	H	600	-	-	1/24/28/28	0/6/6/6

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	600	VFV	NAY-NAZ	-12.59	1.13	1.37
3	A	600	VFV	NAY-NAZ	-10.53	1.17	1.37
3	B	600	VFV	NAY-NAZ	-10.31	1.17	1.37
3	F	600	VFV	NAY-NAZ	-9.70	1.18	1.37
3	F	600	VFV	CBK-CBN	-9.46	1.37	1.52
3	C	600	VFV	CBK-CBN	-9.24	1.37	1.52
3	D	600	VFV	NAY-NAZ	-9.21	1.19	1.37
3	C	600	VFV	NAY-NAZ	-9.18	1.19	1.37
3	G	600	VFV	CBK-CBN	-8.88	1.38	1.52
3	G	600	VFV	NAY-NAZ	-8.69	1.20	1.37
3	H	600	VFV	CBK-CBN	-8.53	1.39	1.52
3	E	600	VFV	NAY-NAZ	-8.52	1.20	1.37
3	A	600	VFV	CBK-CBN	-8.27	1.39	1.52
3	E	600	VFV	CBK-CBN	-8.22	1.39	1.52
3	D	600	VFV	CBK-CBN	-8.02	1.39	1.52
3	E	580	VFV	CBK-CBN	-7.96	1.39	1.52
3	B	600	VFV	CBK-CBN	-7.90	1.39	1.52
3	F	580	VFV	CBK-CBN	-7.61	1.40	1.52
3	C	580	VFV	CBK-CBN	-7.55	1.40	1.52
3	B	580	VFV	CBK-CBN	-7.49	1.40	1.52
3	A	580	VFV	CBK-CBN	-7.46	1.40	1.52
3	D	580	VFV	CBK-CBN	-7.41	1.40	1.52
3	H	580	VFV	CBK-CBN	-7.36	1.40	1.52
3	E	580	VFV	NAY-NAZ	-7.04	1.23	1.37
3	G	580	VFV	CBK-CBN	-6.58	1.41	1.52
3	D	580	VFV	NAY-NAZ	-6.08	1.25	1.37
3	A	580	VFV	NAY-NAZ	-5.74	1.26	1.37
3	G	600	VFV	CBF-CBC	-5.43	1.38	1.50
3	F	600	VFV	CBF-CBC	-5.28	1.39	1.50
3	F	580	VFV	NAY-NAZ	-5.26	1.27	1.37
3	D	580	VFV	CBF-CBC	-5.16	1.39	1.50
3	A	600	VFV	CBF-CBC	-5.15	1.39	1.50
3	G	580	VFV	NAY-NAZ	-5.15	1.27	1.37
3	C	580	VFV	CBF-CBC	-5.10	1.39	1.50
3	C	580	VFV	NAY-NAZ	-5.07	1.27	1.37
3	C	600	VFV	CBF-CBC	-5.06	1.39	1.50
3	H	600	VFV	CBF-CBC	-5.05	1.39	1.50
3	E	600	VFV	CBF-CBC	-5.05	1.39	1.50
3	D	600	VFV	CBF-CBC	-5.02	1.39	1.50
3	B	600	VFV	CBF-CBC	-4.98	1.39	1.50
3	A	580	VFV	CBF-CBC	-4.96	1.39	1.50
3	E	580	VFV	CBF-CBC	-4.82	1.40	1.50
3	B	580	VFV	CBF-CBC	-4.79	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	580	VFV	CBF-CBC	-4.76	1.40	1.50
3	F	600	VFV	CBJ-CBG	-4.70	1.37	1.49
3	G	580	VFV	CBF-CBC	-4.65	1.40	1.50
3	F	580	VFV	CBF-CBC	-4.41	1.41	1.50
3	C	600	VFV	CBJ-CBG	-4.41	1.38	1.49
3	H	580	VFV	NAY-NAZ	-4.20	1.29	1.37
3	G	600	VFV	CBJ-CBG	-4.15	1.38	1.49
3	E	580	VFV	CBJ-CBG	-4.14	1.38	1.49
3	B	580	VFV	CBJ-CBG	-4.11	1.38	1.49
3	A	600	VFV	CBJ-CBG	-4.11	1.38	1.49
3	E	600	VFV	CBJ-CBG	-4.08	1.38	1.49
3	B	600	VFV	CBJ-CBG	-4.03	1.39	1.49
3	A	580	VFV	CBJ-CBG	-4.01	1.39	1.49
3	D	600	VFV	CBJ-CBG	-3.99	1.39	1.49
3	H	600	VFV	CAW-NBO	-3.99	1.44	1.48
2	G	540	HEM	C1B-NB	-3.98	1.33	1.40
3	C	580	VFV	CBJ-CBG	-3.93	1.39	1.49
3	F	580	VFV	CBJ-CBG	-3.92	1.39	1.49
3	H	580	VFV	CBJ-CBG	-3.92	1.39	1.49
3	D	580	VFV	CBJ-CBG	-3.91	1.39	1.49
3	H	600	VFV	CBJ-CBG	-3.91	1.39	1.49
3	G	580	VFV	CBJ-CBG	-3.88	1.39	1.49
2	D	540	HEM	C1B-NB	-3.87	1.33	1.40
2	E	540	HEM	C1B-NB	-3.84	1.33	1.40
2	C	540	HEM	C1B-NB	-3.81	1.33	1.40
2	A	540	HEM	C1B-NB	-3.72	1.33	1.40
2	H	540	HEM	C1B-NB	-3.70	1.33	1.40
2	B	540	HEM	C1B-NB	-3.65	1.34	1.40
2	G	540	HEM	C4D-ND	-3.61	1.34	1.40
3	B	580	VFV	NAY-NAZ	-3.56	1.30	1.37
2	F	540	HEM	C4D-ND	-3.43	1.34	1.40
3	F	600	VFV	CAW-NBO	-3.40	1.44	1.48
2	F	540	HEM	C1B-NB	-3.37	1.34	1.40
2	E	540	HEM	C4D-ND	-3.25	1.34	1.40
2	H	540	HEM	C4D-ND	-3.24	1.34	1.40
2	B	540	HEM	C4D-ND	-3.23	1.34	1.40
2	D	540	HEM	C4D-ND	-3.21	1.34	1.40
2	A	540	HEM	C4D-ND	-3.20	1.34	1.40
3	H	600	VFV	FAB-CBD	-3.20	1.28	1.36
2	C	540	HEM	C4D-ND	-3.15	1.34	1.40
3	C	600	VFV	FAB-CBD	-3.14	1.28	1.36
3	G	600	VFV	CAW-NBO	-3.12	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	600	VFV	FAC-CBE	-3.12	1.27	1.35
3	G	580	VFV	FAB-CBD	-3.02	1.29	1.36
3	F	580	VFV	FAB-CBD	-2.93	1.29	1.36
3	G	580	VFV	FAC-CBE	-2.86	1.28	1.35
3	F	580	VFV	CAW-NBO	2.83	1.51	1.48
2	F	540	HEM	FE-NB	2.80	2.10	1.96
2	E	540	HEM	FE-NB	2.73	2.10	1.96
3	D	600	VFV	FAC-CBE	-2.70	1.28	1.35
2	G	540	HEM	FE-NB	2.66	2.10	1.96
2	A	540	HEM	FE-NB	2.66	2.10	1.96
2	H	540	HEM	FE-NB	2.63	2.09	1.96
3	B	580	VFV	FAC-CBE	-2.60	1.28	1.35
2	D	540	HEM	FE-NB	2.60	2.09	1.96
2	C	540	HEM	FE-NB	2.60	2.09	1.96
2	H	540	HEM	C4B-NB	-2.55	1.33	1.38
3	H	600	VFV	CAT-NBO	-2.55	1.32	1.37
2	B	540	HEM	FE-NB	2.54	2.09	1.96
3	C	600	VFV	CAT-NBO	-2.50	1.33	1.37
3	H	580	VFV	FAB-CBD	-2.47	1.30	1.36
3	G	600	VFV	FAB-CBD	-2.45	1.30	1.36
3	C	580	VFV	CAT-NBO	-2.43	1.33	1.37
3	G	600	VFV	CAT-NBO	-2.41	1.33	1.37
3	B	600	VFV	CAT-NBO	-2.41	1.33	1.37
3	D	580	VFV	CAT-NBO	-2.41	1.33	1.37
3	A	580	VFV	CAT-NBO	-2.39	1.33	1.37
3	C	600	VFV	FAC-CBE	-2.37	1.29	1.35
3	F	600	VFV	CAT-NBO	-2.36	1.33	1.37
2	D	540	HEM	C4B-NB	-2.36	1.33	1.38
3	B	580	VFV	CAT-NBO	-2.33	1.33	1.37
2	F	540	HEM	CHB-C1B	2.33	1.40	1.35
2	F	540	HEM	C1D-ND	-2.31	1.34	1.38
3	D	600	VFV	CAT-NBO	-2.31	1.33	1.37
3	E	600	VFV	CAT-NBO	-2.30	1.33	1.37
2	A	540	HEM	C4B-NB	-2.29	1.34	1.38
2	C	540	HEM	C4B-NB	-2.29	1.34	1.38
3	A	600	VFV	CAT-NBO	-2.29	1.33	1.37
2	C	540	HEM	C1D-ND	-2.25	1.34	1.38
3	E	580	VFV	CAT-NBO	-2.23	1.33	1.37
2	H	540	HEM	C1D-ND	-2.22	1.34	1.38
3	G	580	VFV	CAT-NBO	-2.20	1.33	1.37
2	C	540	HEM	CHB-C1B	2.20	1.40	1.35
2	B	540	HEM	C4B-NB	-2.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	580	VFV	FAB-CBD	-2.17	1.31	1.36
2	G	540	HEM	C4B-NB	-2.16	1.34	1.38
2	D	540	HEM	CHB-C1B	2.15	1.40	1.35
2	B	540	HEM	C1D-ND	-2.15	1.34	1.38
2	D	540	HEM	C1D-ND	-2.14	1.34	1.38
3	E	580	VFV	FAC-CBE	-2.14	1.30	1.35
2	F	540	HEM	C4B-NB	-2.13	1.34	1.38
3	G	600	VFV	FAC-CBE	-2.12	1.30	1.35
2	A	540	HEM	CHB-C1B	2.12	1.40	1.35
2	E	540	HEM	C4B-NB	-2.10	1.34	1.38
2	A	540	HEM	C1D-ND	-2.07	1.34	1.38
2	E	540	HEM	C1D-ND	-2.05	1.34	1.38
3	H	580	VFV	CAT-NBO	-2.05	1.33	1.37
2	F	540	HEM	FE-ND	-2.03	1.86	1.96
2	B	540	HEM	CHB-C1B	2.03	1.40	1.35
3	A	580	VFV	FAB-CBD	-2.02	1.31	1.36
2	H	540	HEM	FE-ND	-2.01	1.86	1.96
2	B	540	HEM	FE-ND	-2.00	1.87	1.96

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	540	HEM	CHC-C4B-NB	5.98	130.93	124.43
2	H	540	HEM	CHC-C4B-NB	5.60	130.51	124.43
2	G	540	HEM	CHC-C4B-NB	5.50	130.41	124.43
2	B	540	HEM	CHC-C4B-NB	5.46	130.37	124.43
2	A	540	HEM	CHC-C4B-NB	5.41	130.31	124.43
2	C	540	HEM	CHC-C4B-NB	5.36	130.26	124.43
2	D	540	HEM	CHC-C4B-NB	5.29	130.18	124.43
2	E	540	HEM	CHC-C4B-NB	5.19	130.07	124.43
2	C	540	HEM	C1B-NB-C4B	4.95	110.18	105.07
2	B	540	HEM	C1B-NB-C4B	4.93	110.16	105.07
2	C	540	HEM	CHD-C1D-ND	4.87	129.72	124.43
2	A	540	HEM	CHD-C1D-ND	4.75	129.60	124.43
2	D	540	HEM	C1B-NB-C4B	4.73	109.96	105.07
2	H	540	HEM	CHD-C1D-ND	4.71	129.54	124.43
2	B	540	HEM	CHD-C1D-ND	4.67	129.51	124.43
2	F	540	HEM	CHD-C1D-ND	4.66	129.49	124.43
2	F	540	HEM	C1B-NB-C4B	4.61	109.84	105.07
2	E	540	HEM	CHD-C1D-ND	4.48	129.30	124.43
2	G	540	HEM	CHD-C1D-ND	4.46	129.28	124.43
2	D	540	HEM	CHD-C1D-ND	4.37	129.18	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	540	HEM	CHA-C4D-ND	4.34	129.74	124.38
2	A	540	HEM	C1B-NB-C4B	4.33	109.54	105.07
2	G	540	HEM	C1B-NB-C4B	4.29	109.50	105.07
2	H	540	HEM	C1B-NB-C4B	4.28	109.49	105.07
2	B	540	HEM	CHA-C4D-ND	4.20	129.57	124.38
2	E	540	HEM	C1B-NB-C4B	4.14	109.35	105.07
3	F	600	VFV	CAS-CBK-CBE	3.96	121.21	116.13
3	A	600	VFV	CAV-CBE-CBK	-3.89	119.17	123.83
2	H	540	HEM	CHA-C4D-ND	3.88	129.18	124.38
2	F	540	HEM	CHA-C4D-ND	3.82	129.10	124.38
2	A	540	HEM	CHA-C4D-ND	3.80	129.07	124.38
3	F	600	VFV	CAV-CBE-CBK	-3.75	119.34	123.83
2	B	540	HEM	CHB-C1B-NB	3.57	128.79	124.38
2	D	540	HEM	CHA-C4D-ND	3.55	128.77	124.38
2	H	540	HEM	CHB-C1B-NB	3.44	128.64	124.38
3	C	600	VFV	CAV-CBJ-CBG	-3.44	115.17	120.86
3	C	600	VFV	CAS-CBK-CBE	3.43	120.54	116.13
3	C	600	VFV	CAV-CBE-CBK	-3.31	119.87	123.83
3	A	600	VFV	CAN-CAJ-CBD	3.29	121.77	118.36
3	E	600	VFV	CAV-CBE-CBK	-3.28	119.90	123.83
3	G	600	VFV	CAS-CBK-CBE	3.27	120.33	116.13
2	G	540	HEM	CHA-C4D-ND	3.26	128.41	124.38
2	E	540	HEM	CHA-C4D-ND	3.25	128.40	124.38
2	G	540	HEM	CHB-C1B-NB	3.25	128.40	124.38
2	F	540	HEM	CHD-C1D-C2D	-3.24	119.92	124.98
2	C	540	HEM	CHD-C1D-C2D	-3.17	120.02	124.98
2	A	540	HEM	CHD-C1D-C2D	-3.10	120.13	124.98
3	G	600	VFV	CAV-CBE-CBK	-3.10	120.11	123.83
2	E	540	HEM	CHB-C1B-NB	3.07	128.17	124.38
2	G	540	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
2	C	540	HEM	CHB-C1B-NB	3.03	128.12	124.38
2	D	540	HEM	CHB-C1B-NB	3.02	128.11	124.38
2	C	540	HEM	CHA-C4D-C3D	-3.00	119.70	125.33
2	D	540	HEM	CHD-C1D-C2D	-3.00	120.30	124.98
2	B	540	HEM	CHD-C1D-C2D	-2.97	120.34	124.98
2	H	540	HEM	CHD-C1D-C2D	-2.94	120.39	124.98
3	E	600	VFV	CAS-CBK-CBE	2.91	119.86	116.13
3	F	600	VFV	CAW-CBN-CBK	-2.90	103.00	112.25
2	F	540	HEM	CHB-C1B-NB	2.88	127.94	124.38
2	A	540	HEM	CHB-C1B-NB	2.85	127.90	124.38
3	B	600	VFV	CAS-CBK-CBE	2.82	119.75	116.13
3	H	600	VFV	CAV-CBE-CBK	-2.81	120.46	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	600	VFV	CAV-CBJ-CBG	-2.81	116.22	120.86
3	C	600	VFV	CAN-CBG-CBJ	-2.81	116.49	121.36
2	E	540	HEM	CHD-C1D-C2D	-2.78	120.63	124.98
3	B	600	VFV	CAV-CBE-CBK	-2.77	120.50	123.83
3	D	600	VFV	CAS-CBK-CBE	2.77	119.69	116.13
3	E	600	VFV	CAV-CBJ-CBG	-2.77	116.29	120.86
3	D	600	VFV	CAV-CBE-CBK	-2.76	120.52	123.83
3	A	600	VFV	CAS-CBK-CBE	2.75	119.67	116.13
2	D	540	HEM	CHA-C4D-C3D	-2.75	120.16	125.33
3	H	600	VFV	CAW-CBN-CBK	-2.73	103.55	112.25
3	H	600	VFV	CAS-CBK-CBE	2.72	119.62	116.13
3	A	600	VFV	CBJ-CAV-CBE	2.71	121.90	119.59
3	A	600	VFV	CBL-NAY-NAZ	2.70	110.85	105.29
3	H	580	VFV	CAW-NBO-CAU	-2.69	120.47	125.76
3	E	580	VFV	CAV-CBE-CBK	-2.68	120.62	123.83
3	E	580	VFV	CAS-CBK-CBE	2.67	119.56	116.13
3	F	600	VFV	CAR-CBJ-CAV	2.65	121.91	118.16
2	B	540	HEM	CHA-C4D-C3D	-2.64	120.36	125.33
3	H	580	VFV	CAW-NBO-CAT	2.62	131.31	125.92
3	B	580	VFV	CAV-CBE-CBK	-2.62	120.70	123.83
3	F	580	VFV	CAW-NBO-CAT	2.61	131.29	125.92
2	A	540	HEM	CHA-C4D-C3D	-2.60	120.45	125.33
3	B	580	VFV	CAS-CBK-CBE	2.59	119.46	116.13
2	F	540	HEM	CHA-C4D-C3D	-2.58	120.49	125.33
3	D	580	VFV	CAW-CBN-NBA	-2.57	105.96	110.45
2	C	540	HEM	CAD-CBD-CGD	-2.55	108.12	113.60
3	G	580	VFV	CAW-NBO-CAT	2.54	131.15	125.92
3	C	580	VFV	CAS-CBK-CBE	2.53	119.38	116.13
3	H	580	VFV	CAS-CBK-CBE	2.53	119.38	116.13
3	F	580	VFV	CBN-CAW-NBO	2.53	115.53	112.25
3	C	580	VFV	CAV-CBJ-CBG	-2.52	116.70	120.86
3	B	580	VFV	CBI-CBM-NAZ	2.52	128.39	124.12
3	D	580	VFV	CAV-CBE-CBK	-2.51	120.82	123.83
3	A	600	VFV	CAJ-CBD-CAK	-2.50	119.50	122.83
3	G	580	VFV	CAW-NBO-CAU	-2.49	120.85	125.76
3	B	580	VFV	CAW-CBN-NBA	-2.49	106.11	110.45
3	C	580	VFV	CAV-CBE-CBK	-2.48	120.86	123.83
3	G	580	VFV	CAW-CBN-NBA	-2.48	106.13	110.45
2	G	540	HEM	CHA-C4D-C3D	-2.47	120.69	125.33
2	B	540	HEM	CAD-CBD-CGD	-2.47	108.29	113.60
3	F	580	VFV	CAW-NBO-CAU	-2.47	120.91	125.76
3	C	600	VFV	CAW-CBN-CBK	-2.45	104.45	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	580	VFV	CAS-CBK-CBE	2.44	119.27	116.13
2	E	540	HEM	CHA-C4D-C3D	-2.43	120.77	125.33
2	H	540	HEM	CHA-C4D-C3D	-2.38	120.86	125.33
3	A	600	VFV	CBH-CBL-NAY	2.38	128.15	124.12
3	A	580	VFV	CAS-CBK-CBE	2.36	119.16	116.13
2	F	540	HEM	CBA-CAA-C2A	-2.31	108.68	112.62
3	F	580	VFV	CBE-CBK-CBN	-2.28	117.43	120.83
3	C	580	VFV	CAW-CBN-NBA	-2.26	106.51	110.45
3	C	580	VFV	CAN-CBG-CBJ	-2.24	117.47	121.36
3	A	580	VFV	CAW-CBN-NBA	-2.24	106.54	110.45
2	H	540	HEM	C4D-ND-C1D	2.24	107.39	105.07
3	D	580	VFV	CAS-CBK-CBE	2.23	119.00	116.13
3	G	600	VFV	CAW-CBN-CBK	-2.23	105.14	112.25
3	A	580	VFV	CAV-CBE-CBK	-2.23	121.16	123.83
3	E	580	VFV	CAW-CBN-NBA	-2.23	106.57	110.45
3	C	600	VFV	CBN-NBA-CBC	-2.22	119.48	122.34
2	A	540	HEM	CAD-CBD-CGD	-2.21	108.84	113.60
2	H	540	HEM	CAD-CBD-CGD	-2.21	108.84	113.60
3	H	580	VFV	CAV-CBE-CBK	-2.19	121.21	123.83
3	D	580	VFV	CAV-CBJ-CBG	-2.18	117.26	120.86
2	G	540	HEM	O2D-CGD-CBD	2.15	120.93	114.03
3	E	580	VFV	CAV-CBJ-CBG	-2.13	117.34	120.86
2	E	540	HEM	O2D-CGD-CBD	2.12	120.85	114.03
3	H	600	VFV	CBN-NBA-CBC	-2.11	119.62	122.34
2	B	540	HEM	O2A-CGA-CBA	2.11	120.79	114.03
3	H	580	VFV	CBE-CBK-CBN	-2.10	117.69	120.83
3	D	600	VFV	CAW-CBN-CBK	-2.10	105.56	112.25
3	F	600	VFV	CAN-CBG-CAO	2.06	121.69	117.59
2	D	540	HEM	CAD-C3D-C4D	2.04	128.23	124.66
2	F	540	HEM	CHC-C4B-C3B	-2.04	121.44	124.57
3	F	600	VFV	CBN-NBA-CBC	-2.04	119.71	122.34
3	H	580	VFV	CAW-CBN-NBA	-2.04	106.89	110.45
3	E	600	VFV	CAW-CBN-CBK	-2.04	105.74	112.25
2	H	540	HEM	CMC-C2C-C3C	2.03	128.48	124.68
3	B	600	VFV	CAW-CBN-CBK	-2.03	105.77	112.25
3	E	580	VFV	CAN-CBG-CBJ	-2.02	117.86	121.36
2	F	540	HEM	O2D-CGD-CBD	2.01	120.50	114.03
3	B	580	VFV	CBH-CBL-NAY	2.01	127.53	124.12
2	A	540	HEM	O2A-CGA-CBA	2.01	120.49	114.03
2	A	540	HEM	C4B-C3B-C2B	-2.01	105.52	107.11
3	A	600	VFV	CAW-CBN-CBK	-2.00	105.86	112.25
2	D	540	HEM	O2D-CGD-CBD	2.00	120.47	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	600	VFV	CAR-CBJ-CAV	2.00	121.00	118.16
3	G	580	VFV	CAV-CBE-CBK	-2.00	121.43	123.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	540	HEM	C2D-C3D-CAD-CBD
2	D	540	HEM	C4D-C3D-CAD-CBD
2	E	540	HEM	C2D-C3D-CAD-CBD
3	A	580	VFV	CAW-CBN-NBA-CBC
2	E	540	HEM	C4D-C3D-CAD-CBD
3	C	580	VFV	CAW-CBN-NBA-CBC
3	F	580	VFV	CAW-CBN-NBA-CBC
3	G	580	VFV	CAW-CBN-NBA-CBC
3	H	600	VFV	CAW-CBN-NBA-CBC
2	F	540	HEM	CAA-CBA-CGA-O1A
2	F	540	HEM	CAA-CBA-CGA-O2A
2	H	540	HEM	CAA-CBA-CGA-O2A
2	E	540	HEM	CAA-CBA-CGA-O2A
2	G	540	HEM	CAD-CBD-CGD-O2D
2	H	540	HEM	CAA-CBA-CGA-O1A
3	C	580	VFV	CBN-CAW-NBO-CAT
2	D	540	HEM	CAD-CBD-CGD-O2D
2	G	540	HEM	CAA-CBA-CGA-O2A
2	D	540	HEM	CAA-CBA-CGA-O2A
2	D	540	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

23 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	580	VFV	6	0
2	F	540	HEM	7	0
2	E	540	HEM	9	0
3	E	580	VFV	2	0
3	E	600	VFV	3	0
3	A	580	VFV	1	0
3	G	580	VFV	4	0
3	F	580	VFV	1	0
3	A	600	VFV	4	0

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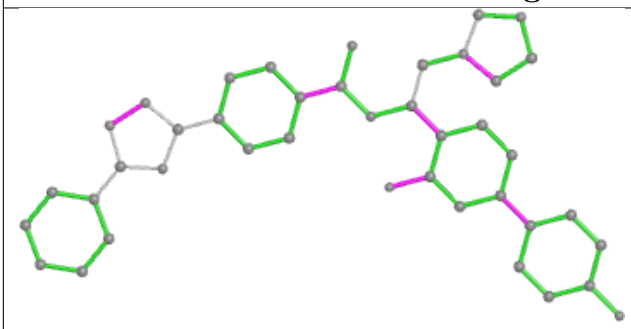
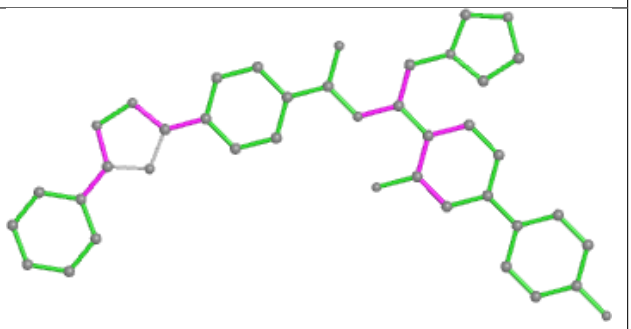
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	600	VFV	5	0
3	B	600	VFV	1	0
2	D	540	HEM	4	0
3	C	600	VFV	10	0
2	C	540	HEM	7	0
2	A	540	HEM	7	0
3	G	600	VFV	1	0
3	C	580	VFV	7	0
2	H	540	HEM	8	0
2	G	540	HEM	5	0
3	F	600	VFV	16	0
3	H	580	VFV	3	0
2	B	540	HEM	2	0
3	H	600	VFV	9	0

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.

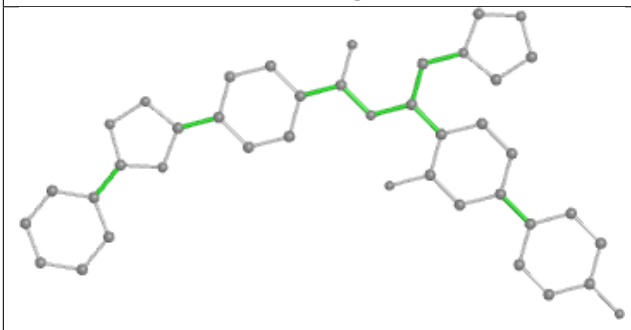
Ligand VFV B 580



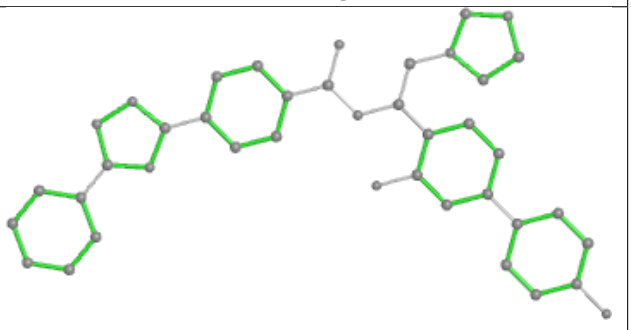
Bond lengths



Bond angles

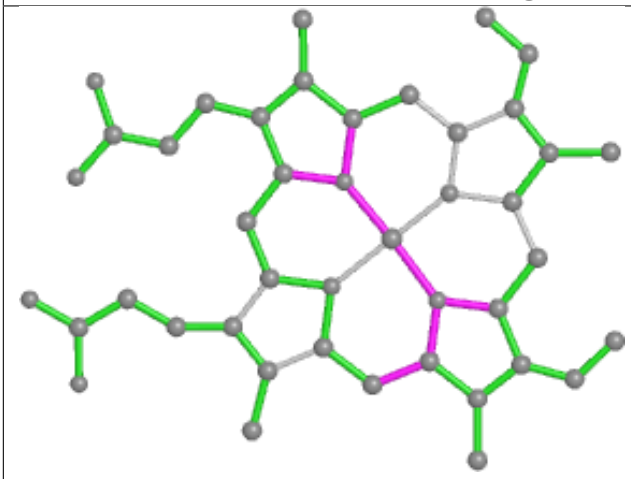


Torsions

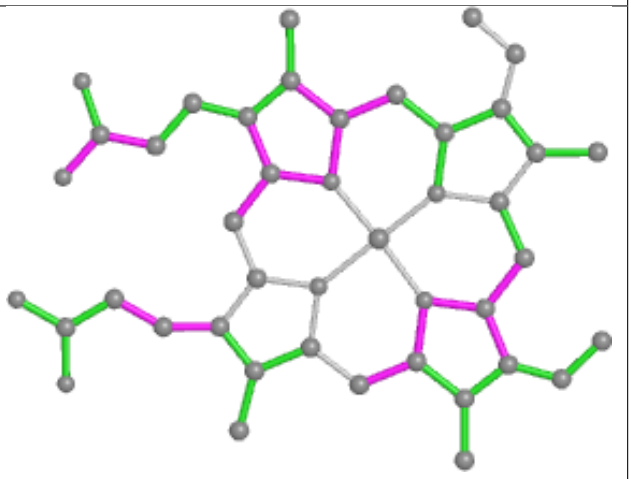


Rings

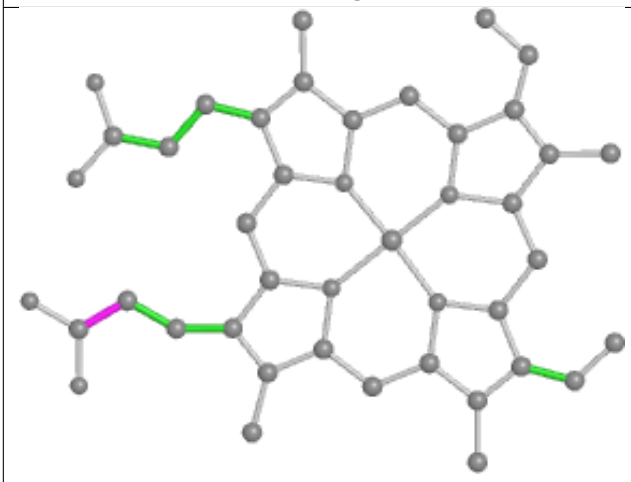
Ligand HEM F 540



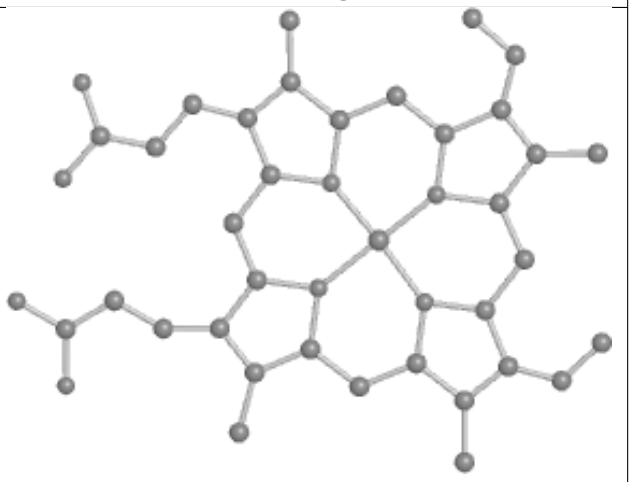
Bond lengths



Bond angles

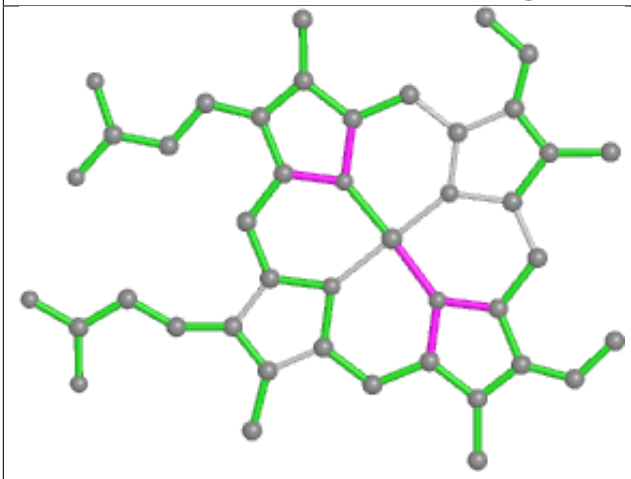


Torsions

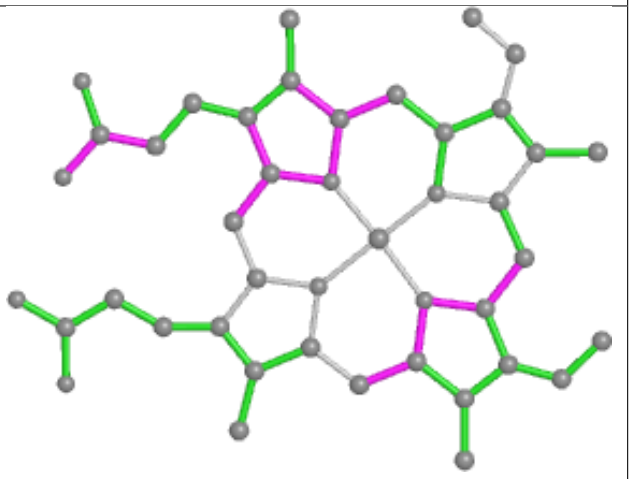


Rings

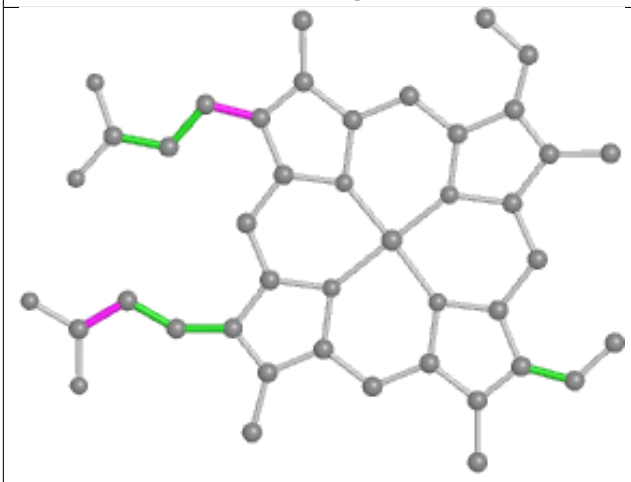
Ligand HEM E 540



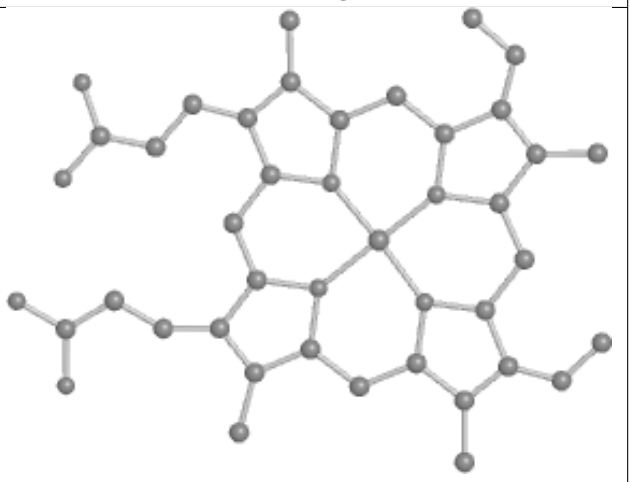
Bond lengths



Bond angles

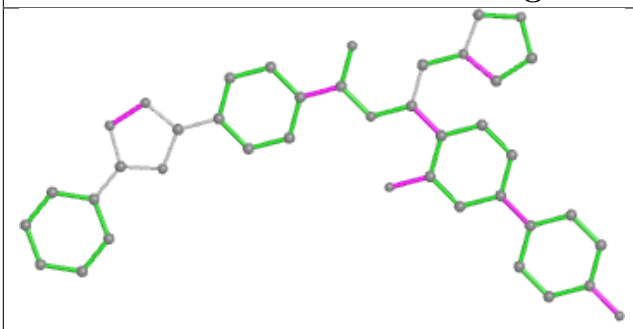


Torsions

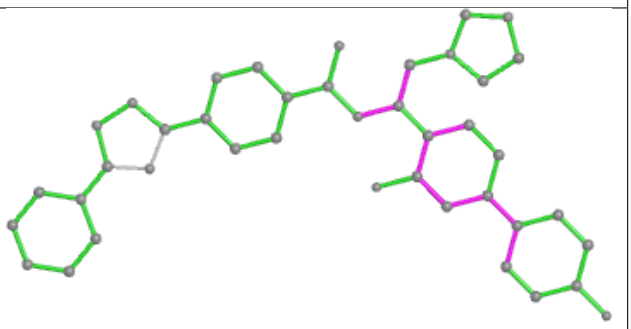


Rings

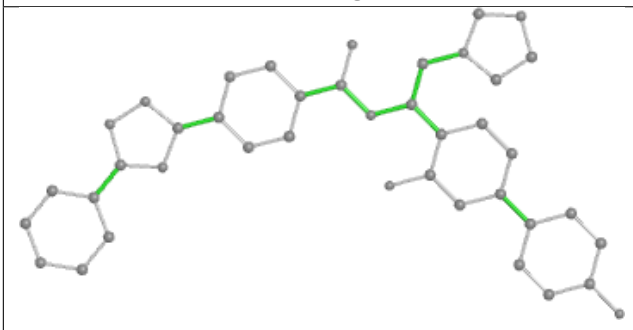
Ligand VFV E 580



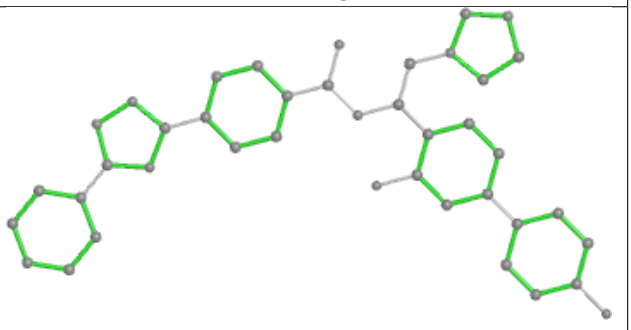
Bond lengths



Bond angles

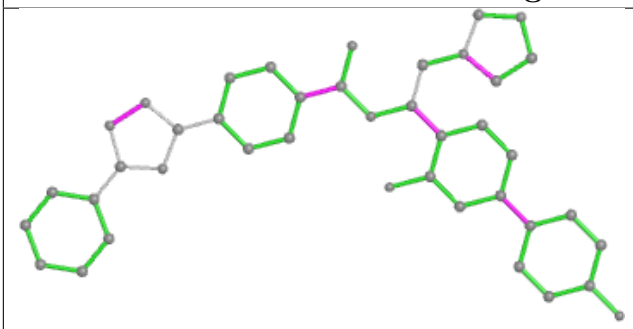


Torsions

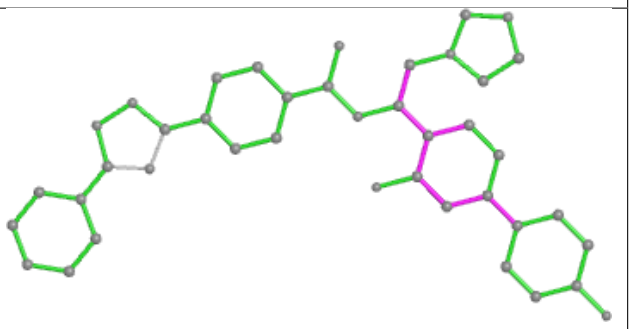


Rings

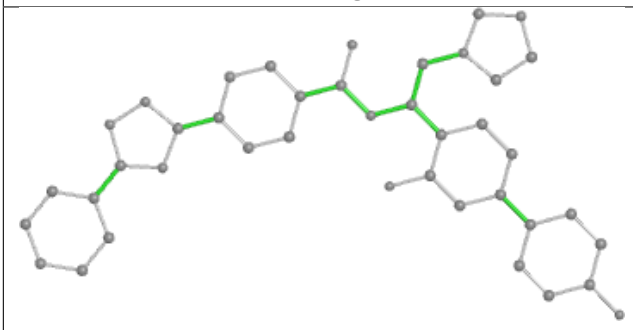
Ligand VFV E 600



Bond lengths



Bond angles



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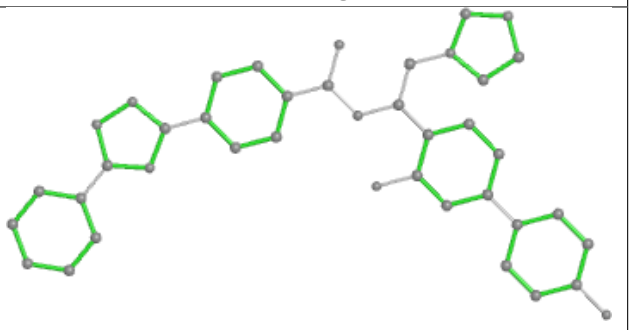
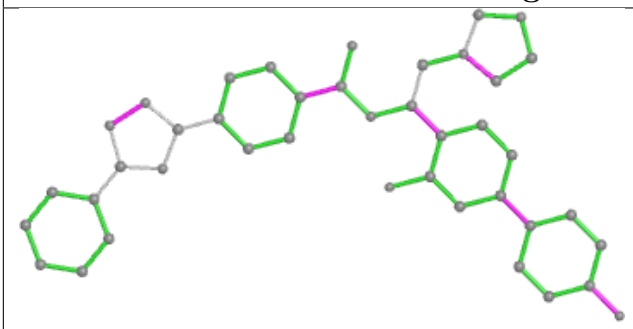


Rings

Ligand VFV A 580



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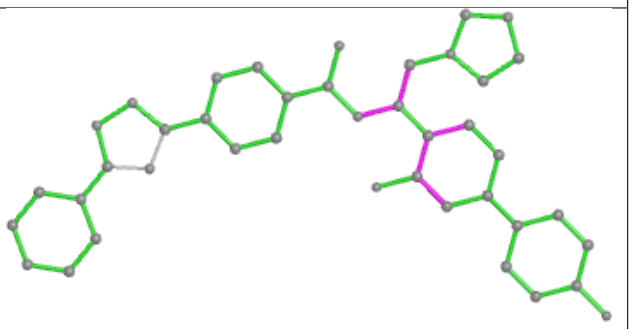
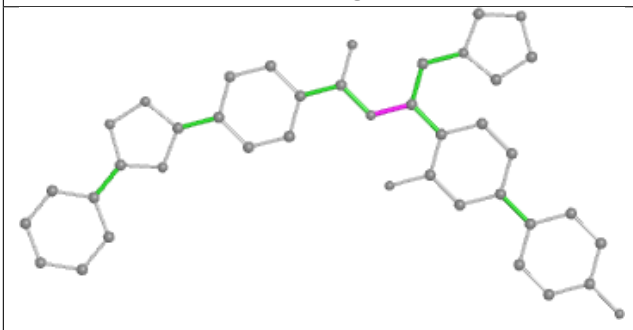


Bond angles



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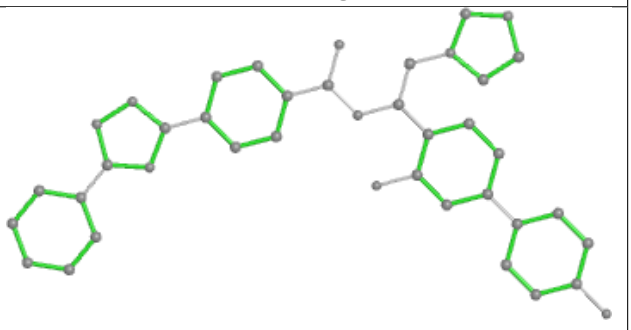
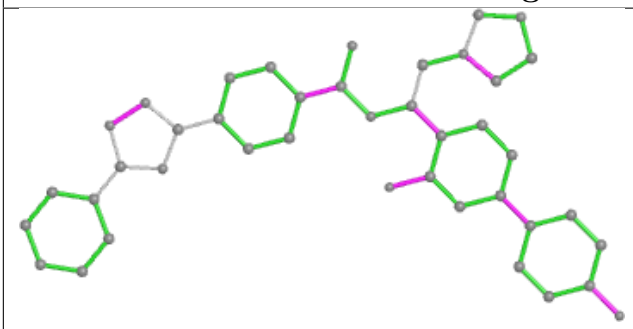
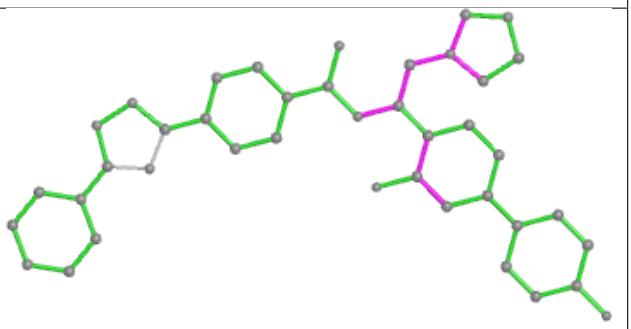


Rings

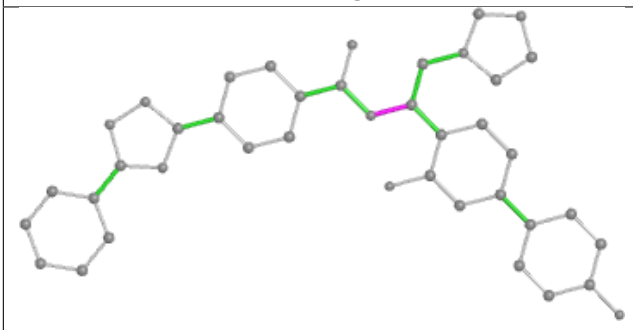
Ligand VFV G 580



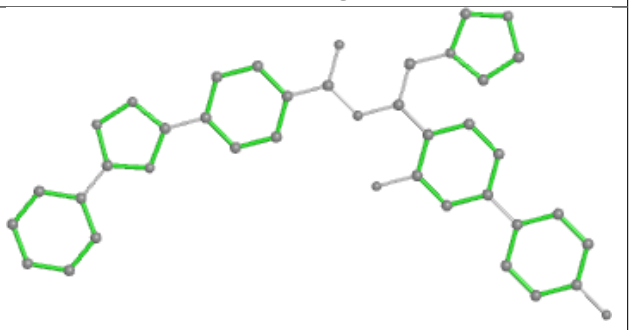
Bond lengths



Bond angles

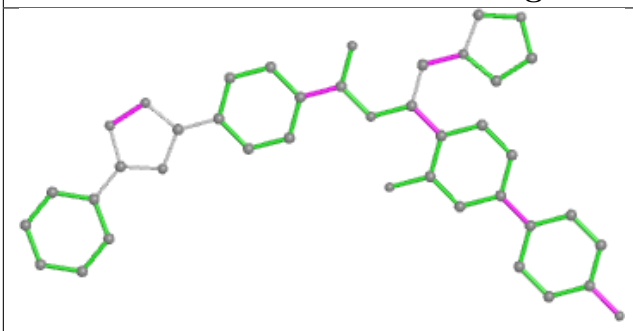


Torsions



Rings

Ligand VFV F 580



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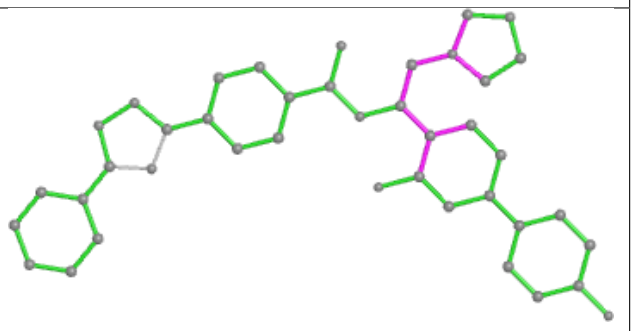
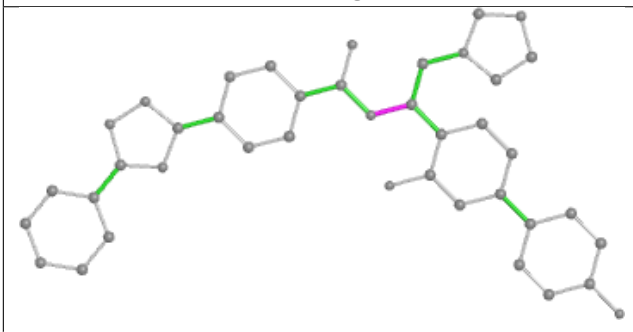


Bond angles



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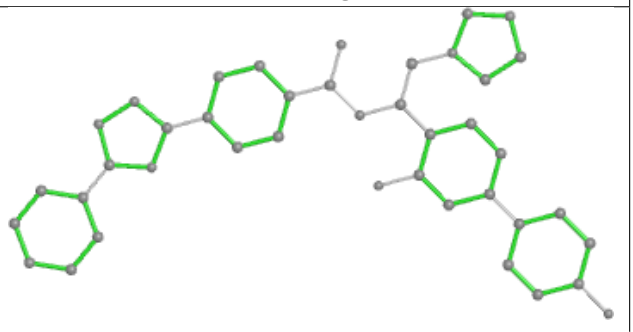
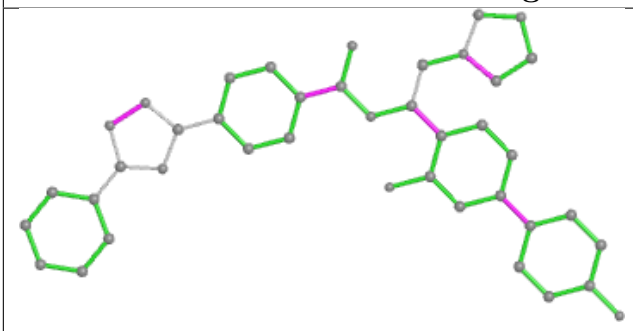


Rings

Ligand VFV D 580



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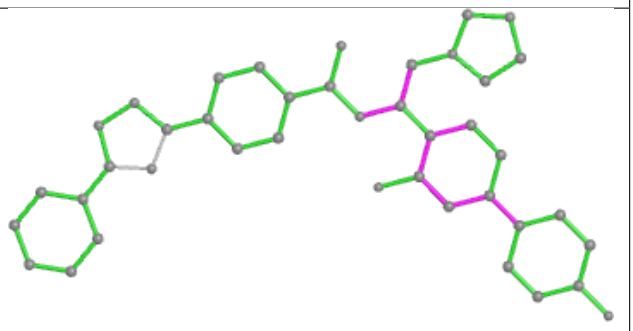

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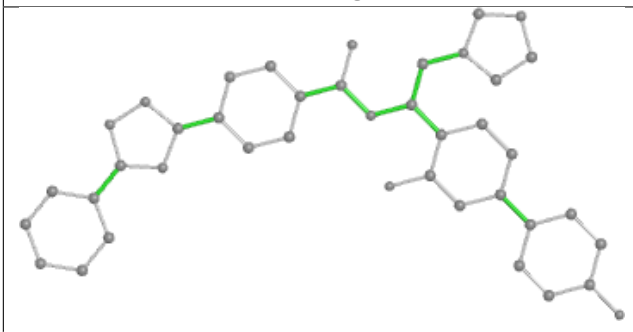

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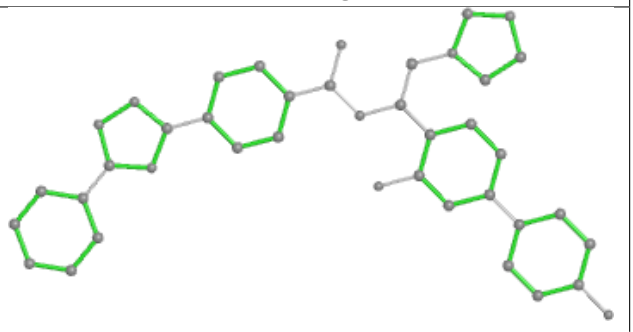
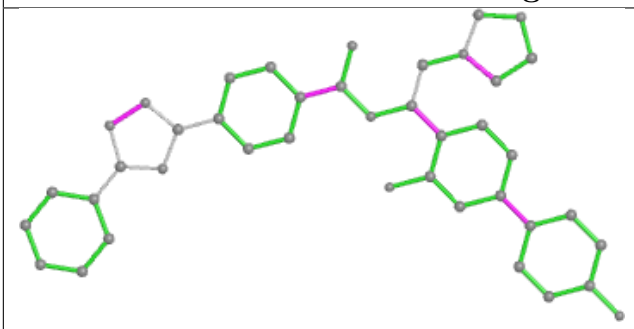


Rings

Ligand VFV A 600



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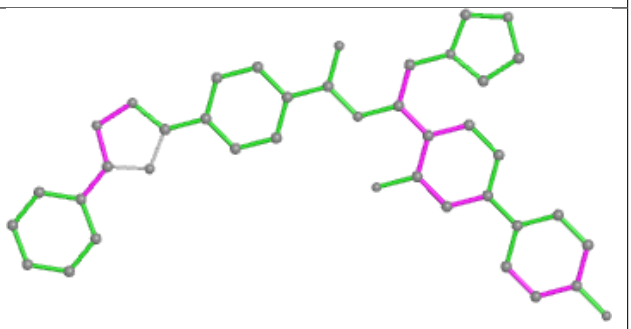
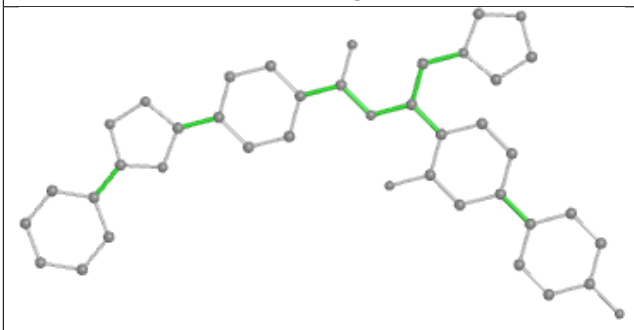


Bond angles



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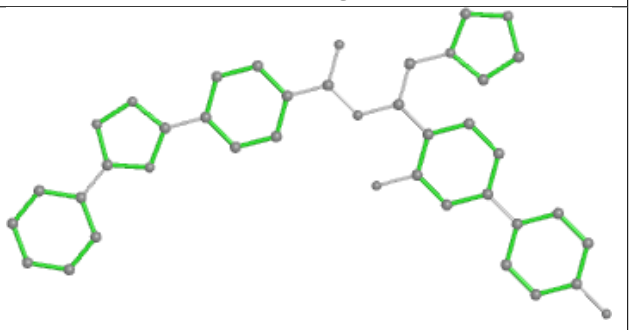
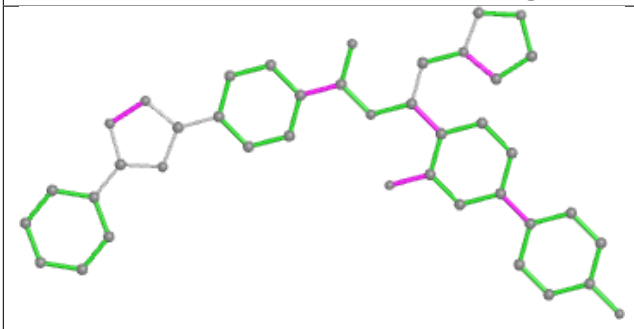


Rings

Ligand VFV D 600



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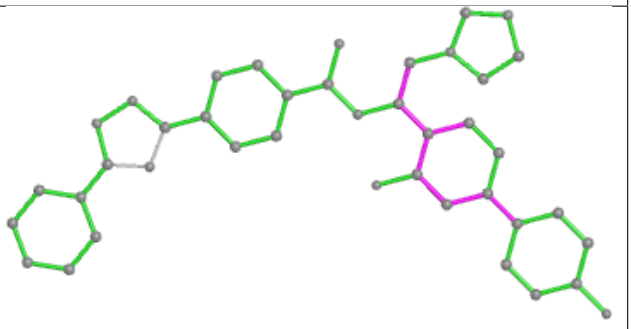
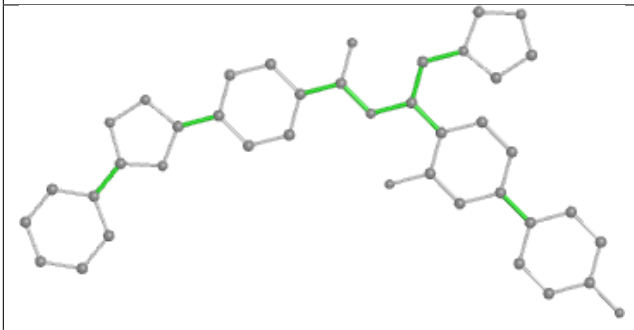


Bond angles



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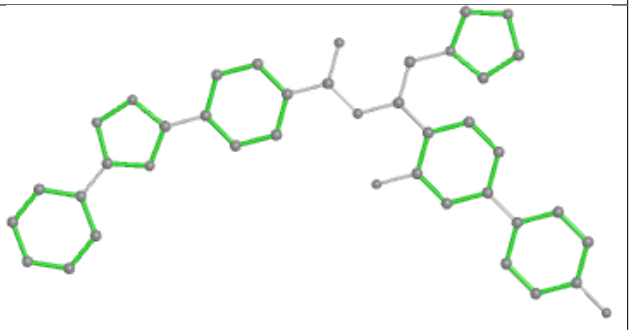
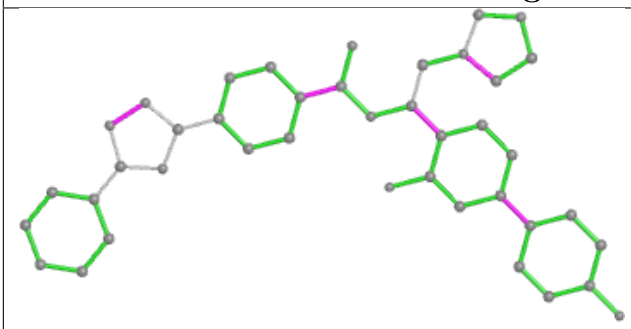


Rings

Ligand VFV B 600



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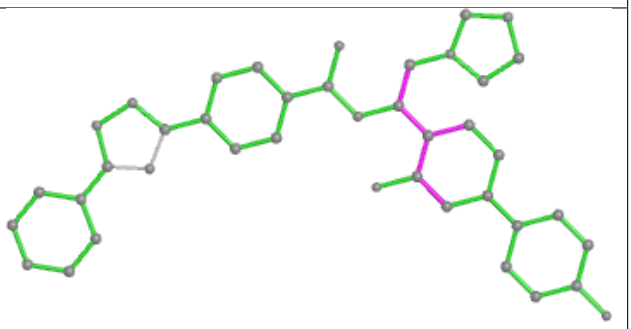
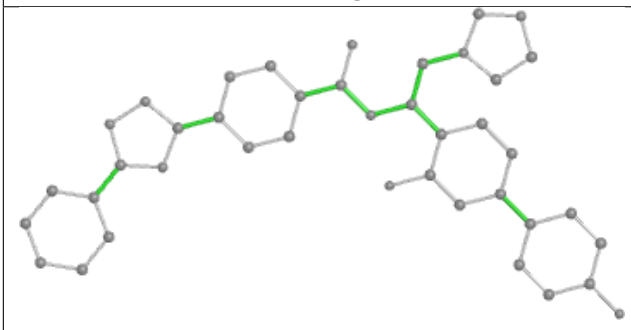


Bond angles



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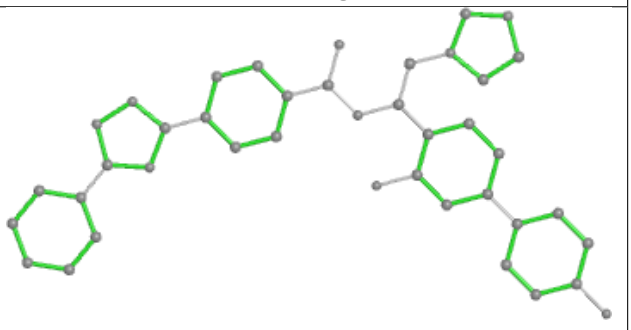
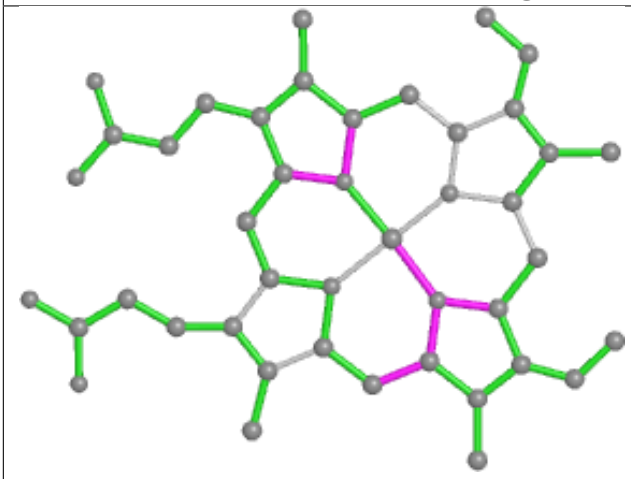


Rings

Ligand HEM D 540



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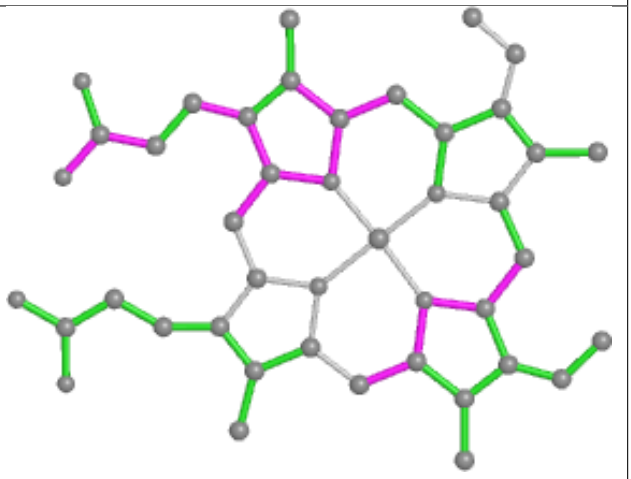
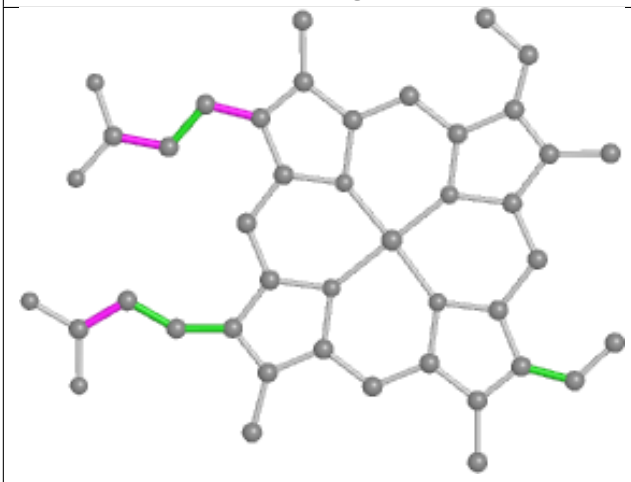


Bond angles



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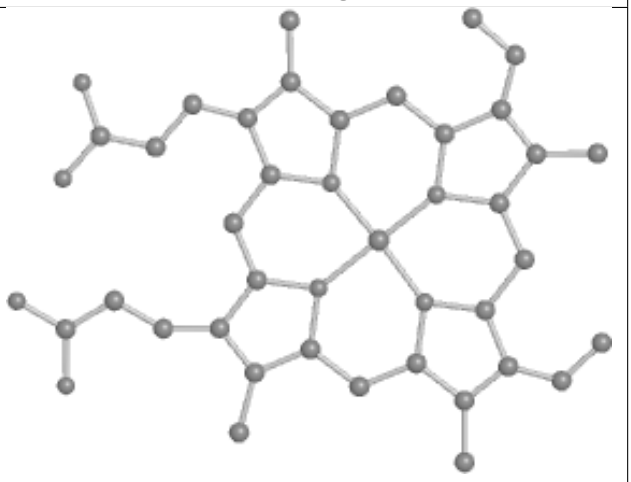
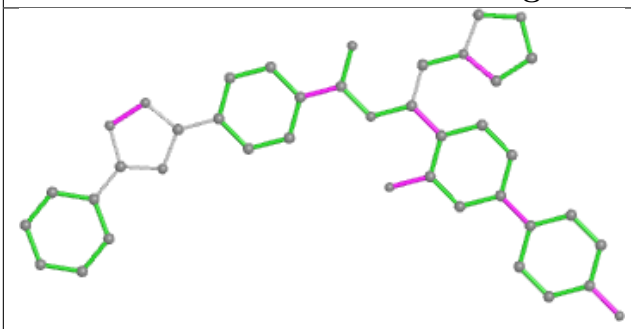


Rings

Ligand VFV C 600



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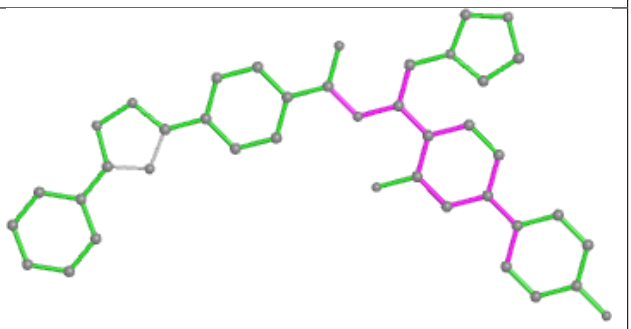

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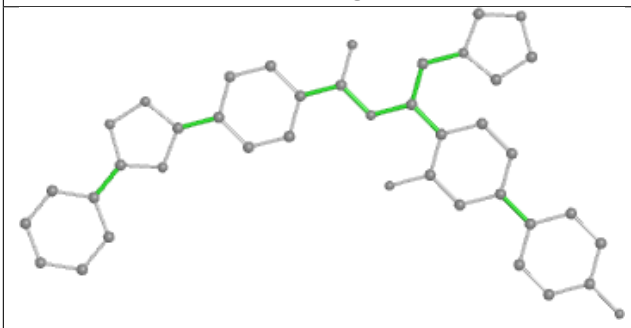

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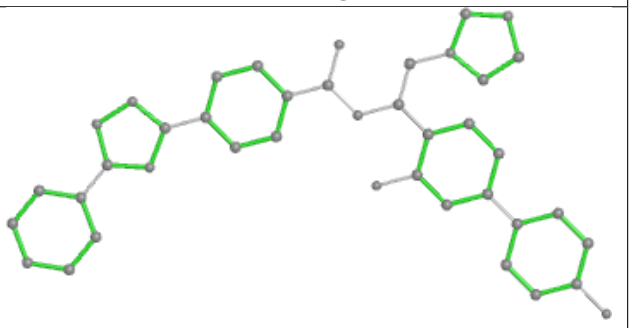
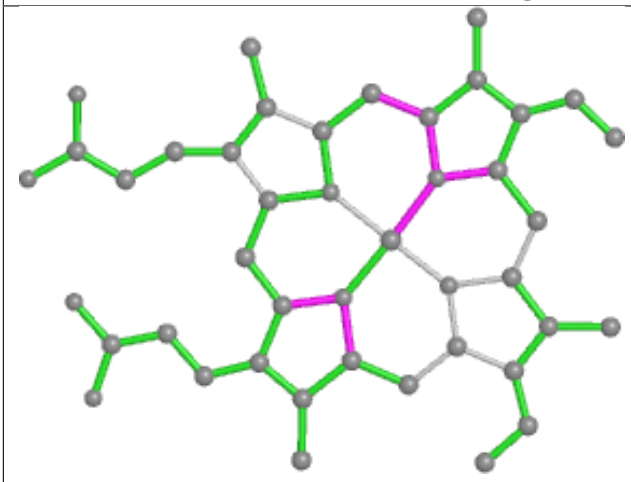


Rings

Ligand HEM C 540



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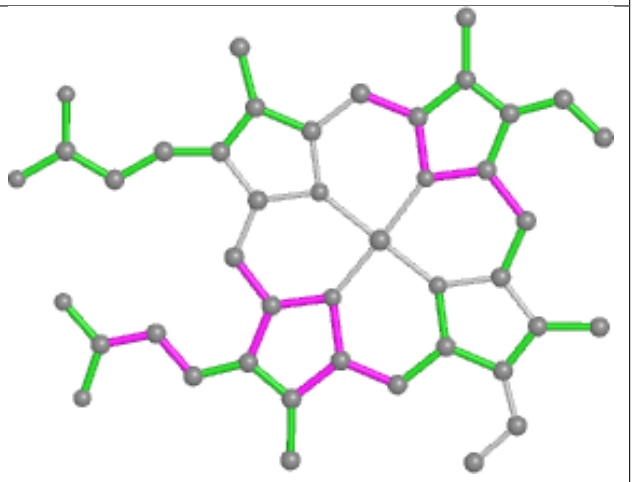
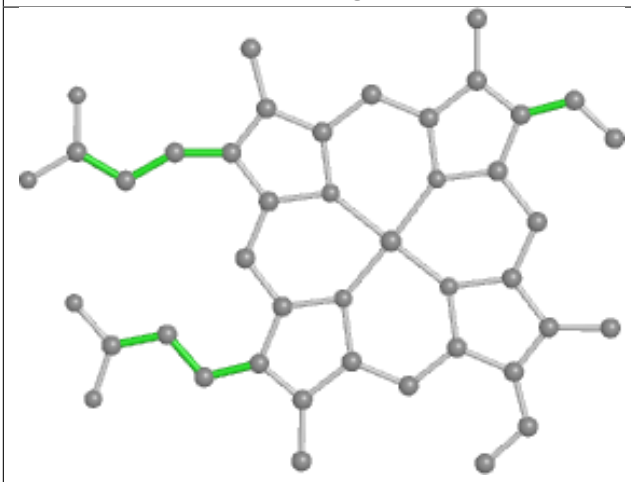
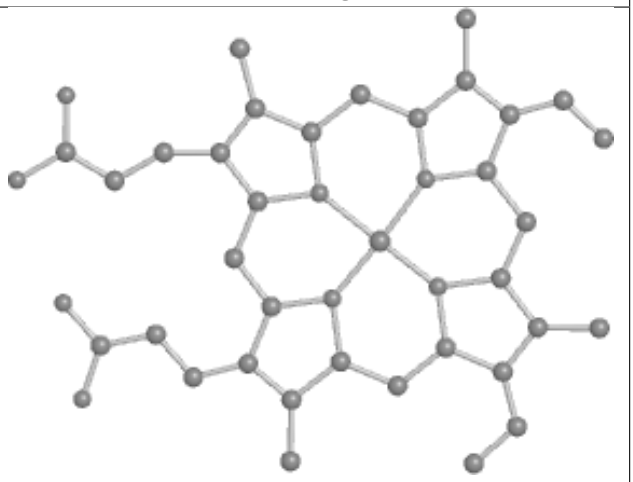


Bond angles

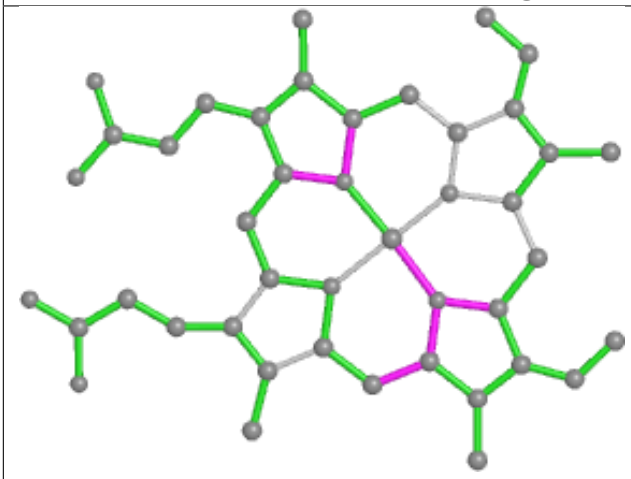


Torsions

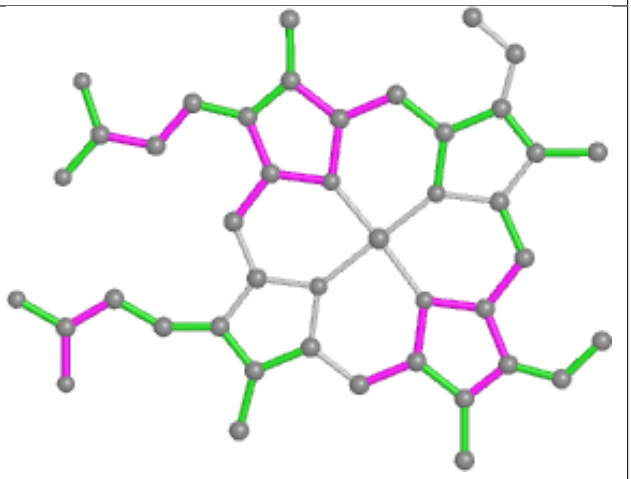


Rings

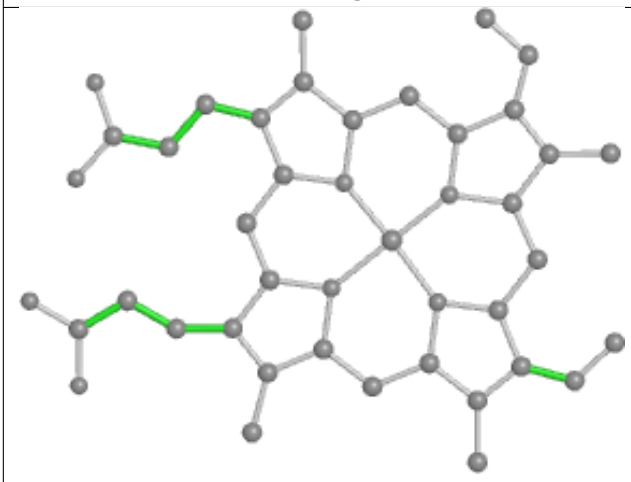
Ligand HEM A 540



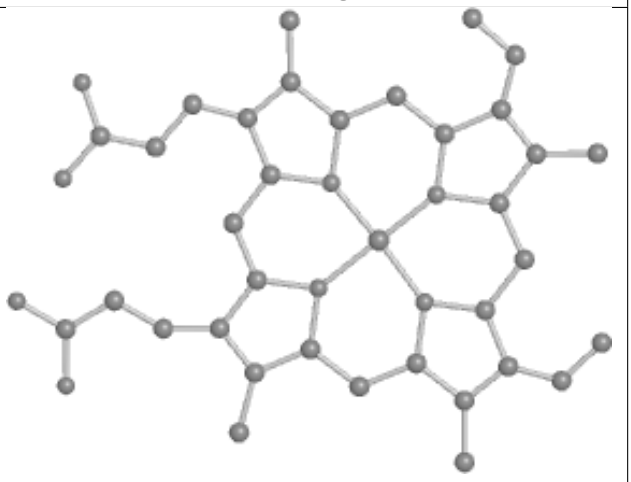
Bond lengths



Bond angles

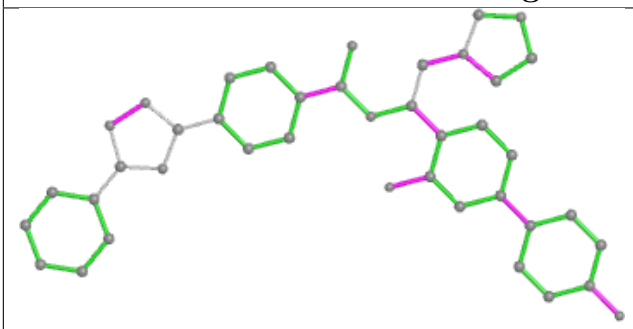


Torsions



Rings

Ligand VFV G 600



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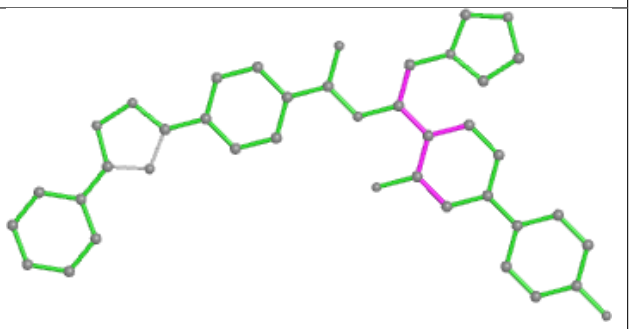
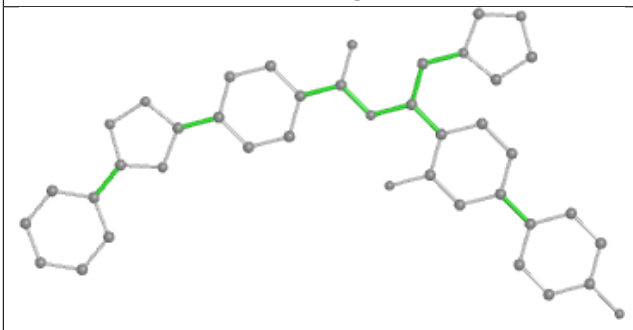


Bond angles



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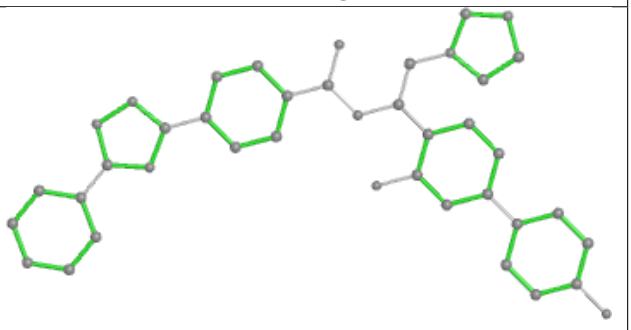
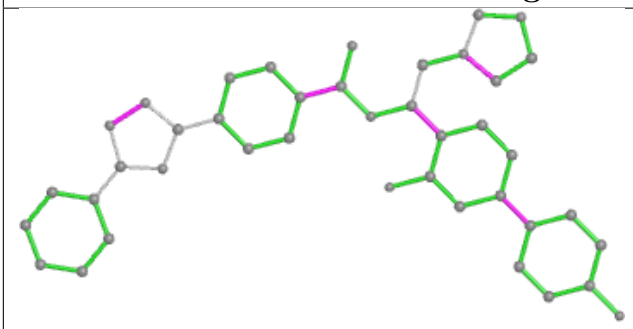


Rings

Ligand VFV C 580



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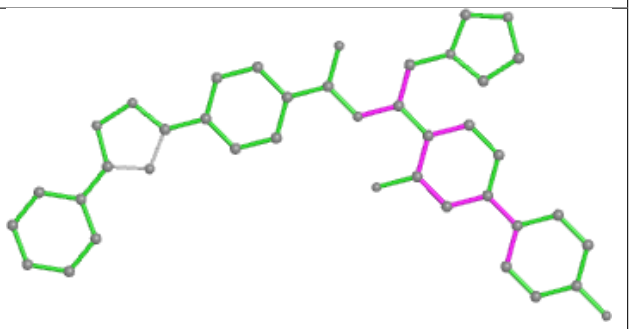
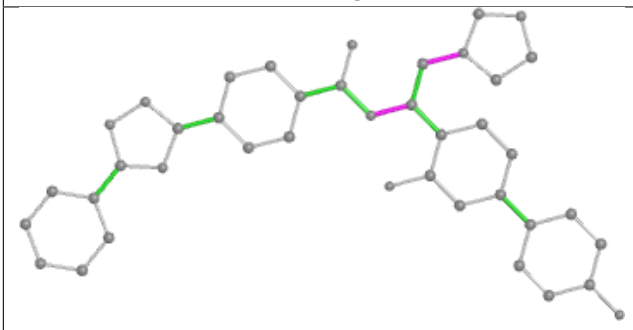


Bond angles



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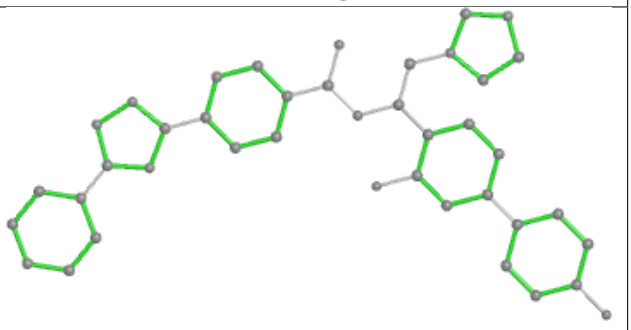
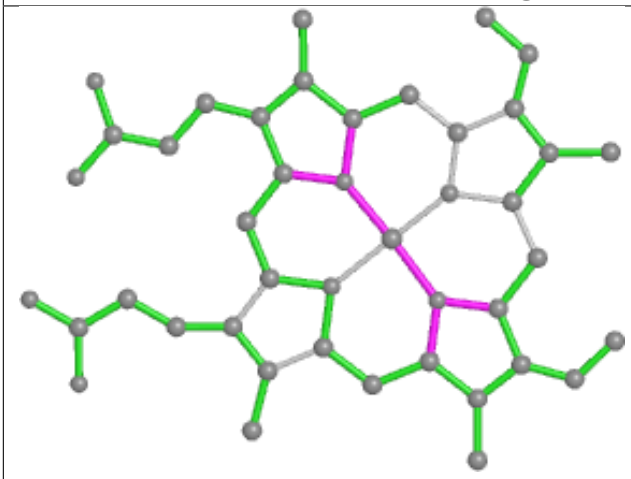


Rings

Ligand HEM H 540



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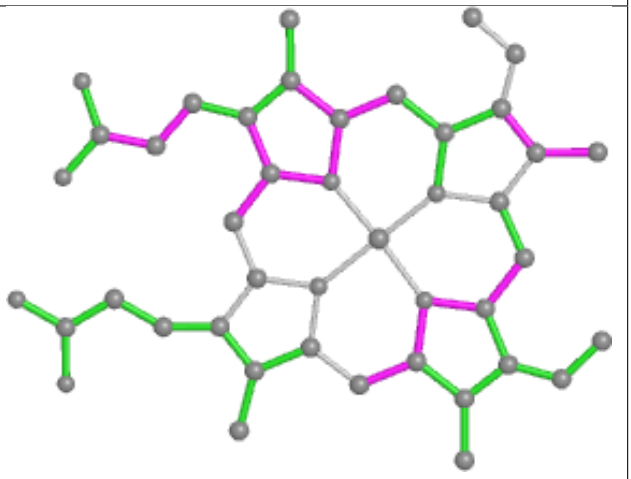
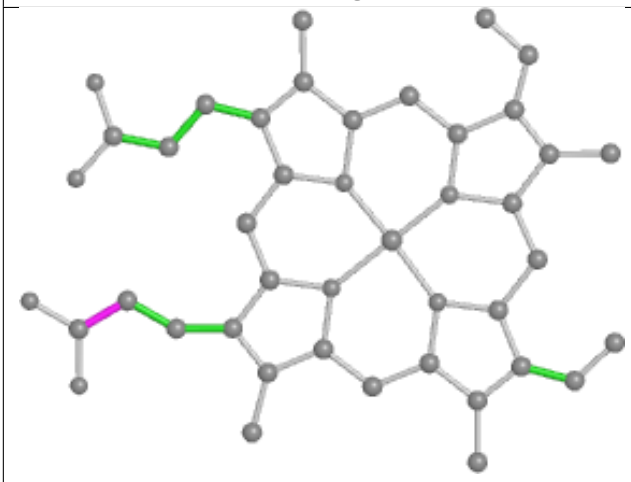
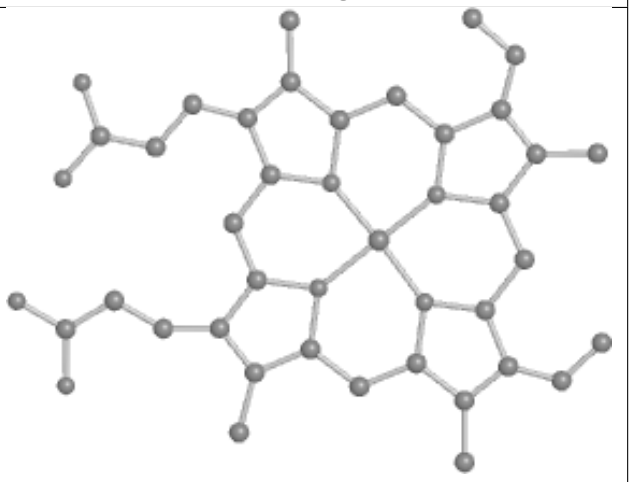


Bond angles

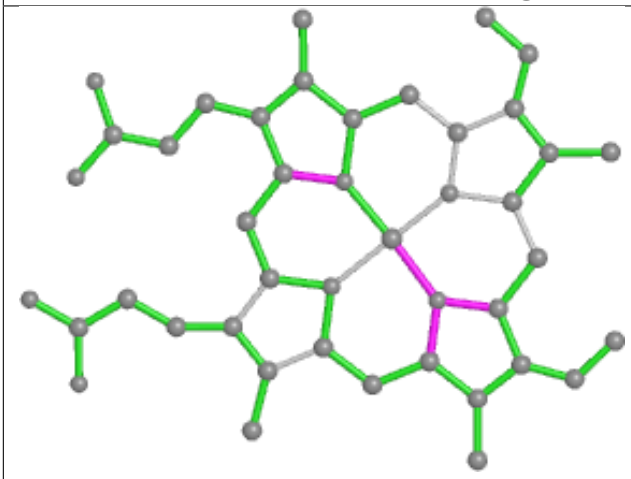


Torsions



Rings

Ligand HEM G 540



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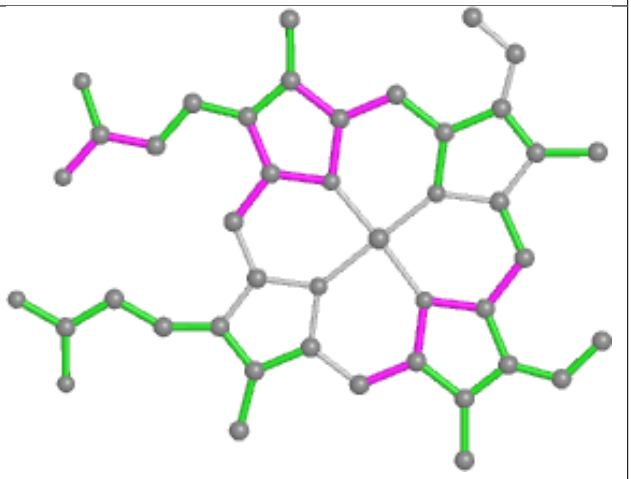
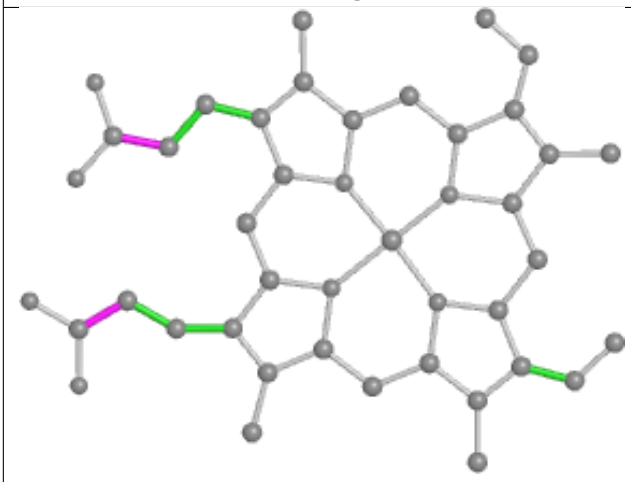


Bond angles



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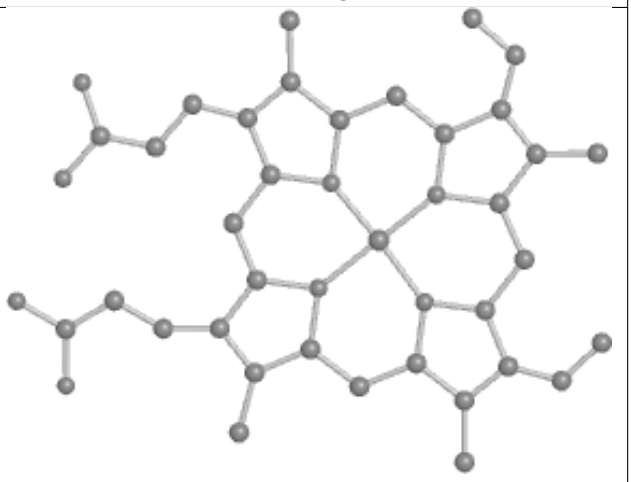
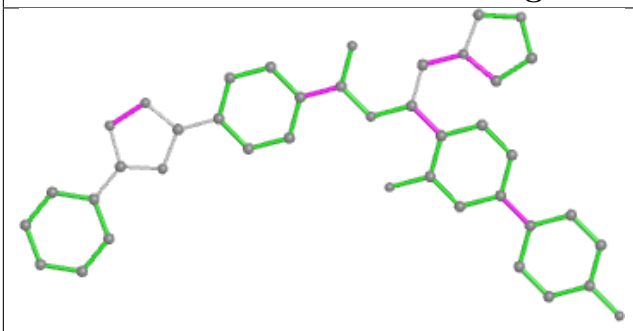
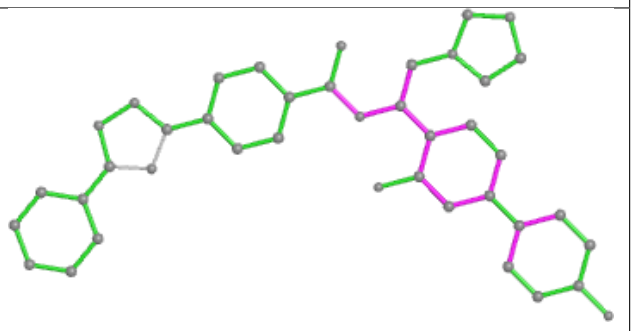


Rings

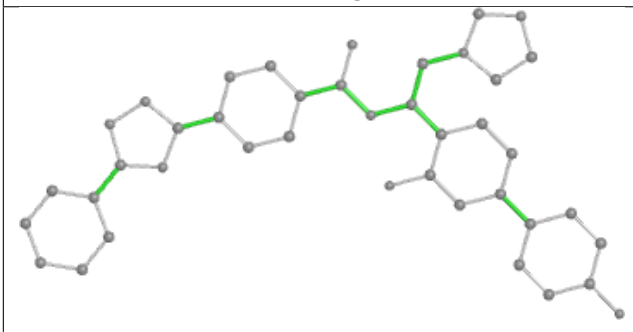
Ligand VFV F 600



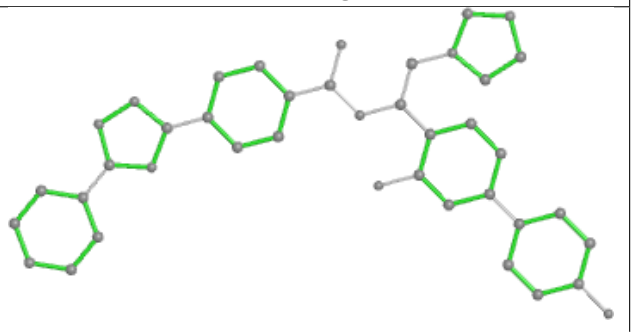
Bond lengths



Bond angles

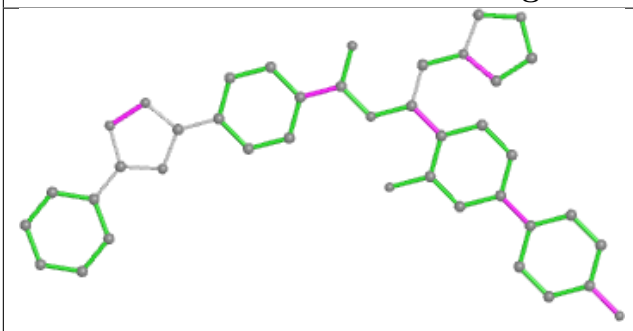


Torsions

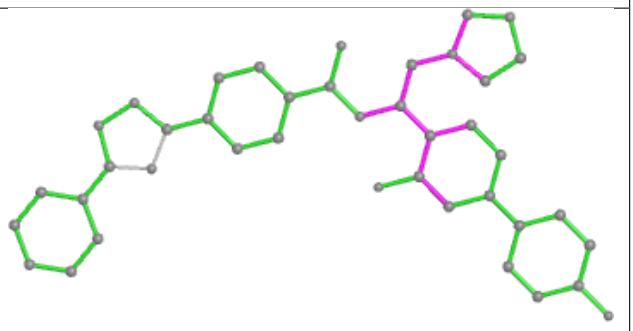


Rings

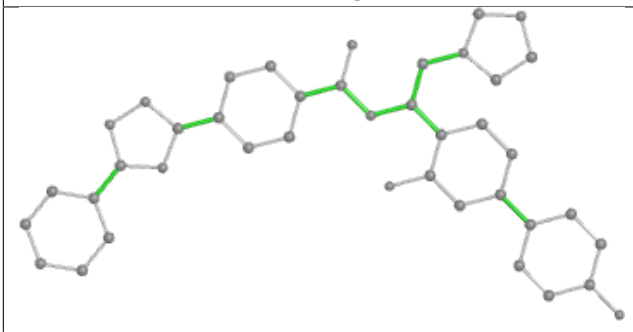
Ligand VFV H 580



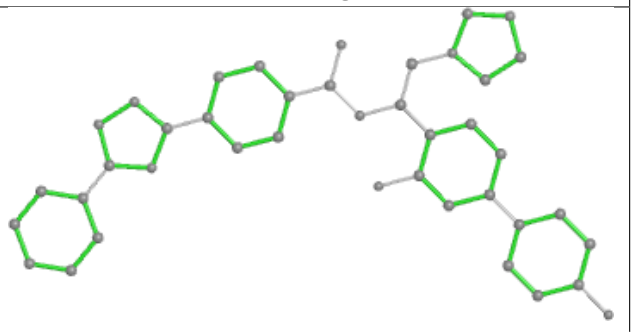
Bond lengths



Bond angles

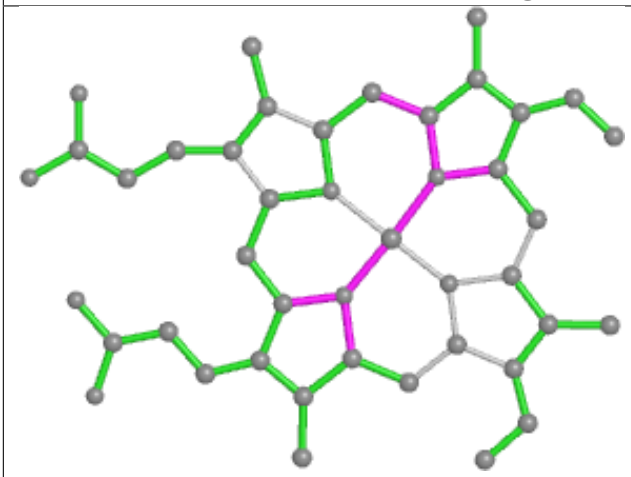


Torsions

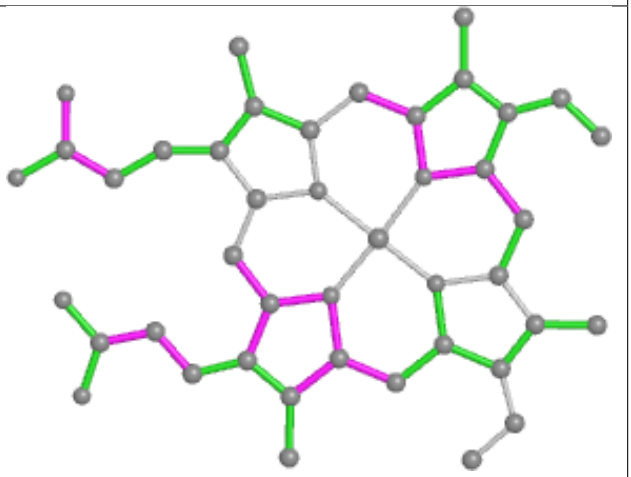


Rings

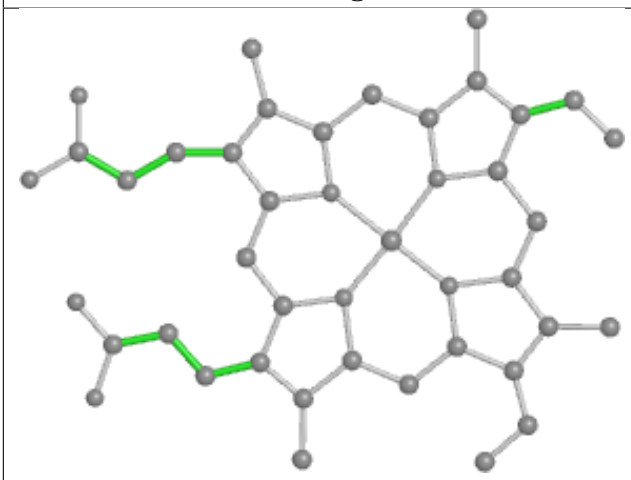
Ligand HEM B 540



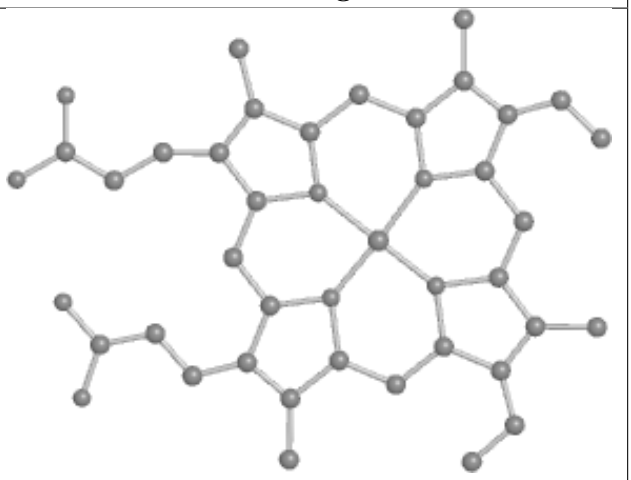
Bond lengths



Bond angles

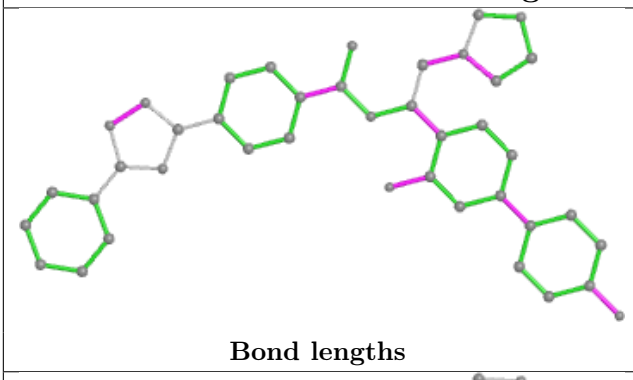


Torsions

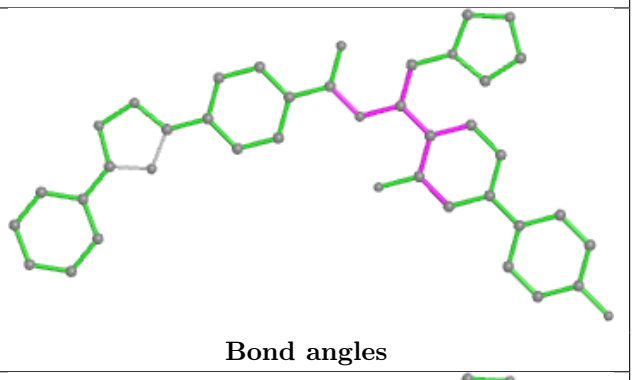


Rings

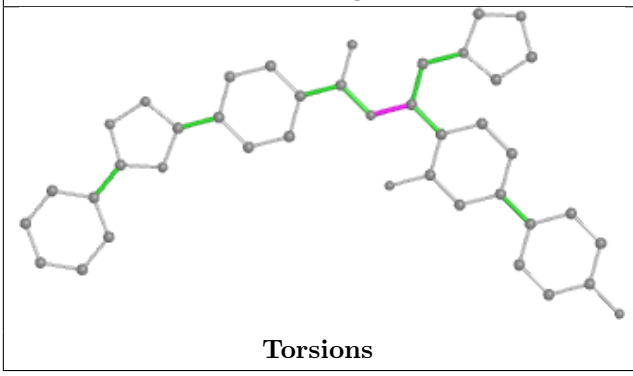
Ligand VFV H 600



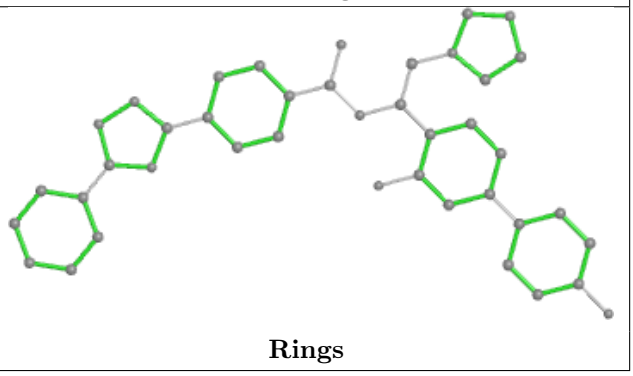
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	445/446 (99%)	-0.06	4 (0%)	84	86	46, 61, 81, 110	0
1	B	445/446 (99%)	0.01	6 (1%)	77	79	40, 57, 82, 126	0
1	C	445/446 (99%)	-0.10	5 (1%)	80	82	43, 57, 80, 122	0
1	D	445/446 (99%)	-0.08	4 (0%)	84	86	42, 55, 78, 112	0
1	E	445/446 (99%)	0.23	12 (2%)	54	58	43, 65, 92, 126	0
1	F	445/446 (99%)	0.39	30 (6%)	17	18	48, 76, 102, 132	0
1	G	445/446 (99%)	0.05	8 (1%)	68	71	42, 62, 86, 139	0
1	H	445/446 (99%)	-0.03	10 (2%)	62	65	45, 68, 96, 120	0
All	All	3560/3568 (99%)	0.05	79 (2%)	62	65	40, 62, 91, 139	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	277	LYS	5.6
1	B	278	ILE	5.1
1	F	392	GLY	4.5
1	B	275	GLN	4.4
1	G	278	ILE	4.3
1	C	277	LYS	4.2
1	F	65	PHE	3.9
1	E	275	GLN	3.9
1	F	278	ILE	3.8
1	F	446	ARG	3.7
1	F	291	LYS	3.7
1	F	96	PHE	3.5
1	A	277	LYS	3.5
1	D	277	LYS	3.5
1	H	275	GLN	3.4
1	G	276	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	91	LYS	3.4
1	E	351	PRO	3.4
1	H	277	LYS	3.2
1	H	276	GLU	3.2
1	B	277	LYS	3.1
1	A	335	LYS	3.0
1	F	288	ALA	2.9
1	B	58	GLY	2.9
1	E	65	PHE	2.9
1	E	247	LEU	2.9
1	C	502	SER	2.9
1	E	429	ASP	2.8
1	C	275	GLN	2.8
1	F	290	TYR	2.8
1	F	391	ALA	2.8
1	F	276	GLU	2.8
1	C	487	MET	2.7
1	B	273	GLN	2.7
1	G	277	LYS	2.7
1	D	487	MET	2.6
1	F	157	LYS	2.6
1	E	276	GLU	2.6
1	F	67	PRO	2.6
1	G	487	MET	2.5
1	E	502	SER	2.5
1	G	291	LYS	2.5
1	E	90	GLU	2.5
1	F	68	ILE	2.4
1	F	58	GLY	2.4
1	F	107	TYR	2.4
1	H	91	LYS	2.4
1	F	243	GLY	2.3
1	H	290	TYR	2.3
1	C	276	GLU	2.3
1	H	273	GLN	2.3
1	F	275	GLN	2.3
1	E	213	LYS	2.3
1	F	98	PHE	2.3
1	B	276	GLU	2.3
1	A	427	LEU	2.2
1	F	285	LEU	2.2
1	F	429	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	286	LEU	2.2
1	D	502	SER	2.2
1	D	275	GLN	2.2
1	G	446	ARG	2.2
1	G	237	ALA	2.2
1	F	284	THR	2.2
1	H	264	PHE	2.2
1	H	270	LYS	2.1
1	A	278	ILE	2.1
1	F	90	GLU	2.1
1	E	291	LYS	2.1
1	E	488	ILE	2.1
1	G	269	GLN	2.1
1	F	121	LYS	2.1
1	F	378	MET	2.0
1	H	278	ILE	2.0
1	F	274	SER	2.0
1	H	268	ILE	2.0
1	E	248	PRO	2.0
1	F	158	MET	2.0
1	F	351	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	VFV	F	600	41/41	0.91	0.19	44,58,84,87	0
3	VFV	F	580	41/41	0.94	0.15	36,46,68,70	0

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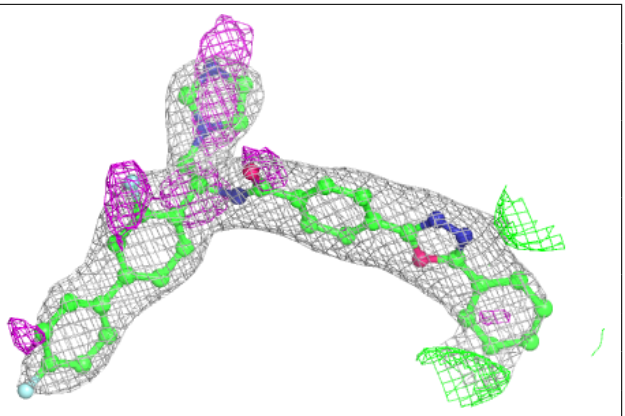
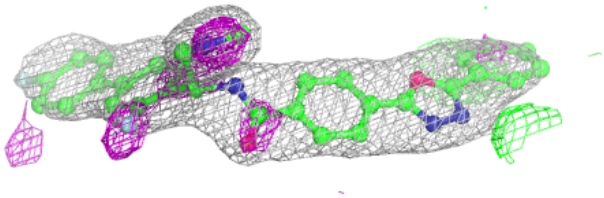
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	VFV	A	600	41/41	0.94	0.16	37,53,73,81	0
3	VFV	H	580	41/41	0.94	0.17	36,45,71,78	0
3	VFV	H	600	41/41	0.94	0.15	38,51,73,88	0
3	VFV	C	600	41/41	0.95	0.16	41,53,78,87	0
3	VFV	D	580	41/41	0.95	0.14	35,42,57,63	0
3	VFV	D	600	41/41	0.95	0.15	38,52,74,89	0
3	VFV	E	600	41/41	0.95	0.16	37,55,76,99	0
3	VFV	A	580	41/41	0.95	0.13	34,43,66,70	0
3	VFV	B	580	41/41	0.95	0.14	34,40,64,73	0
3	VFV	G	600	41/41	0.95	0.18	38,49,71,77	0
3	VFV	B	600	41/41	0.95	0.15	40,53,71,78	0
3	VFV	C	580	41/41	0.95	0.13	36,43,64,71	0
3	VFV	G	580	41/41	0.96	0.15	36,41,69,77	0
3	VFV	E	580	41/41	0.96	0.15	36,41,61,70	0
2	HEM	B	540	43/43	0.98	0.17	39,45,50,55	0
2	HEM	E	540	43/43	0.98	0.15	46,53,60,65	0
2	HEM	F	540	43/43	0.98	0.16	53,63,75,81	0
2	HEM	G	540	43/43	0.98	0.18	44,51,58,61	0
2	HEM	A	540	43/43	0.98	0.16	45,51,59,61	0
2	HEM	C	540	43/43	0.99	0.14	41,48,54,56	0
2	HEM	H	540	43/43	0.99	0.16	45,52,63,71	0
2	HEM	D	540	43/43	0.99	0.18	38,44,54,59	0

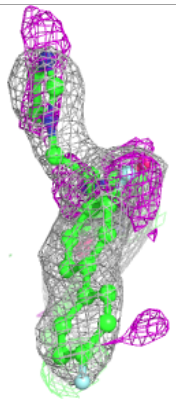
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VFV F 600:

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

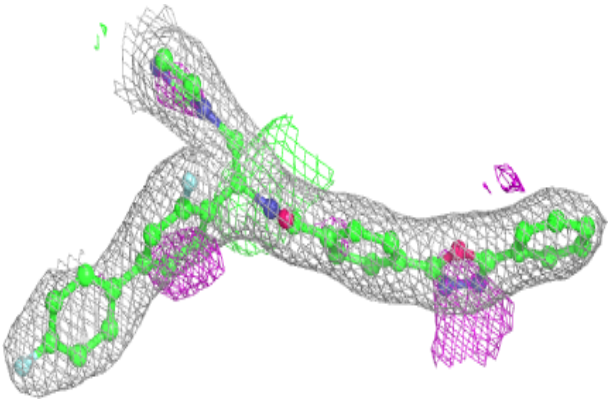


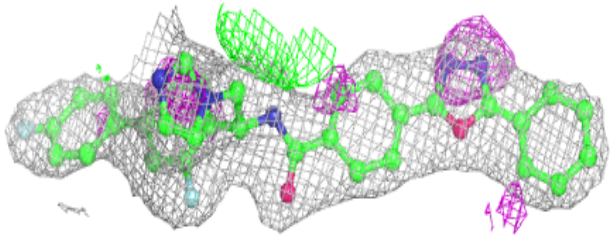


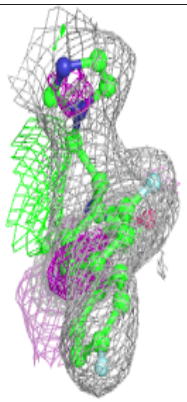


Electron density around VFV F 580:

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

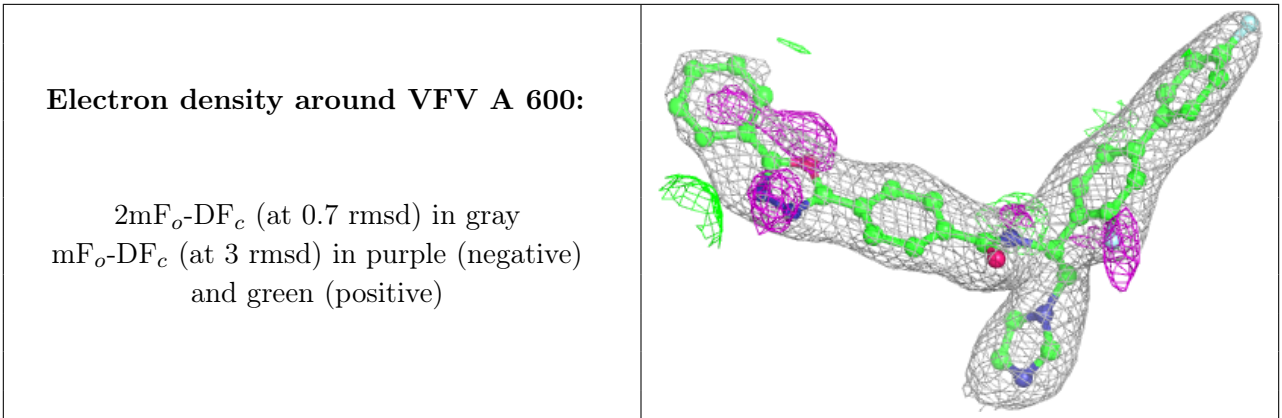


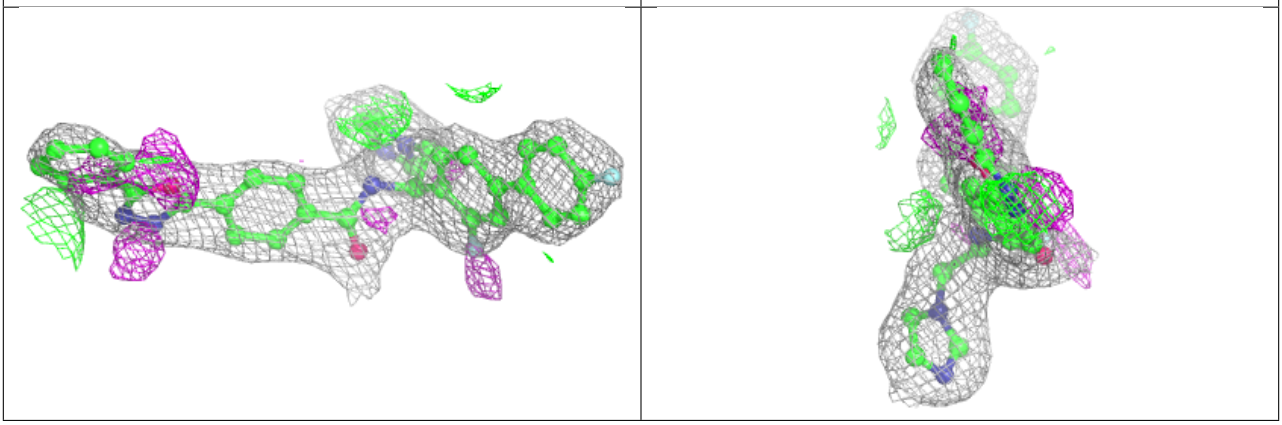




Electron density around VFV A 600:

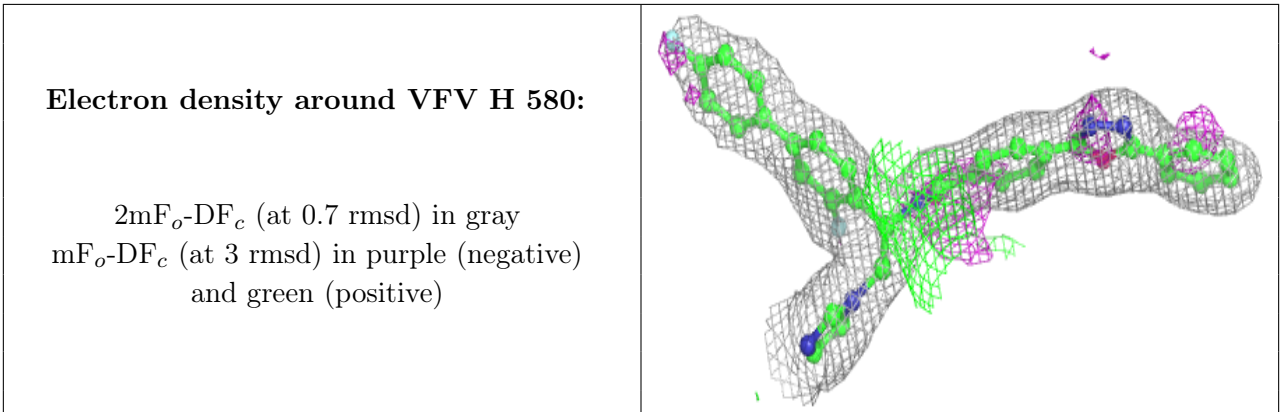
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

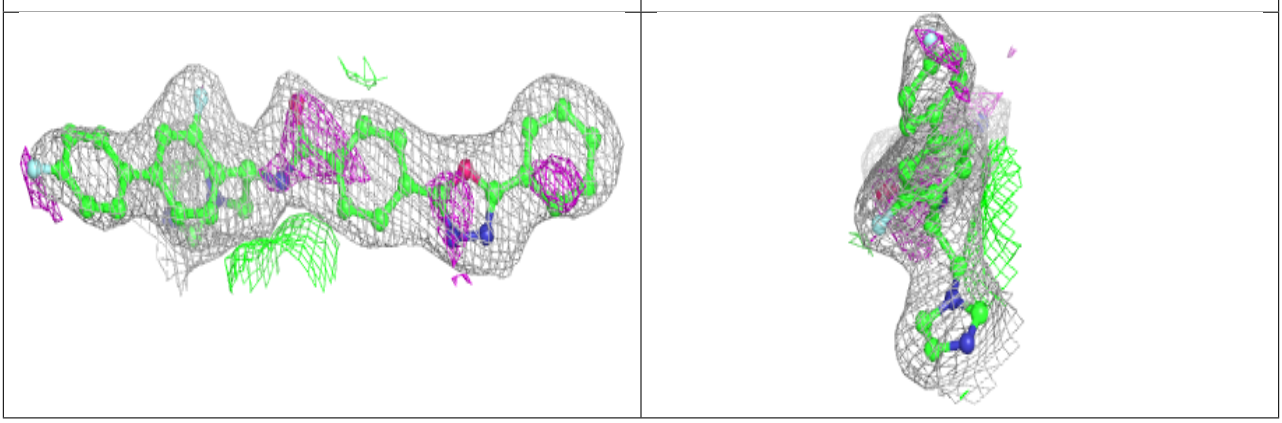




Electron density around VFV H 580:

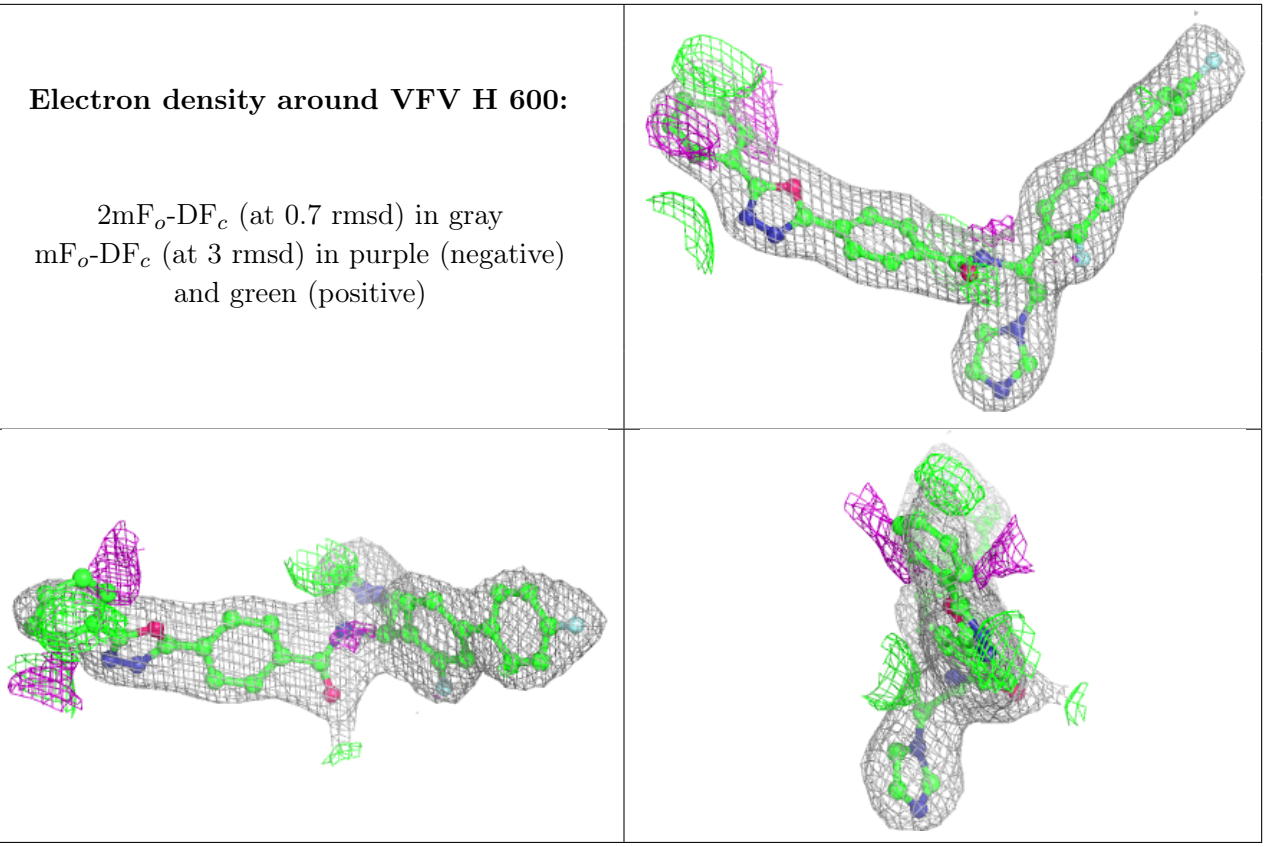
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





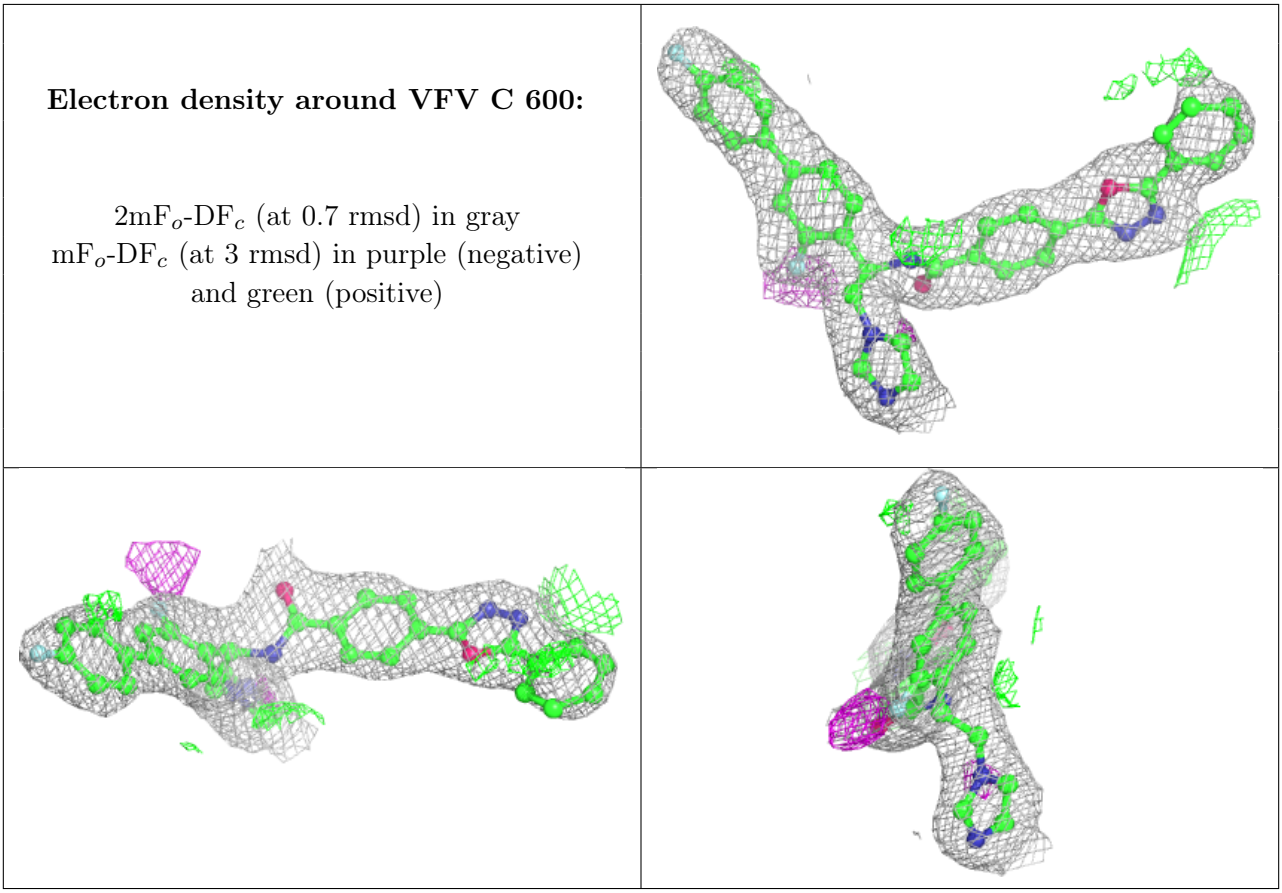
Electron density around VFV H 600:

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



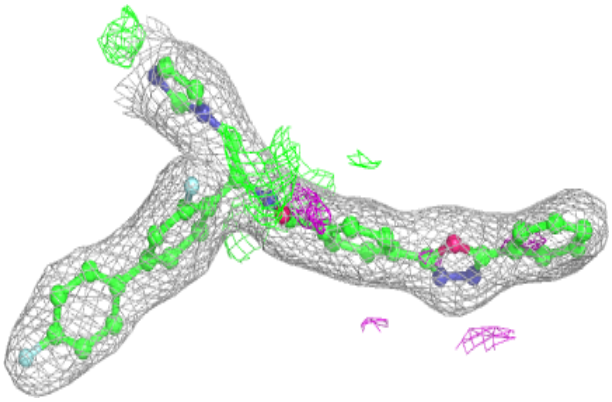
Electron density around VFV C 600:

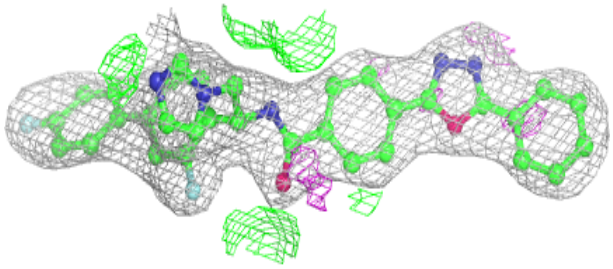
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

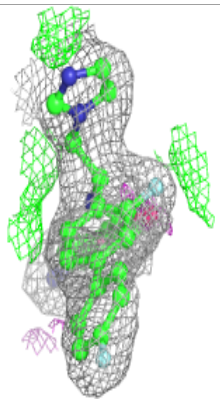


Electron density around VFV D 580:

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

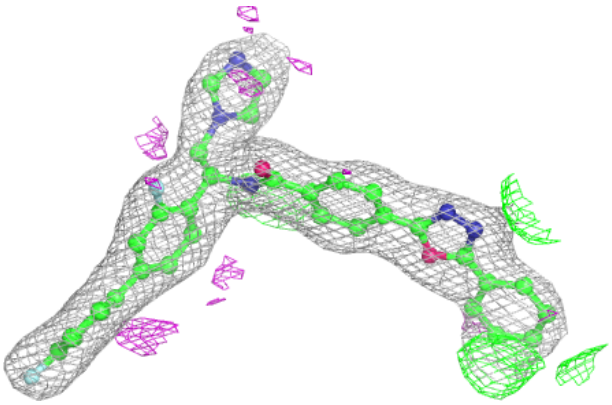


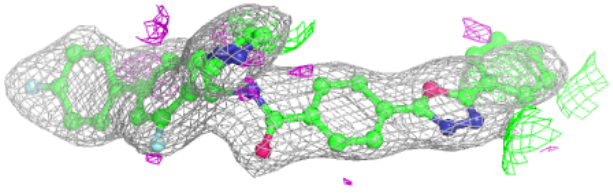


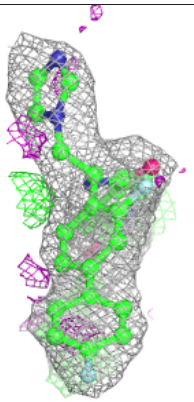


Electron density around VFV D 600:

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

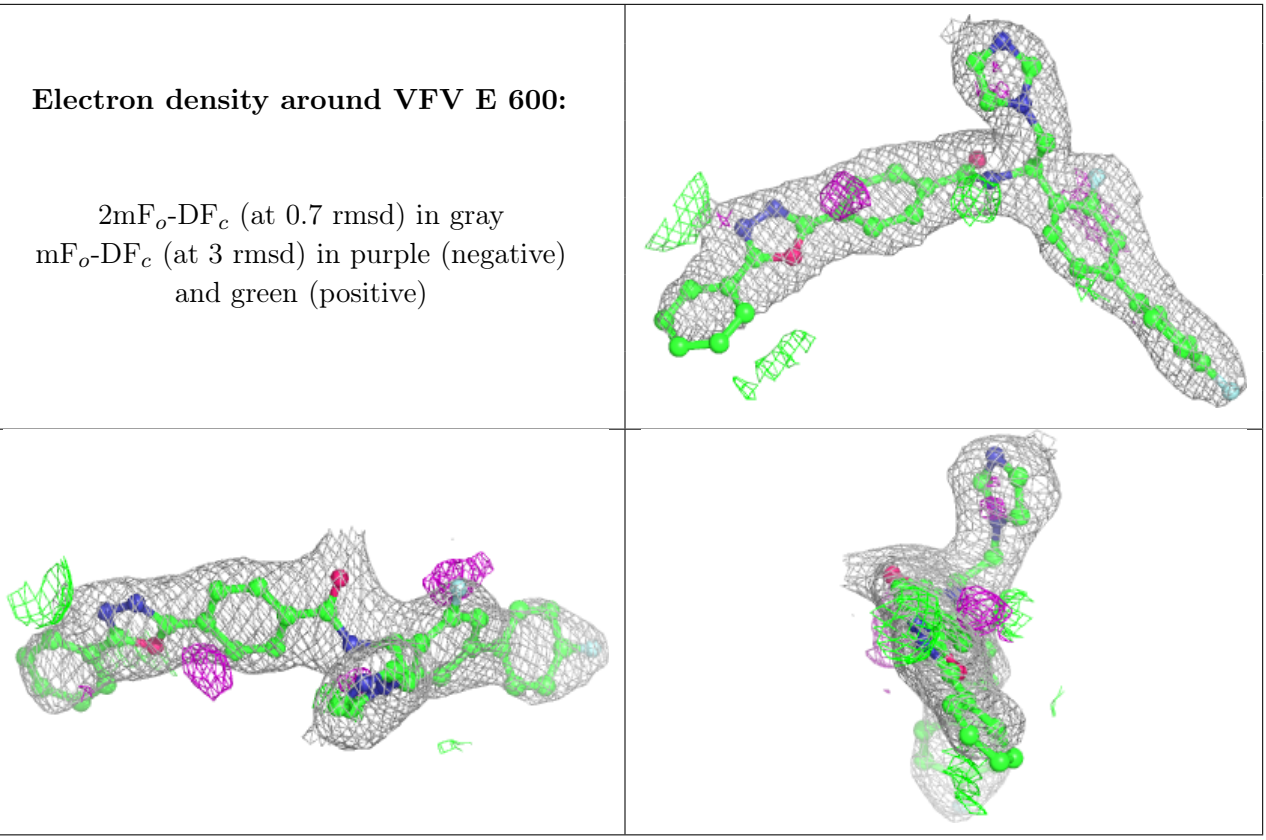






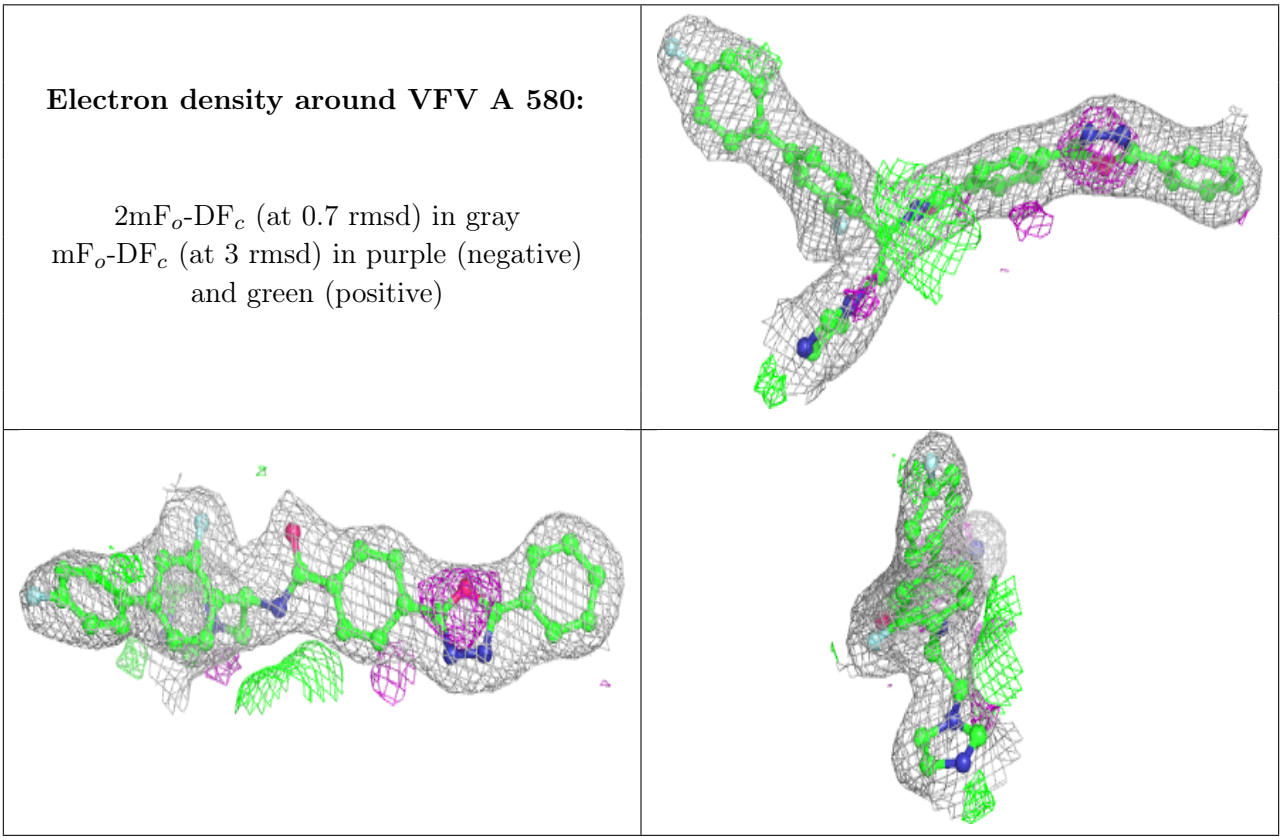
Electron density around VFV E 600:

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



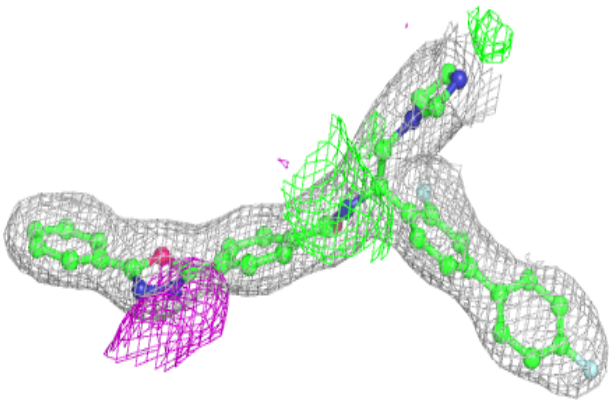
Electron density around VFV A 580:

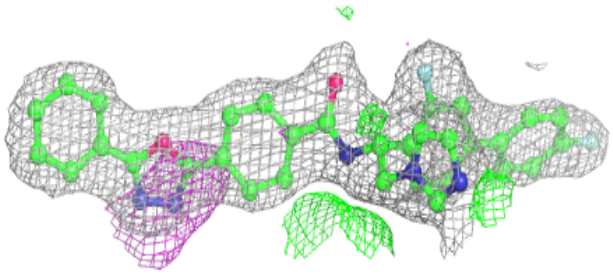
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

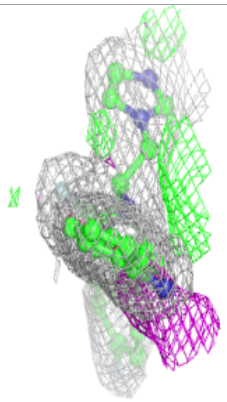


Electron density around VFV B 580:

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

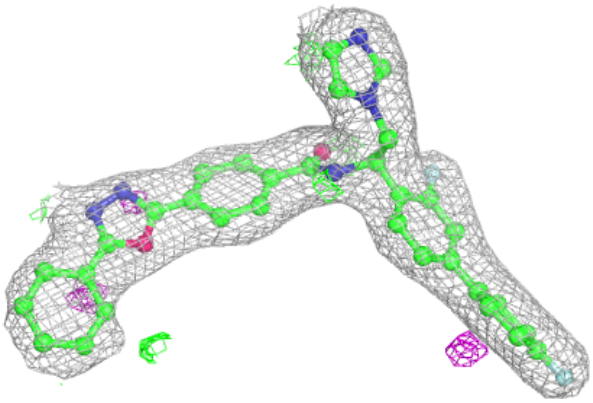


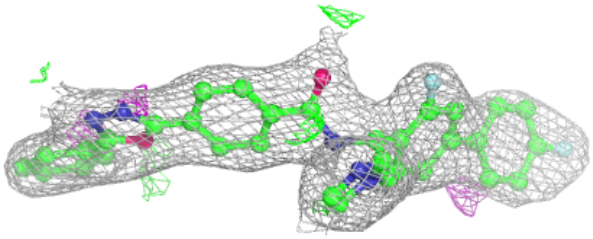


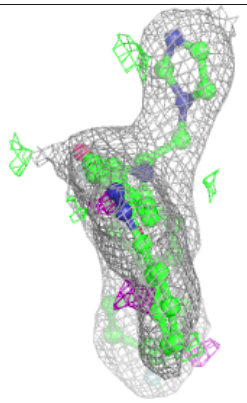


Electron density around VFV G 600:

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

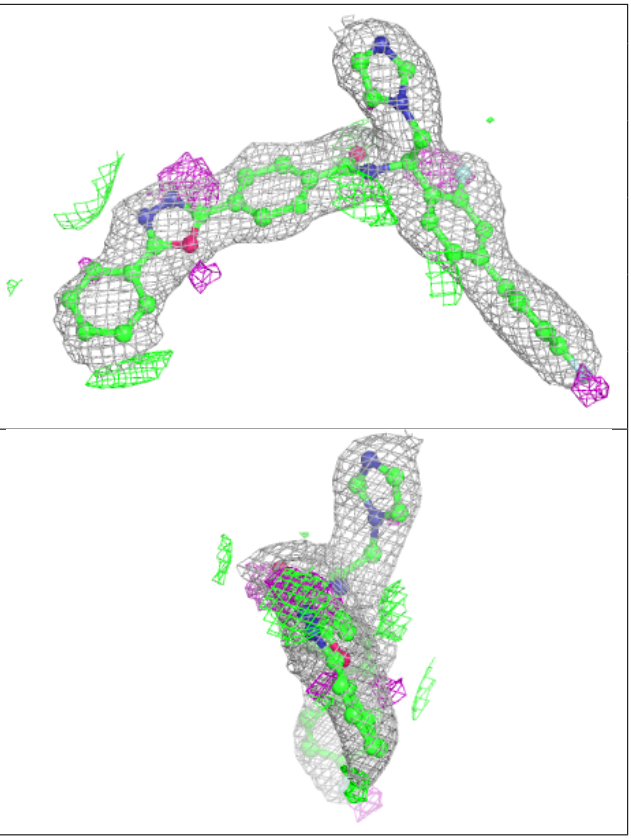






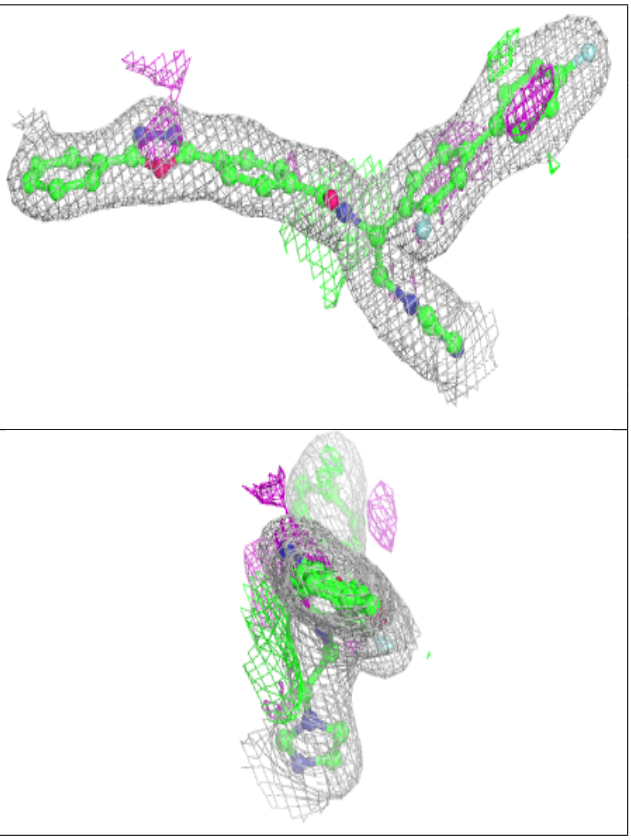
Electron density around VFV B 600:

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



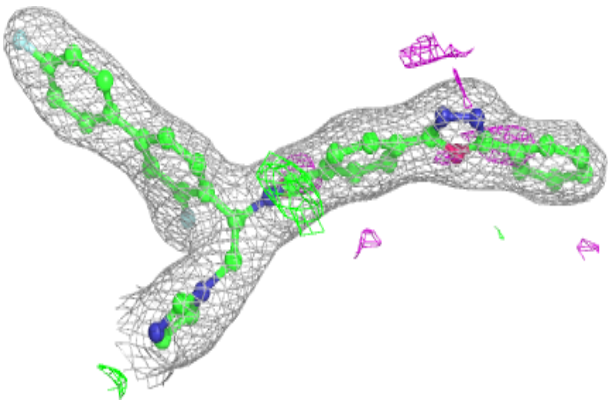
Electron density around VFV C 580:

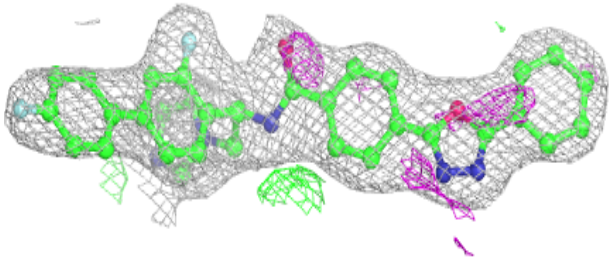
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

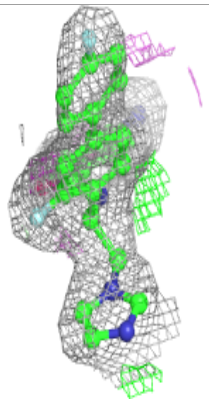


Electron density around VFV G 580:

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

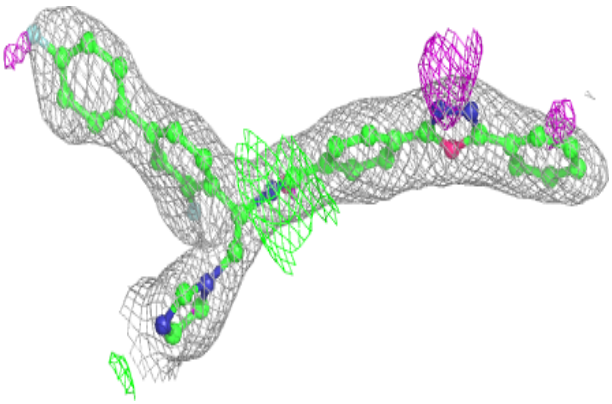


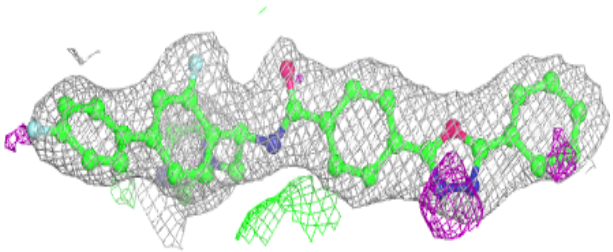


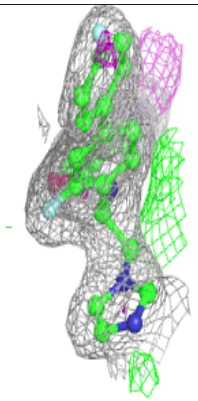


Electron density around VFV E 580:

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

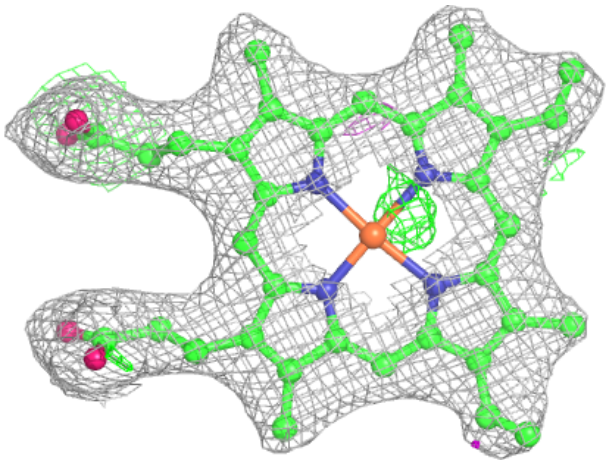


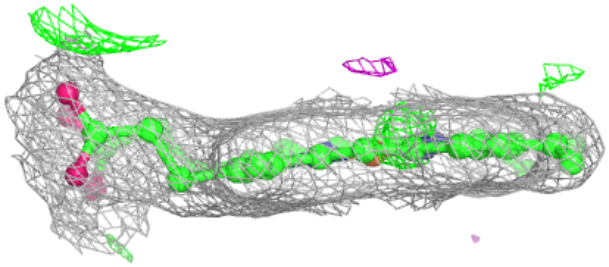


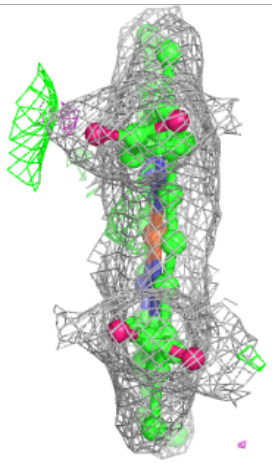


Electron density around HEM B 540:

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

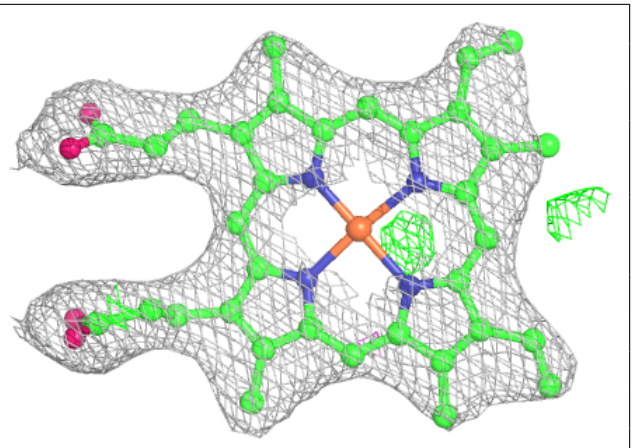


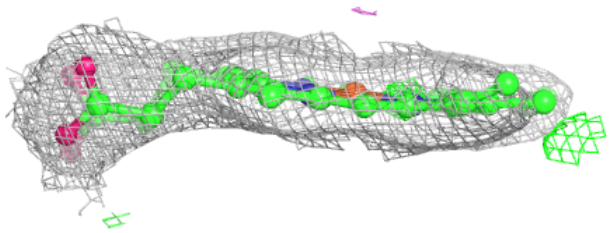


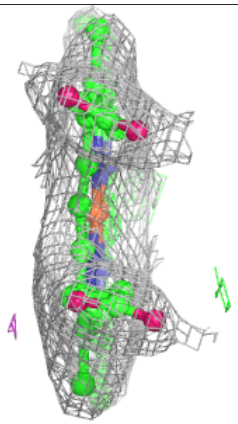


Electron density around HEM E 540:

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

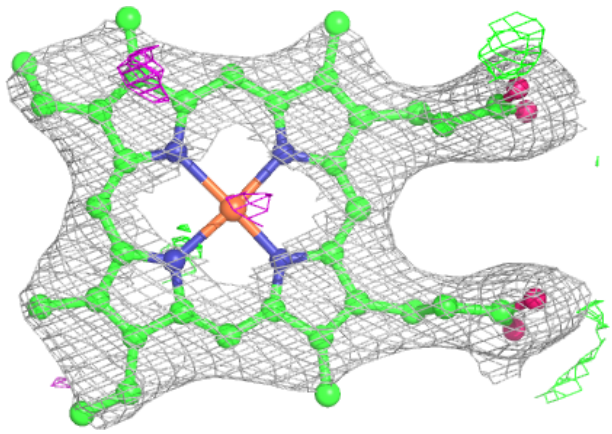


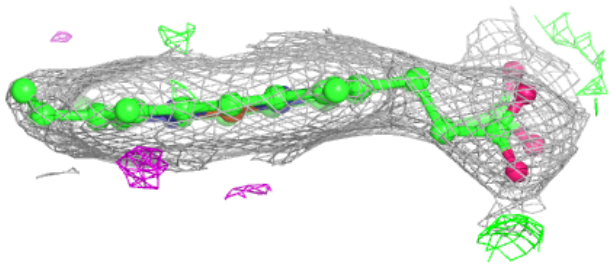


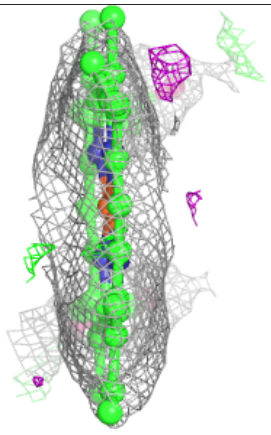


Electron density around HEM F 540:

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

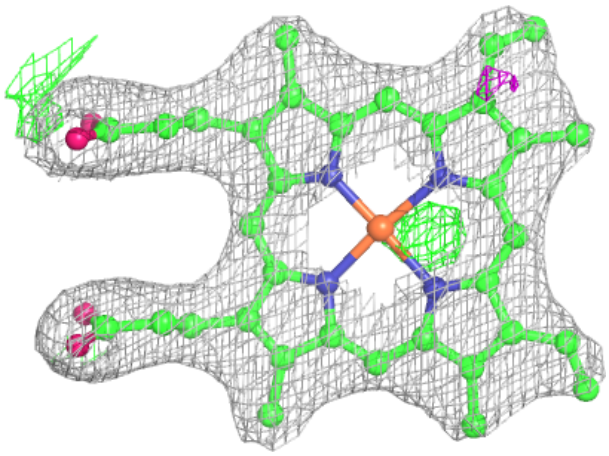


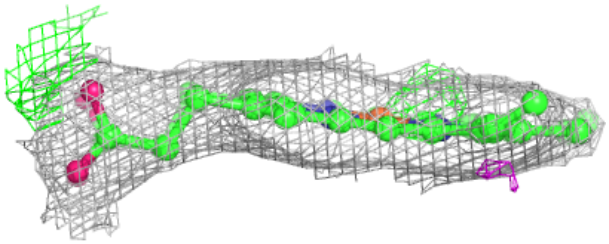


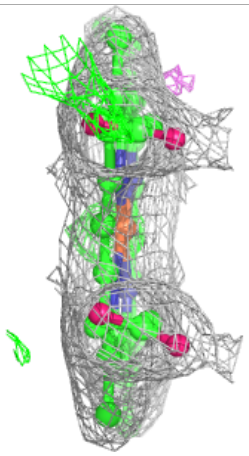


Electron density around HEM G 540:

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

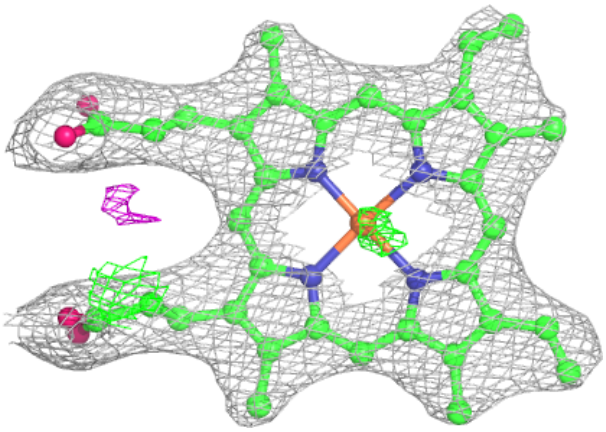


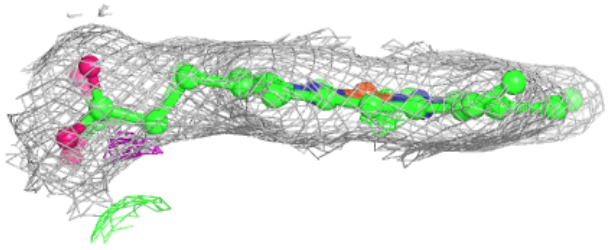


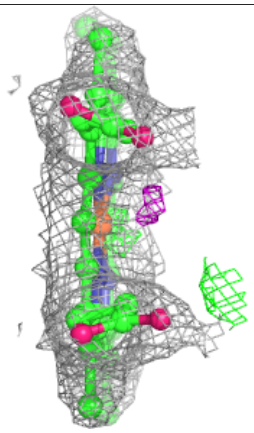


Electron density around HEM A 540:

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

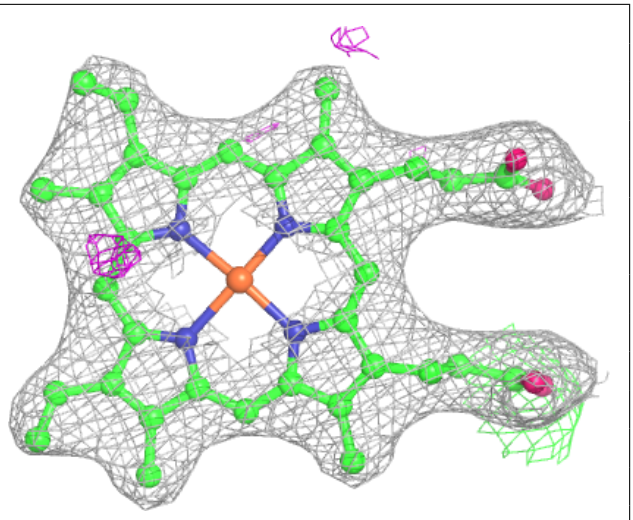


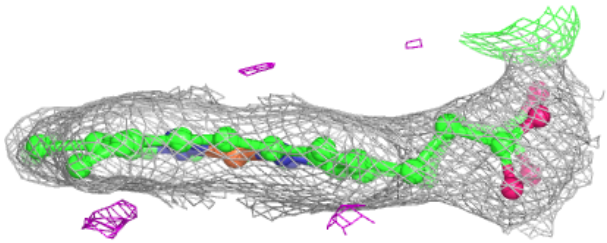


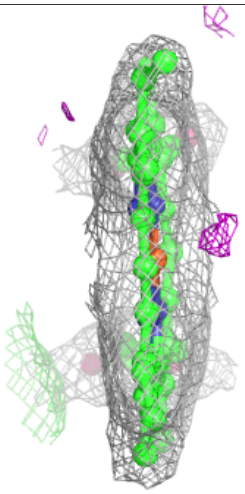


Electron density around HEM C 540:

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

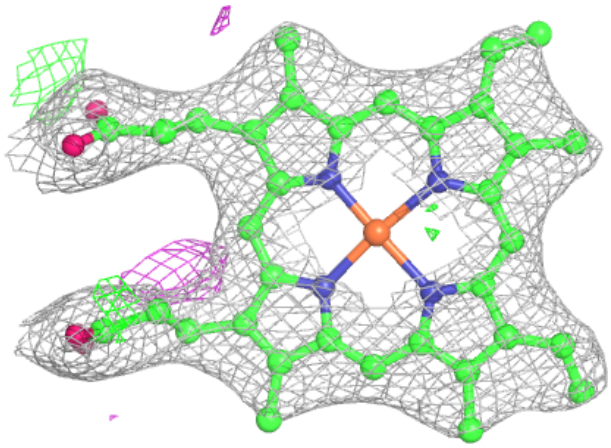


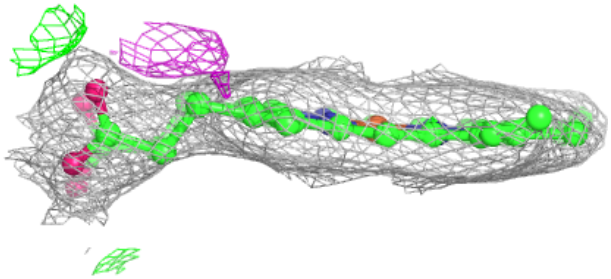


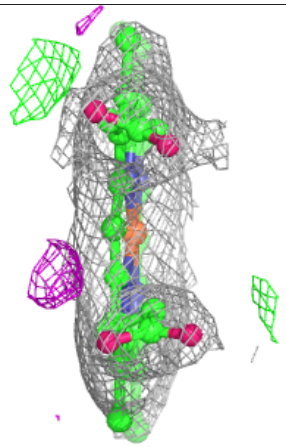


Electron density around HEM H 540:

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

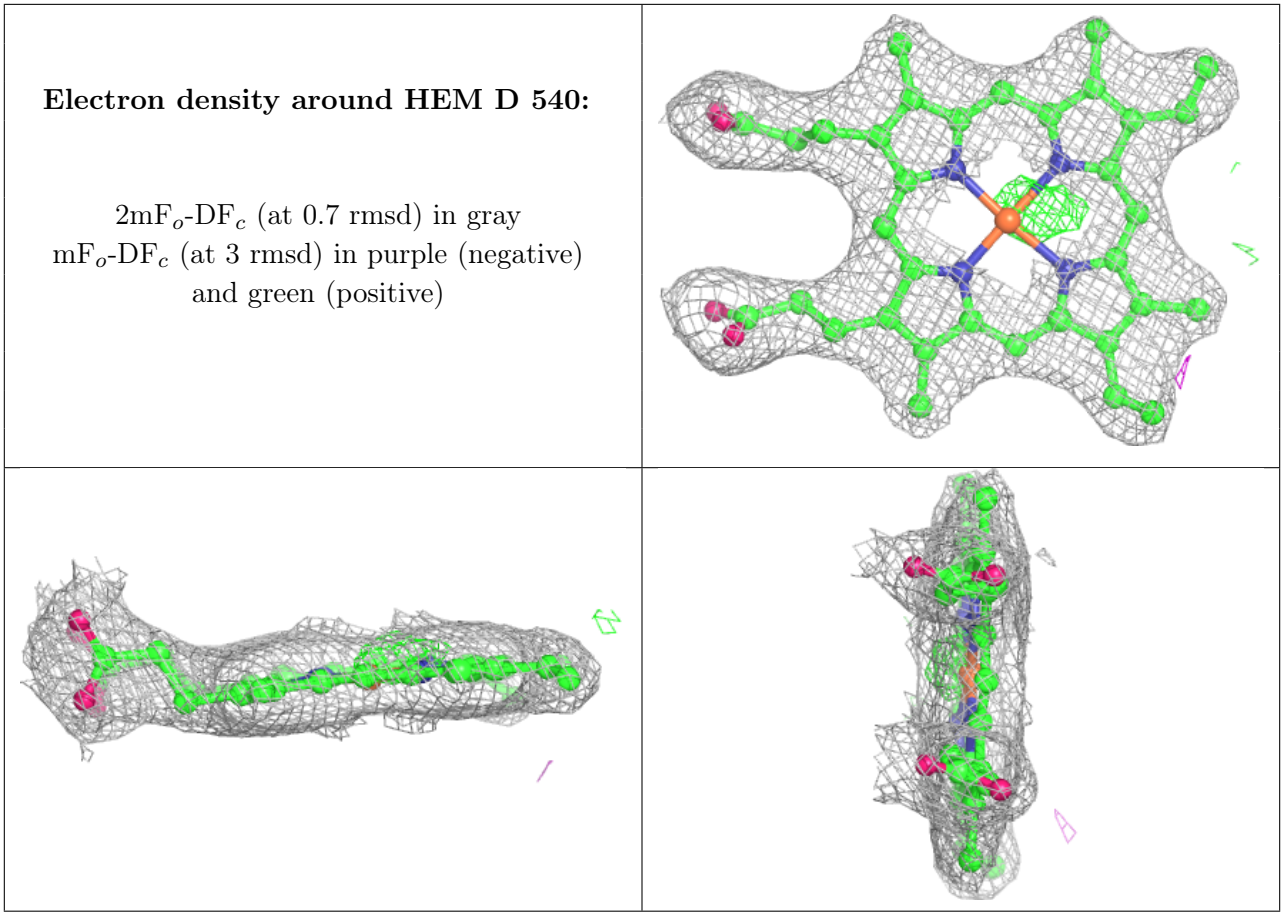






Electron density around HEM D 540:

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



6.5 Other polymers

There are no such residues in this entry.