



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 11:42 PM JST

PDB ID : 8K1X / pdb_00008k1x
Title : Biochemical and structural characterization of a multifunctional cytochrome P450 SpcN in staurosporine biosynthesis
Authors : Xiao, F.; Dong, S.; Feng, Y.; Li, W.
Deposited on : 2023-07-11
Resolution : 2.27 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 : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

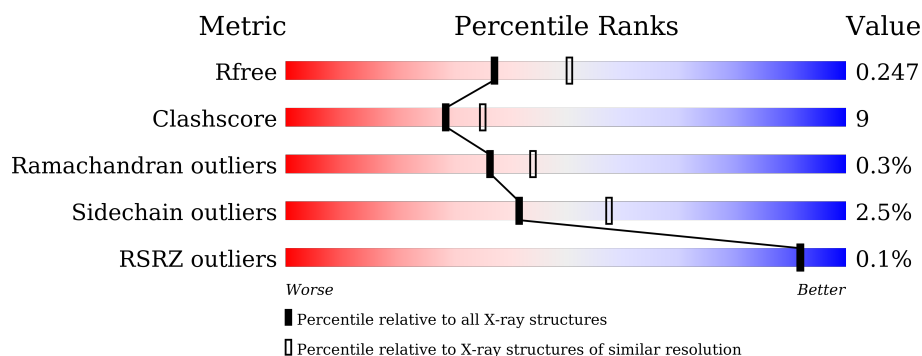
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 $\leq 5\%$. 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	440	70% 18% • 11%
1	B	440	70% 17% 12%
1	C	440	68% 18% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9344 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2969	1893	529	532	15			
1	B	387	Total	C	N	O	S	0	0	0
			2921	1865	520	521	15			
1	C	381	Total	C	N	O	S	0	0	0
			2896	1849	520	512	15			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP W5R4Y8
A	-14	HIS	-	expression tag	UNP W5R4Y8
A	-13	HIS	-	expression tag	UNP W5R4Y8
A	-12	HIS	-	expression tag	UNP W5R4Y8
A	-11	HIS	-	expression tag	UNP W5R4Y8
A	-10	HIS	-	expression tag	UNP W5R4Y8
A	-9	SER	-	expression tag	UNP W5R4Y8
A	-8	SER	-	expression tag	UNP W5R4Y8
A	-7	GLY	-	expression tag	UNP W5R4Y8
A	-6	LEU	-	expression tag	UNP W5R4Y8
A	-5	VAL	-	expression tag	UNP W5R4Y8
A	-4	PRO	-	expression tag	UNP W5R4Y8
A	-3	ARG	-	expression tag	UNP W5R4Y8
A	-2	GLY	-	expression tag	UNP W5R4Y8
A	-1	SER	-	expression tag	UNP W5R4Y8
A	0	HIS	-	expression tag	UNP W5R4Y8
A	1	MET	-	expression tag	UNP W5R4Y8
A	2	ASN	-	expression tag	UNP W5R4Y8
A	3	VAL	-	expression tag	UNP W5R4Y8
A	4	THR	-	expression tag	UNP W5R4Y8
A	5	THR	-	expression tag	UNP W5R4Y8
A	6	LYS	-	expression tag	UNP W5R4Y8
A	7	THR	-	expression tag	UNP W5R4Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP W5R4Y8
A	9	LEU	-	expression tag	UNP W5R4Y8
A	10	ALA	-	expression tag	UNP W5R4Y8
A	11	GLU	-	expression tag	UNP W5R4Y8
A	12	ALA	-	expression tag	UNP W5R4Y8
A	13	PRO	-	expression tag	UNP W5R4Y8
A	14	GLU	-	expression tag	UNP W5R4Y8
A	15	ALA	-	expression tag	UNP W5R4Y8
A	16	HIS	-	expression tag	UNP W5R4Y8
A	17	MET	-	expression tag	UNP W5R4Y8
A	18	PRO	-	expression tag	UNP W5R4Y8
A	19	THR	-	expression tag	UNP W5R4Y8
A	20	ASP	-	expression tag	UNP W5R4Y8
A	21	PRO	-	expression tag	UNP W5R4Y8
A	22	GLY	-	expression tag	UNP W5R4Y8
A	23	PRO	-	expression tag	UNP W5R4Y8
A	24	PHE	-	expression tag	UNP W5R4Y8
A	25	ASP	-	expression tag	UNP W5R4Y8
A	26	CYS	-	expression tag	UNP W5R4Y8
A	417	LEU	-	expression tag	UNP W5R4Y8
A	418	GLU	-	expression tag	UNP W5R4Y8
A	419	HIS	-	expression tag	UNP W5R4Y8
A	420	HIS	-	expression tag	UNP W5R4Y8
A	421	HIS	-	expression tag	UNP W5R4Y8
A	422	HIS	-	expression tag	UNP W5R4Y8
A	423	HIS	-	expression tag	UNP W5R4Y8
A	424	HIS	-	expression tag	UNP W5R4Y8
B	-15	HIS	-	expression tag	UNP W5R4Y8
B	-14	HIS	-	expression tag	UNP W5R4Y8
B	-13	HIS	-	expression tag	UNP W5R4Y8
B	-12	HIS	-	expression tag	UNP W5R4Y8
B	-11	HIS	-	expression tag	UNP W5R4Y8
B	-10	HIS	-	expression tag	UNP W5R4Y8
B	-9	SER	-	expression tag	UNP W5R4Y8
B	-8	SER	-	expression tag	UNP W5R4Y8
B	-7	GLY	-	expression tag	UNP W5R4Y8
B	-6	LEU	-	expression tag	UNP W5R4Y8
B	-5	VAL	-	expression tag	UNP W5R4Y8
B	-4	PRO	-	expression tag	UNP W5R4Y8
B	-3	ARG	-	expression tag	UNP W5R4Y8
B	-2	GLY	-	expression tag	UNP W5R4Y8
B	-1	SER	-	expression tag	UNP W5R4Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP W5R4Y8
B	1	MET	-	expression tag	UNP W5R4Y8
B	2	ASN	-	expression tag	UNP W5R4Y8
B	3	VAL	-	expression tag	UNP W5R4Y8
B	4	THR	-	expression tag	UNP W5R4Y8
B	5	THR	-	expression tag	UNP W5R4Y8
B	6	LYS	-	expression tag	UNP W5R4Y8
B	7	THR	-	expression tag	UNP W5R4Y8
B	8	GLY	-	expression tag	UNP W5R4Y8
B	9	LEU	-	expression tag	UNP W5R4Y8
B	10	ALA	-	expression tag	UNP W5R4Y8
B	11	GLU	-	expression tag	UNP W5R4Y8
B	12	ALA	-	expression tag	UNP W5R4Y8
B	13	PRO	-	expression tag	UNP W5R4Y8
B	14	GLU	-	expression tag	UNP W5R4Y8
B	15	ALA	-	expression tag	UNP W5R4Y8
B	16	HIS	-	expression tag	UNP W5R4Y8
B	17	MET	-	expression tag	UNP W5R4Y8
B	18	PRO	-	expression tag	UNP W5R4Y8
B	19	THR	-	expression tag	UNP W5R4Y8
B	20	ASP	-	expression tag	UNP W5R4Y8
B	21	PRO	-	expression tag	UNP W5R4Y8
B	22	GLY	-	expression tag	UNP W5R4Y8
B	23	PRO	-	expression tag	UNP W5R4Y8
B	24	PHE	-	expression tag	UNP W5R4Y8
B	25	ASP	-	expression tag	UNP W5R4Y8
B	26	CYS	-	expression tag	UNP W5R4Y8
B	417	LEU	-	expression tag	UNP W5R4Y8
B	418	GLU	-	expression tag	UNP W5R4Y8
B	419	HIS	-	expression tag	UNP W5R4Y8
B	420	HIS	-	expression tag	UNP W5R4Y8
B	421	HIS	-	expression tag	UNP W5R4Y8
B	422	HIS	-	expression tag	UNP W5R4Y8
B	423	HIS	-	expression tag	UNP W5R4Y8
B	424	HIS	-	expression tag	UNP W5R4Y8
C	-15	HIS	-	expression tag	UNP W5R4Y8
C	-14	HIS	-	expression tag	UNP W5R4Y8
C	-13	HIS	-	expression tag	UNP W5R4Y8
C	-12	HIS	-	expression tag	UNP W5R4Y8
C	-11	HIS	-	expression tag	UNP W5R4Y8
C	-10	HIS	-	expression tag	UNP W5R4Y8
C	-9	SER	-	expression tag	UNP W5R4Y8

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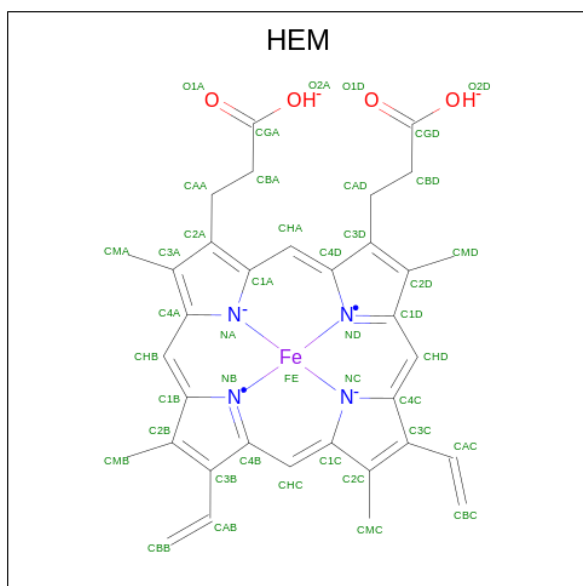
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP W5R4Y8
C	-7	GLY	-	expression tag	UNP W5R4Y8
C	-6	LEU	-	expression tag	UNP W5R4Y8
C	-5	VAL	-	expression tag	UNP W5R4Y8
C	-4	PRO	-	expression tag	UNP W5R4Y8
C	-3	ARG	-	expression tag	UNP W5R4Y8
C	-2	GLY	-	expression tag	UNP W5R4Y8
C	-1	SER	-	expression tag	UNP W5R4Y8
C	0	HIS	-	expression tag	UNP W5R4Y8
C	1	MET	-	expression tag	UNP W5R4Y8
C	2	ASN	-	expression tag	UNP W5R4Y8
C	3	VAL	-	expression tag	UNP W5R4Y8
C	4	THR	-	expression tag	UNP W5R4Y8
C	5	THR	-	expression tag	UNP W5R4Y8
C	6	LYS	-	expression tag	UNP W5R4Y8
C	7	THR	-	expression tag	UNP W5R4Y8
C	8	GLY	-	expression tag	UNP W5R4Y8
C	9	LEU	-	expression tag	UNP W5R4Y8
C	10	ALA	-	expression tag	UNP W5R4Y8
C	11	GLU	-	expression tag	UNP W5R4Y8
C	12	ALA	-	expression tag	UNP W5R4Y8
C	13	PRO	-	expression tag	UNP W5R4Y8
C	14	GLU	-	expression tag	UNP W5R4Y8
C	15	ALA	-	expression tag	UNP W5R4Y8
C	16	HIS	-	expression tag	UNP W5R4Y8
C	17	MET	-	expression tag	UNP W5R4Y8
C	18	PRO	-	expression tag	UNP W5R4Y8
C	19	THR	-	expression tag	UNP W5R4Y8
C	20	ASP	-	expression tag	UNP W5R4Y8
C	21	PRO	-	expression tag	UNP W5R4Y8
C	22	GLY	-	expression tag	UNP W5R4Y8
C	23	PRO	-	expression tag	UNP W5R4Y8
C	24	PHE	-	expression tag	UNP W5R4Y8
C	25	ASP	-	expression tag	UNP W5R4Y8
C	26	CYS	-	expression tag	UNP W5R4Y8
C	417	LEU	-	expression tag	UNP W5R4Y8
C	418	GLU	-	expression tag	UNP W5R4Y8
C	419	HIS	-	expression tag	UNP W5R4Y8
C	420	HIS	-	expression tag	UNP W5R4Y8
C	421	HIS	-	expression tag	UNP W5R4Y8
C	422	HIS	-	expression tag	UNP W5R4Y8
C	423	HIS	-	expression tag	UNP W5R4Y8

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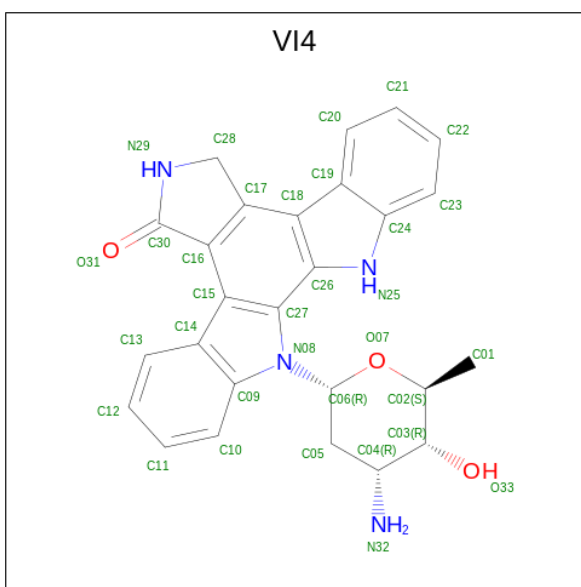
Chain	Residue	Modelled	Actual	Comment	Reference
C	424	HIS	-	expression tag	UNP W5R4Y8

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



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

- Molecule 3 is 13-(3-Amino-2,3,6-trideoxy-alpha-L-ribo-hexopyranosyl)-6,7,12,13-tetrahydro-5H-indolo[2,3-a]pyrrolo[3,4-c]carbazol-5-one (CCD ID: VI4) (formula: $C_{26}H_{24}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	26	4	3		
3	A	1	Total	C	N	O	0	0
			33	26	4	3		
3	B	1	Total	C	N	O	0	0
			33	26	4	3		
3	B	1	Total	C	N	O	0	0
			33	26	4	3		
3	B	1	Total	C	N	O	0	0
			33	26	4	3		
3	C	1	Total	C	N	O	0	0
			33	26	4	3		

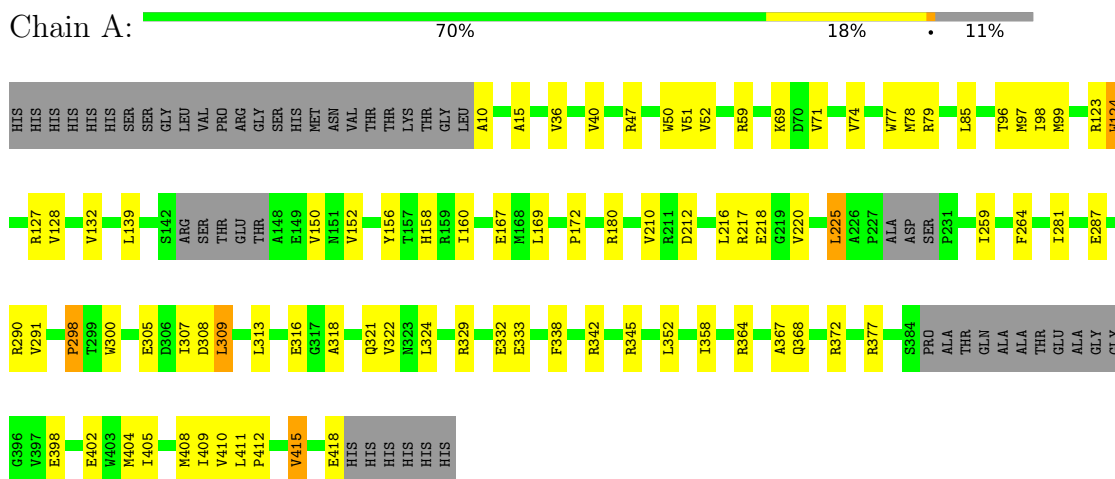
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	74	Total	O	0	0
			74	74		
4	C	72	Total	O	0	0
			72	72		

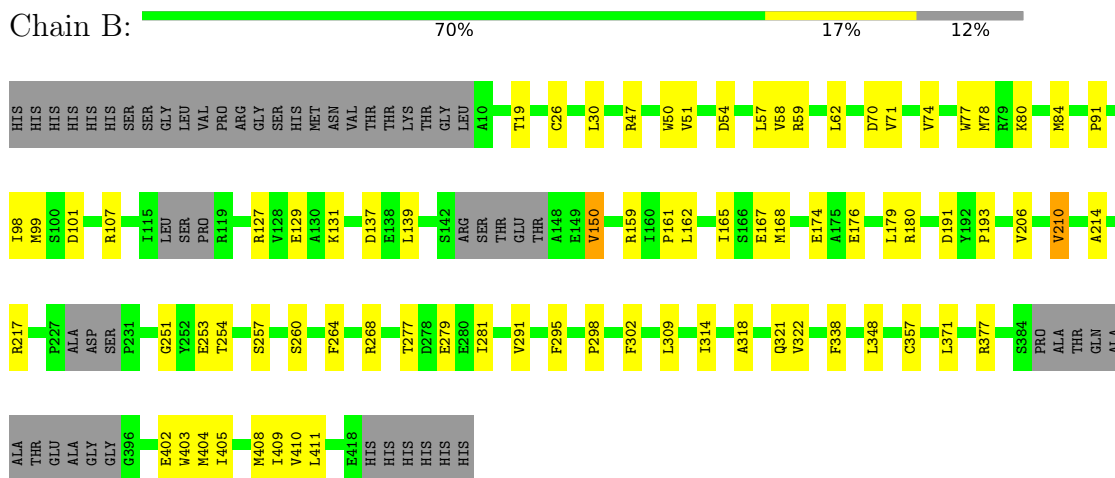
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome P450

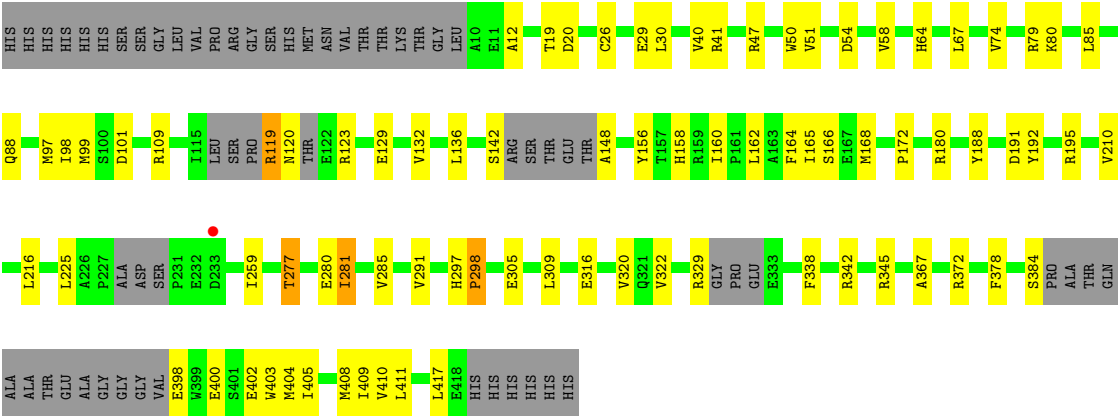


• Molecule 1: Cytochrome P450



• Molecule 1: Cytochrome P450





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.96Å 121.79Å 64.21Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	55.17 – 2.27 55.17 – 2.27	Depositor EDS
% Data completeness (in resolution range)	96.5 (55.17-2.27) 96.5 (55.17-2.27)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.211 , 0.234 0.225 , 0.247	Depositor DCC
R_{free} test set	3657 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.011 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.176 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.089 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9344	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VI4, 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	0.40	1/3048 (0.0%)	0.58	3/4162 (0.1%)
1	B	0.25	0/2998	0.44	0/4095
1	C	0.39	0/2970	0.48	1/4050 (0.0%)
All	All	0.35	1/9016 (0.0%)	0.50	4/12307 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	PRO	CA-C	-5.54	1.47	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ASP	N-CA-C	-5.53	100.38	109.40
1	C	123	ARG	N-CA-C	-5.10	106.84	113.16
1	A	225	LEU	N-CA-C	-5.01	107.00	112.72
1	A	415	VAL	N-CA-C	5.01	118.15	111.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2969	0	2896	47	0
1	B	2921	0	2838	46	0
1	C	2896	0	2825	54	0
2	A	43	0	30	3	0
2	B	43	0	30	7	0
2	C	43	0	30	6	0
3	A	66	0	0	0	0
3	B	99	0	0	3	0
3	C	33	0	0	0	0
4	A	85	0	0	4	0
4	B	74	0	0	1	0
4	C	72	0	0	8	0
All	All	9344	0	8649	157	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 9.

All (157) 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)
2:C:501:HEM:HBB2	2:C:501:HEM:HMB1	1.51	0.91
2:B:501:HEM:HMB1	2:B:501:HEM:HBB2	1.63	0.80
1:C:402:GLU:HG3	1:C:404:MET:H	1.48	0.78
1:B:137:ASP:OD1	1:B:377:ARG:NH2	2.17	0.78
1:C:398:GLU:HA	1:C:410:VAL:HG22	1.66	0.77
1:B:62:LEU:HD21	1:B:322:VAL:HG21	1.66	0.76
1:A:78:MET:HE3	1:A:85:LEU:HD13	1.69	0.72
1:A:398:GLU:HG2	1:A:410:VAL:HG22	1.73	0.71
1:C:20:ASP:OD1	4:C:601:HOH:O	2.09	0.71
1:A:313:LEU:O	4:A:601:HOH:O	2.09	0.70
1:B:174:GLU:N	1:B:174:GLU:OE2	2.23	0.70
2:C:501:HEM:HBB2	2:C:501:HEM:CMB	2.22	0.69
1:A:10:ALA:N	4:A:603:HOH:O	2.25	0.69
1:C:398:GLU:N	4:C:605:HOH:O	2.25	0.69
2:B:501:HEM:CMC	2:B:501:HEM:HBC2	2.24	0.68
1:C:58:VAL:HG13	1:C:322:VAL:HB	1.76	0.67
1:C:408:MET:HE1	1:C:411:LEU:HD22	1.76	0.67
1:C:402:GLU:HG2	1:C:405:ILE:HG22	1.76	0.67
1:B:165:ILE:HD13	1:B:251:GLY:HA3	1.75	0.67
1:A:158:HIS:O	1:A:180:ARG:NH2	2.28	0.66
1:A:287:GLU:OE2	1:A:290:ARG:NH2	2.28	0.65
1:C:305:GLU:HA	1:C:316:GLU:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LEU:O	1:C:166:SER:OG	2.15	0.64
1:A:281:ILE:HD13	1:A:372:ARG:HB2	1.80	0.64
1:A:74:VAL:HG23	1:A:78:MET:HE2	1.81	0.63
1:C:88:GLN:HG3	1:C:99:MET:HE1	1.81	0.63
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.79	0.62
2:B:501:HEM:HMB1	2:B:501:HEM:CBB	2.29	0.62
3:B:503:VI4:O07	3:B:503:VI4:N25	2.33	0.61
1:B:402:GLU:HG2	1:B:405:ILE:HG22	1.82	0.61
1:B:59:ARG:HG3	1:B:348:LEU:HD11	1.82	0.60
1:A:329:ARG:HB3	1:A:333:GLU:HG3	1.83	0.59
1:B:180:ARG:NH1	1:B:253:GLU:OE1	2.35	0.59
1:A:332:GLU:N	1:A:332:GLU:OE2	2.36	0.59
1:C:64:HIS:HB3	1:C:67:LEU:HG	1.83	0.58
1:A:368:GLN:NE2	4:A:604:HOH:O	2.25	0.58
3:B:504:VI4:O07	3:B:504:VI4:N25	2.36	0.58
1:C:47:ARG:NH1	4:C:609:HOH:O	2.28	0.58
1:C:29:GLU:N	1:C:29:GLU:OE2	2.37	0.58
1:A:398:GLU:HG3	1:A:409:ILE:HG13	1.84	0.58
1:C:80:LYS:HD3	1:C:192:TYR:CE2	2.39	0.58
1:B:47:ARG:HD3	1:B:77:TRP:CE2	2.38	0.57
1:A:402:GLU:HG3	1:A:404:MET:H	1.69	0.57
1:C:298:PRO:HB2	2:C:501:HEM:O1A	2.05	0.57
1:B:408:MET:HE1	1:B:411:LEU:HD13	1.87	0.57
1:C:74:VAL:O	1:C:79:ARG:NH1	2.37	0.57
1:B:71:VAL:HG13	1:B:91:PRO:HG3	1.85	0.56
1:B:47:ARG:HD3	1:B:77:TRP:CD2	2.41	0.56
1:A:172:PRO:HD3	1:A:216:LEU:HD23	1.88	0.56
1:C:97:MET:HE2	1:C:109:ARG:HA	1.88	0.55
1:C:297:HIS:ND1	1:C:403:TRP:O	2.27	0.55
1:C:148:ALA:N	4:C:611:HOH:O	2.39	0.55
1:C:30:LEU:HD12	1:C:297:HIS:HE1	1.72	0.54
1:A:264:PHE:HB2	1:A:408:MET:HE1	1.89	0.54
1:A:291:VAL:HG21	1:A:338:PHE:HA	1.89	0.53
1:B:277:THR:OG1	1:B:279:GLU:OE1	2.24	0.53
1:C:277:THR:HG23	1:C:280:GLU:H	1.74	0.52
1:C:40:VAL:HG13	1:C:51:VAL:HB	1.92	0.52
2:C:501:HEM:HBC2	2:C:501:HEM:HHD	1.90	0.52
1:C:132:VAL:O	1:C:136:LEU:HG	2.10	0.51
1:C:384:SER:O	4:C:602:HOH:O	2.19	0.51
1:A:97:MET:HG2	2:A:501:HEM:CGD	2.41	0.51
1:C:74:VAL:HG11	1:C:85:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HB	1:A:322:VAL:HG12	1.93	0.51
1:C:188:TYR:HB3	1:C:400:GLU:OE1	2.11	0.51
2:B:501:HEM:HMC1	2:B:501:HEM:CBC	2.40	0.51
1:A:402:GLU:HG2	1:A:405:ILE:HG22	1.93	0.51
1:A:298:PRO:HD3	1:A:324:LEU:HG	1.93	0.50
1:C:259:ILE:HG12	1:C:367:ALA:HA	1.94	0.50
1:A:123:ARG:O	1:A:127:ARG:HG3	2.11	0.50
1:B:162:LEU:HD22	1:B:176:GLU:HG2	1.92	0.50
1:B:78:MET:HE1	1:B:302:PHE:HE1	1.77	0.49
1:C:164:PHE:CE2	1:C:168:MET:HE2	2.47	0.49
1:B:281:ILE:HG23	1:B:371:LEU:HD23	1.93	0.49
1:B:291:VAL:HG21	1:B:338:PHE:HA	1.93	0.49
1:B:191:ASP:OD1	1:B:193:PRO:HD2	2.12	0.49
1:C:12:ALA:O	1:C:41:ARG:NH1	2.43	0.49
1:A:50:TRP:CE3	1:A:318:ALA:HB1	2.47	0.48
1:B:214:ALA:O	4:B:601:HOH:O	2.20	0.48
1:A:139:LEU:HD21	1:A:150:VAL:HG21	1.94	0.48
1:B:74:VAL:HG22	1:B:302:PHE:CZ	2.48	0.48
1:B:167:GLU:HA	1:B:217:ARG:NH2	2.28	0.48
1:C:378:PHE:HA	1:C:417:LEU:CB	2.44	0.48
1:B:402:GLU:HG3	1:B:404:MET:H	1.78	0.48
1:A:210:VAL:HG13	1:A:225:LEU:HD21	1.95	0.48
1:B:51:VAL:HG12	1:B:321:GLN:HB2	1.96	0.48
1:A:69:LYS:HE3	1:A:98:ILE:O	2.14	0.48
1:C:156:TYR:CE1	1:C:160:ILE:HD11	2.49	0.47
1:B:254:THR:HG21	1:B:295:PHE:CZ	2.50	0.47
1:B:179:LEU:HD23	1:B:179:LEU:HA	1.77	0.47
1:A:69:LYS:NZ	1:A:300:TRP:O	2.48	0.47
1:C:101:ASP:OD1	4:C:603:HOH:O	2.20	0.47
1:C:98:ILE:HD13	2:C:501:HEM:HAD2	1.96	0.47
1:A:47:ARG:HB2	1:A:77:TRP:CZ3	2.50	0.47
1:C:19:THR:HA	1:C:403:TRP:CD1	2.49	0.47
1:C:291:VAL:HG21	1:C:338:PHE:HA	1.96	0.47
1:C:54:ASP:O	1:C:58:VAL:HG23	2.15	0.46
1:B:70:ASP:HB2	1:B:101:ASP:OD2	2.16	0.46
1:B:50:TRP:CE3	1:B:318:ALA:HB1	2.50	0.46
1:C:97:MET:SD	2:C:501:HEM:HBD2	2.56	0.46
1:B:19:THR:HA	1:B:403:TRP:CD1	2.51	0.46
1:B:98:ILE:HD13	2:B:501:HEM:HAD2	1.97	0.45
1:C:119:ARG:HG2	1:C:120:ASN:N	2.31	0.45
1:C:195:ARG:NH2	4:C:601:HOH:O	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HD11	1:B:180:ARG:HB2	1.99	0.45
1:C:291:VAL:O	1:C:329:ARG:NH2	2.46	0.45
1:B:80:LYS:HA	1:B:80:LYS:HD3	1.69	0.44
1:B:409:ILE:HA	1:B:409:ILE:HD13	1.85	0.44
1:B:54:ASP:HB3	1:B:57:LEU:HB2	2.00	0.44
1:B:309:LEU:HD12	1:B:314:ILE:HD11	1.99	0.44
1:C:210:VAL:HG13	1:C:225:LEU:HD21	2.00	0.44
1:C:409:ILE:HG13	1:C:410:VAL:HG13	1.98	0.44
1:B:139:LEU:HD21	1:B:150:VAL:HG11	2.00	0.43
1:B:264:PHE:CE1	1:B:268:ARG:HD3	2.53	0.43
1:A:377:ARG:O	1:A:418:GLU:HA	2.18	0.43
1:B:99:MET:HE2	1:B:99:MET:HB3	1.75	0.43
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.85	0.43
1:C:342:ARG:O	1:C:345:ARG:HD3	2.18	0.43
1:B:84:MET:HB2	3:B:502:VI4:C09	2.49	0.43
1:A:59:ARG:HG3	1:A:352:LEU:HD22	2.00	0.43
1:A:345:ARG:HG2	1:B:107:ARG:NH2	2.33	0.43
1:A:372:ARG:HH11	1:A:372:ARG:HG2	1.84	0.43
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.48	0.43
1:A:71:VAL:O	1:A:79:ARG:NH2	2.52	0.43
1:B:167:GLU:HG3	1:B:168:MET:N	2.34	0.43
1:C:41:ARG:HD2	1:C:50:TRP:NE1	2.34	0.43
1:A:51:VAL:HG12	1:A:321:GLN:HB2	2.00	0.42
1:C:309:LEU:HD23	1:C:309:LEU:HA	1.88	0.42
1:A:152:VAL:HG12	1:A:411:LEU:O	2.19	0.42
1:C:136:LEU:CD2	1:C:156:TYR:CE1	3.02	0.42
1:A:358:ILE:HG22	2:A:501:HEM:C2D	2.53	0.42
1:C:88:GLN:HG3	1:C:99:MET:CE	2.48	0.42
1:A:156:TYR:CE1	1:A:160:ILE:HD11	2.55	0.42
1:A:167:GLU:HG3	1:A:217:ARG:HH12	1.84	0.42
1:C:191:ASP:OD2	4:C:604:HOH:O	2.22	0.42
1:A:96:THR:HG22	1:A:99:MET:HB2	2.01	0.42
1:B:58:VAL:O	1:B:62:LEU:HD23	2.20	0.42
1:C:26:CYS:SG	1:C:30:LEU:HD21	2.60	0.42
1:A:305:GLU:HA	1:A:316:GLU:HG3	2.02	0.42
1:A:364:ARG:NH1	4:A:607:HOH:O	2.33	0.41
1:B:161:PRO:O	1:B:165:ILE:HG22	2.19	0.41
1:B:206:VAL:O	1:B:210:VAL:HG13	2.20	0.41
1:C:408:MET:HE3	1:C:408:MET:HB3	1.79	0.41
1:B:409:ILE:HG22	1:B:410:VAL:HG23	2.03	0.41
1:C:281:ILE:HD13	1:C:372:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LEU:HD23	1:C:156:TYR:CE1	2.56	0.41
1:A:15:ALA:HB2	1:A:36:VAL:HG21	2.03	0.41
1:A:132:VAL:HG22	1:A:160:ILE:HD13	2.03	0.41
1:A:169:LEU:HA	1:A:220:VAL:HB	2.03	0.41
1:B:260:SER:HB3	1:B:408:MET:HE2	2.03	0.41
1:C:172:PRO:HD3	1:C:216:LEU:HD23	2.03	0.41
1:A:259:ILE:HG12	1:A:367:ALA:HA	2.03	0.41
1:B:26:CYS:O	1:B:30:LEU:HG	2.21	0.41
1:B:357:CYS:HB2	2:B:501:HEM:NA	2.37	0.40
1:A:342:ARG:O	1:A:345:ARG:HD3	2.22	0.40
1:A:124:TRP:O	1:A:128:VAL:HG23	2.21	0.40
1:C:158:HIS:O	1:C:180:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	382/440 (87%)	367 (96%)	14 (4%)	1 (0%)	36	44
1	B	377/440 (86%)	362 (96%)	14 (4%)	1 (0%)	36	44
1	C	367/440 (83%)	348 (95%)	18 (5%)	1 (0%)	36	44
All	All	1126/1320 (85%)	1077 (96%)	46 (4%)	3 (0%)	36	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	PRO
1	B	298	PRO
1	C	298	PRO

5.3.2 Protein sidechains ⓘ

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	298/357 (84%)	291 (98%)	7 (2%)	44	60
1	B	290/357 (81%)	283 (98%)	7 (2%)	43	59
1	C	288/357 (81%)	280 (97%)	8 (3%)	38	53
All	All	876/1071 (82%)	854 (98%)	22 (2%)	42	58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	124	TRP
1	A	212	ASP
1	A	218	GLU
1	A	307	ILE
1	A	309	LEU
1	A	415	VAL
1	B	127	ARG
1	B	129	GLU
1	B	131	LYS
1	B	150	VAL
1	B	159	ARG
1	B	210	VAL
1	B	257	SER
1	C	119	ARG
1	C	129	GLU
1	C	142	SER
1	C	165	ILE
1	C	277	THR
1	C	281	ILE
1	C	285	VAL
1	C	320	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	HIS
1	C	48	HIS
1	C	158	HIS
1	C	343	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	VI4	A	502	-	39,39,39	2.89	12 (30%)	51,61,61	1.95	9 (17%)
2	HEM	B	501	-	50,50,50	2.82	25 (50%)	66,82,82	2.14	23 (34%)
2	HEM	C	501	-	50,50,50	2.64	23 (46%)	66,82,82	2.19	23 (34%)
3	VI4	B	503	-	39,39,39	2.92	12 (30%)	51,61,61	2.03	10 (19%)
3	VI4	C	502	-	39,39,39	2.86	11 (28%)	51,61,61	1.95	9 (17%)
3	VI4	B	502	-	39,39,39	2.85	11 (28%)	51,61,61	1.80	6 (11%)
2	HEM	A	501	1	50,50,50	2.45	21 (42%)	66,82,82	1.87	17 (25%)
3	VI4	A	503	1	39,39,39	2.90	10 (25%)	51,61,61	2.01	7 (13%)
3	VI4	B	504	-	39,39,39	3.01	11 (28%)	51,61,61	2.20	10 (19%)

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	VI4	A	502	-	-	0/4/29/29	0/7/7/7
2	HEM	B	501	-	-	0/14/54/54	-
2	HEM	C	501	-	-	1/14/54/54	-
3	VI4	B	503	-	-	2/4/29/29	0/7/7/7
3	VI4	C	502	-	-	0/4/29/29	0/7/7/7
3	VI4	B	502	-	-	0/4/29/29	0/7/7/7
2	HEM	A	501	1	-	2/14/54/54	-
3	VI4	A	503	1	-	0/4/29/29	0/7/7/7
3	VI4	B	504	-	-	2/4/29/29	0/7/7/7

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	504	VI4	C30-N29	13.38	1.46	1.35
3	C	502	VI4	C30-N29	13.26	1.45	1.35
3	B	503	VI4	C30-N29	13.22	1.45	1.35
3	A	503	VI4	C30-N29	13.20	1.45	1.35
3	A	502	VI4	C30-N29	13.10	1.45	1.35
3	B	502	VI4	C30-N29	13.10	1.45	1.35
3	B	504	VI4	O07-C06	7.87	1.52	1.42
3	B	503	VI4	O07-C06	6.98	1.50	1.42
3	A	503	VI4	O07-C06	6.60	1.50	1.42
2	B	501	HEM	C1B-NB	-6.48	1.29	1.40
3	A	502	VI4	O07-C06	6.34	1.50	1.42
3	B	502	VI4	O07-C06	6.26	1.50	1.42
2	C	501	HEM	C1B-NB	-6.25	1.29	1.40
2	B	501	HEM	C4D-ND	-6.09	1.29	1.40
3	C	502	VI4	O07-C06	5.84	1.49	1.42
2	C	501	HEM	FE-ND	-5.64	1.77	1.94
2	A	501	HEM	C4D-ND	-5.38	1.31	1.40
2	C	501	HEM	C1C-C2C	-5.31	1.34	1.45
2	C	501	HEM	C4B-NB	-5.30	1.27	1.38
2	A	501	HEM	C1B-NB	-5.21	1.31	1.40
3	A	502	VI4	C28-C17	5.09	1.54	1.50
2	B	501	HEM	C3C-C4C	-5.06	1.37	1.46
2	B	501	HEM	C1A-C2A	-4.96	1.34	1.44
3	A	503	VI4	C28-C17	4.96	1.54	1.50
2	A	501	HEM	C3C-C4C	-4.94	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	504	VI4	C28-C17	4.91	1.54	1.50
3	C	502	VI4	C28-C17	4.82	1.54	1.50
2	B	501	HEM	C4A-NA	-4.79	1.30	1.39
3	B	502	VI4	C28-C17	4.78	1.54	1.50
2	A	501	HEM	C1C-C2C	-4.71	1.36	1.45
3	B	503	VI4	C28-C17	4.71	1.54	1.50
2	C	501	HEM	C4D-ND	-4.69	1.32	1.40
2	B	501	HEM	C1C-C2C	-4.62	1.36	1.45
2	B	501	HEM	C4C-NC	-4.50	1.31	1.39
2	B	501	HEM	C1D-ND	-4.21	1.30	1.38
2	C	501	HEM	C1C-NC	-4.21	1.31	1.39
2	A	501	HEM	C4B-NB	-4.08	1.30	1.38
2	B	501	HEM	C4B-NB	-4.04	1.30	1.38
2	B	501	HEM	FE-ND	-3.98	1.82	1.94
2	C	501	HEM	C1D-ND	-3.89	1.30	1.38
2	C	501	HEM	C3C-C4C	-3.84	1.39	1.46
2	C	501	HEM	C1A-C2A	-3.84	1.37	1.44
2	C	501	HEM	C4A-NA	-3.84	1.32	1.39
2	B	501	HEM	C1A-NA	-3.76	1.32	1.39
2	A	501	HEM	C1A-C2A	-3.76	1.37	1.44
2	A	501	HEM	FE-NB	3.72	2.06	1.94
2	A	501	HEM	FE-ND	-3.67	1.83	1.94
2	C	501	HEM	C1B-C2B	-3.56	1.37	1.44
2	A	501	HEM	C4A-NA	-3.45	1.33	1.39
2	A	501	HEM	C3D-C2D	-3.42	1.29	1.36
3	B	504	VI4	C05-C04	-3.39	1.46	1.53
2	B	501	HEM	CHD-C4C	-3.34	1.31	1.38
2	C	501	HEM	C2A-C3A	-3.34	1.29	1.38
2	C	501	HEM	CHC-C1C	-3.30	1.32	1.38
2	A	501	HEM	C1B-C2B	-3.29	1.38	1.44
3	B	504	VI4	C15-C16	3.28	1.46	1.40
2	A	501	HEM	C1D-ND	-3.26	1.32	1.38
2	A	501	HEM	C1C-NC	-3.25	1.33	1.39
3	B	503	VI4	C05-C04	-3.23	1.46	1.53
2	A	501	HEM	O2D-CGD	-3.22	1.19	1.30
2	B	501	HEM	O2A-CGA	-3.17	1.20	1.30
2	C	501	HEM	C4C-NC	-3.11	1.33	1.39
3	A	503	VI4	C15-C16	3.11	1.46	1.40
2	B	501	HEM	CHA-C1A	-3.11	1.32	1.39
2	B	501	HEM	O2D-CGD	-3.09	1.20	1.30
3	A	502	VI4	C15-C16	3.07	1.45	1.40
2	B	501	HEM	FE-NB	3.05	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	VI4	C15-C16	3.04	1.45	1.40
2	B	501	HEM	C2A-C3A	-3.01	1.30	1.38
2	B	501	HEM	C1B-C2B	-2.99	1.38	1.44
2	A	501	HEM	C2A-C3A	-2.99	1.30	1.38
3	A	502	VI4	C05-C04	-2.94	1.47	1.53
2	B	501	HEM	C3D-C2D	-2.93	1.30	1.36
2	B	501	HEM	C1C-NC	-2.93	1.34	1.39
2	A	501	HEM	C4C-NC	-2.91	1.34	1.39
3	B	502	VI4	C05-C04	-2.90	1.47	1.53
3	C	502	VI4	C15-C16	2.83	1.45	1.40
2	C	501	HEM	C3B-C2B	-2.79	1.31	1.37
2	C	501	HEM	C3D-C2D	-2.78	1.30	1.36
3	C	502	VI4	C05-C04	-2.76	1.47	1.53
3	B	503	VI4	C26-C27	2.75	1.49	1.41
3	A	503	VI4	C05-C04	-2.71	1.47	1.53
2	A	501	HEM	O2A-CGA	-2.69	1.21	1.30
3	A	503	VI4	C26-C27	2.65	1.48	1.41
3	B	502	VI4	C18-C17	2.63	1.45	1.40
2	B	501	HEM	C3B-C2B	-2.61	1.32	1.37
3	B	504	VI4	C03-C04	-2.60	1.48	1.53
3	B	502	VI4	C06-N08	-2.58	1.43	1.46
3	A	503	VI4	C19-C24	-2.56	1.37	1.41
2	B	501	HEM	C4A-C3A	-2.54	1.37	1.43
3	B	504	VI4	C10-C09	2.53	1.43	1.39
2	A	501	HEM	CHA-C1A	-2.52	1.33	1.39
3	A	502	VI4	C06-N08	-2.51	1.43	1.46
2	C	501	HEM	CHA-C1A	-2.49	1.33	1.39
3	B	503	VI4	C19-C24	-2.49	1.37	1.41
3	C	502	VI4	C19-C24	-2.49	1.37	1.41
3	A	502	VI4	C18-C17	2.49	1.45	1.40
3	C	502	VI4	C06-N08	-2.48	1.43	1.46
3	B	504	VI4	C26-C27	2.48	1.48	1.41
3	B	503	VI4	C10-C09	2.47	1.43	1.39
2	A	501	HEM	C1A-NA	-2.47	1.35	1.39
3	B	504	VI4	C19-C24	-2.47	1.37	1.41
3	C	502	VI4	C26-C27	2.45	1.48	1.41
3	B	502	VI4	C26-C27	2.45	1.48	1.41
2	C	501	HEM	O2A-CGA	-2.45	1.22	1.30
2	A	501	HEM	C3B-C2B	-2.44	1.32	1.37
3	A	503	VI4	C18-C17	2.43	1.45	1.40
3	B	502	VI4	C15-C16	2.41	1.44	1.40
3	B	503	VI4	C18-C17	2.39	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	VI4	C14-C09	-2.37	1.37	1.41
3	C	502	VI4	C14-C09	-2.35	1.37	1.41
3	C	502	VI4	C18-C17	2.35	1.45	1.40
2	C	501	HEM	O2D-CGD	-2.35	1.22	1.30
3	A	502	VI4	C26-C27	2.33	1.47	1.41
2	B	501	HEM	FE-NA	-2.33	1.87	1.95
3	A	502	VI4	C14-C09	-2.32	1.37	1.41
3	B	502	VI4	C14-C09	-2.31	1.37	1.41
2	B	501	HEM	CHA-C4D	-2.30	1.33	1.38
3	A	502	VI4	C19-C24	-2.30	1.37	1.41
2	C	501	HEM	CHB-C4A	-2.29	1.34	1.39
3	B	504	VI4	C18-C17	2.29	1.45	1.40
3	A	502	VI4	C09-N08	-2.28	1.37	1.40
3	B	503	VI4	C03-C04	-2.28	1.48	1.53
3	B	502	VI4	C19-C24	-2.27	1.37	1.41
2	C	501	HEM	CHD-C4C	-2.25	1.34	1.38
2	C	501	HEM	CHC-C4B	-2.23	1.34	1.39
3	A	502	VI4	O31-C30	-2.15	1.18	1.23
3	B	503	VI4	C14-C09	-2.14	1.37	1.41
3	C	502	VI4	O31-C30	-2.12	1.19	1.23
2	C	501	HEM	FE-NB	2.08	2.01	1.94
2	A	501	HEM	C4A-C3A	-2.05	1.38	1.43
3	B	504	VI4	O31-C30	-2.05	1.19	1.23
3	B	502	VI4	O31-C30	-2.04	1.19	1.23
2	B	501	HEM	CHD-C1D	-2.03	1.34	1.39
3	A	503	VI4	C10-C09	2.01	1.43	1.39
3	B	503	VI4	O31-C30	-2.00	1.19	1.23

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	VI4	O07-C06-N08	7.31	114.16	105.85
3	A	503	VI4	O07-C06-N08	7.17	114.00	105.85
2	C	501	HEM	CHC-C4B-NB	6.60	131.59	124.42
3	A	502	VI4	C28-N29-C30	-6.57	107.53	113.85
3	A	502	VI4	O07-C06-N08	6.48	113.22	105.85
3	C	502	VI4	C28-N29-C30	-6.44	107.66	113.85
3	B	504	VI4	C28-N29-C30	-6.35	107.75	113.85
3	A	503	VI4	C28-N29-C30	-6.12	107.97	113.85
3	B	502	VI4	C28-N29-C30	-6.07	108.01	113.85
3	A	502	VI4	C17-C28-N29	6.06	108.05	101.77
3	C	502	VI4	O07-C06-N08	6.06	112.74	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	VI4	C28-N29-C30	-6.06	108.02	113.85
3	A	503	VI4	C17-C28-N29	6.00	107.98	101.77
3	B	502	VI4	C17-C28-N29	5.98	107.96	101.77
3	C	502	VI4	C17-C28-N29	5.96	107.94	101.77
2	B	501	HEM	CHC-C4B-NB	5.95	130.88	124.42
3	B	503	VI4	C17-C28-N29	5.89	107.86	101.77
2	C	501	HEM	CHD-C1D-ND	5.86	130.79	124.42
3	B	504	VI4	C17-C28-N29	5.86	107.84	101.77
2	B	501	HEM	C1B-NB-C4B	5.42	110.67	105.07
3	B	503	VI4	C02-O07-C06	5.37	120.48	112.90
2	A	501	HEM	CHC-C4B-NB	5.23	130.10	124.42
3	B	504	VI4	C02-O07-C06	5.18	120.21	112.90
3	B	502	VI4	O07-C06-N08	5.16	111.72	105.85
2	A	501	HEM	C1B-NB-C4B	5.15	110.39	105.07
2	B	501	HEM	CHD-C4C-NC	5.07	129.92	124.44
3	B	503	VI4	O07-C06-N08	4.81	111.32	105.85
3	B	503	VI4	O07-C02-C03	4.60	117.77	109.52
2	A	501	HEM	CHD-C4C-NC	4.30	129.09	124.44
2	C	501	HEM	C1B-NB-C4B	4.29	109.50	105.07
2	C	501	HEM	CAC-C3C-C4C	3.91	134.34	124.90
2	C	501	HEM	CHA-C4D-ND	3.83	129.10	124.37
2	B	501	HEM	CHD-C1D-C2D	-3.83	118.99	124.98
3	B	504	VI4	O07-C02-C03	3.82	116.38	109.52
2	A	501	HEM	CHB-C1B-NB	3.68	128.92	124.37
2	A	501	HEM	C4C-NC-C1C	3.68	108.95	105.35
3	B	504	VI4	C10-C09-C14	-3.66	117.33	121.60
2	C	501	HEM	C4C-CHD-C1D	-3.44	118.64	126.06
2	C	501	HEM	CHD-C1D-C2D	-3.35	119.74	124.98
3	A	503	VI4	C26-N25-C24	3.34	112.23	108.83
2	C	501	HEM	CHB-C1B-NB	3.34	128.49	124.37
2	A	501	HEM	CHD-C1D-ND	3.33	128.03	124.42
2	A	501	HEM	C4C-CHD-C1D	-3.21	119.14	126.06
2	B	501	HEM	O2A-CGA-O1A	-3.21	115.31	123.30
3	B	504	VI4	C01-C02-C03	-3.19	107.17	113.07
2	C	501	HEM	CMA-C3A-C4A	3.14	130.16	125.37
2	C	501	HEM	O2A-CGA-CBA	3.14	124.12	114.03
2	B	501	HEM	CHA-C1A-NA	3.14	129.62	123.85
3	B	503	VI4	C10-C09-C14	-3.13	117.94	121.60
2	C	501	HEM	O2D-CGD-O1D	-3.12	115.53	123.30
2	B	501	HEM	O2D-CGD-O1D	-3.07	115.65	123.30
2	B	501	HEM	O2A-CGA-CBA	3.06	123.86	114.03
2	B	501	HEM	CHD-C1D-ND	3.06	127.74	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	VI4	C18-C17-C16	-3.05	119.24	121.18
2	C	501	HEM	C1A-CHA-C4D	-3.05	119.11	126.34
2	A	501	HEM	CHA-C4D-ND	3.02	128.10	124.37
2	C	501	HEM	C4C-NC-C1C	3.01	108.29	105.35
3	A	503	VI4	O07-C02-C03	2.99	114.89	109.52
2	C	501	HEM	C4A-CHB-C1B	-2.99	119.26	126.34
2	B	501	HEM	CHB-C1B-NB	2.98	128.04	124.37
2	B	501	HEM	C4C-CHD-C1D	-2.93	119.75	126.06
3	B	504	VI4	C18-C17-C16	-2.88	119.35	121.18
2	C	501	HEM	CAC-C3C-C2C	-2.84	119.24	128.60
2	B	501	HEM	C2D-C1D-ND	2.82	113.26	109.88
3	A	503	VI4	C09-N08-C06	-2.82	120.42	126.83
3	C	502	VI4	C05-C04-C03	2.77	114.22	110.04
2	A	501	HEM	O2A-CGA-O1A	-2.75	116.44	123.30
2	C	501	HEM	CHA-C4D-C3D	-2.72	120.22	125.33
3	A	502	VI4	C09-N08-C06	-2.72	120.66	126.83
3	B	503	VI4	C26-N25-C24	2.71	111.58	108.83
2	B	501	HEM	C1A-CHA-C4D	-2.71	119.92	126.34
3	B	504	VI4	C10-C09-N08	2.70	133.58	129.55
3	C	502	VI4	C18-C17-C16	-2.69	119.47	121.18
2	A	501	HEM	O2A-CGA-CBA	2.69	122.67	114.03
2	B	501	HEM	C1C-CHC-C4B	-2.68	120.27	126.06
2	A	501	HEM	C4A-CHB-C1B	-2.67	120.01	126.34
2	B	501	HEM	CHA-C1A-C2A	-2.66	119.54	125.36
2	C	501	HEM	CAA-C2A-C1A	2.62	130.06	124.89
2	C	501	HEM	O2A-CGA-O1A	-2.59	116.85	123.30
2	B	501	HEM	C3B-C2B-C1B	2.58	108.40	106.49
2	B	501	HEM	O2D-CGD-CBD	2.58	122.33	114.03
2	B	501	HEM	C4C-NC-C1C	2.58	107.87	105.35
3	B	502	VI4	C05-C06-N08	-2.57	106.57	113.21
2	A	501	HEM	O2D-CGD-O1D	-2.57	116.90	123.30
2	A	501	HEM	CMD-C2D-C1D	2.54	128.91	125.04
3	C	502	VI4	C23-C24-N25	2.51	132.87	129.07
3	C	502	VI4	C05-C06-N08	-2.50	106.75	113.21
2	C	501	HEM	O2D-CGD-CBD	2.50	122.06	114.03
2	A	501	HEM	CHD-C1D-C2D	-2.48	121.10	124.98
2	B	501	HEM	CAD-C3D-C4D	2.46	128.95	124.66
3	B	503	VI4	C10-C09-N08	2.43	133.17	129.55
3	C	502	VI4	C09-N08-C06	-2.42	121.33	126.83
2	A	501	HEM	CAA-C2A-C1A	2.38	129.58	124.89
3	A	502	VI4	C05-C06-N08	-2.38	107.06	113.21
3	B	503	VI4	C01-C02-C03	-2.37	108.69	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	VI4	C23-C24-N25	2.33	132.60	129.07
2	C	501	HEM	CAD-C3D-C4D	2.31	128.69	124.66
3	C	502	VI4	C23-C24-C19	-2.31	119.16	121.70
3	B	502	VI4	C23-C24-N25	2.29	132.54	129.07
3	B	504	VI4	C26-N25-C24	2.28	111.15	108.83
2	C	501	HEM	CHC-C4B-C3B	-2.27	120.24	125.13
3	A	503	VI4	C05-C04-C03	2.26	113.45	110.04
3	B	503	VI4	C18-C17-C16	-2.20	119.78	121.18
3	B	502	VI4	C18-C17-C16	-2.16	119.81	121.18
2	A	501	HEM	CAD-C3D-C4D	2.15	128.41	124.66
2	C	501	HEM	CMB-C2B-C1B	2.14	128.29	125.04
2	B	501	HEM	CHD-C4C-C3C	-2.13	121.61	125.26
2	B	501	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
3	A	502	VI4	C01-C02-C03	-2.10	109.19	113.07
2	A	501	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
2	B	501	HEM	C4A-CHB-C1B	-2.05	121.47	126.34
2	B	501	HEM	C1D-C2D-C3D	-2.01	104.85	106.96
3	A	502	VI4	C23-C24-C19	-2.00	119.50	121.70
2	C	501	HEM	C4D-ND-C1D	2.00	107.14	105.07

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	VI4	O07-C06-N08-C09
3	B	503	VI4	O07-C06-N08-C27
3	B	504	VI4	O07-C06-N08-C27
2	A	501	HEM	C2B-C3B-CAB-CBB
2	C	501	HEM	C4C-C3C-CAC-CBC
3	B	504	VI4	O07-C06-N08-C09
2	A	501	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	7	0
2	C	501	HEM	6	0
3	B	503	VI4	1	0
3	B	502	VI4	1	0
2	A	501	HEM	3	0

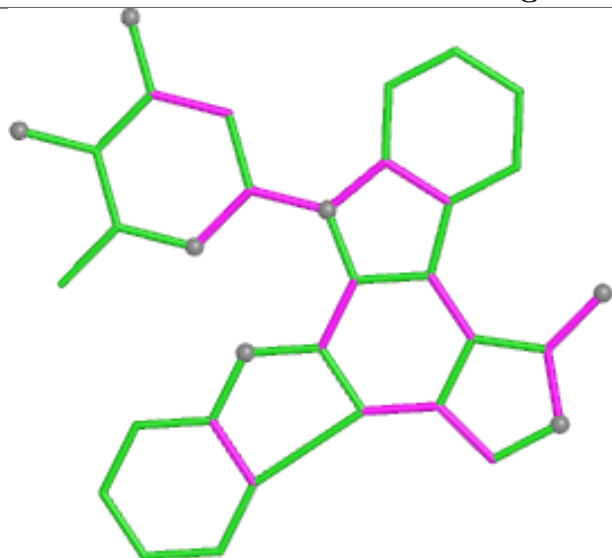
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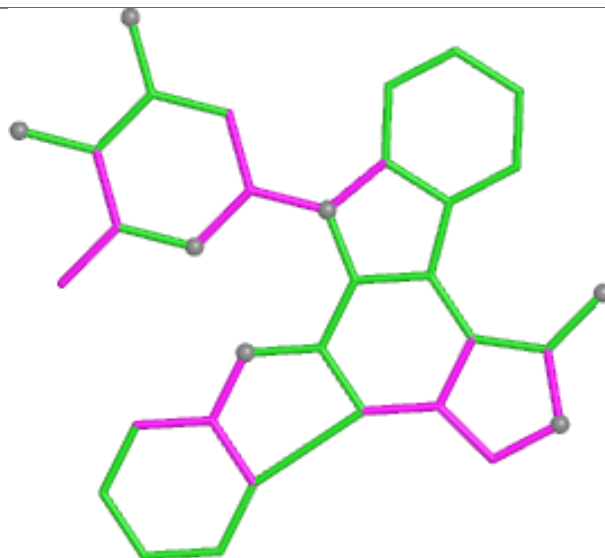
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	VI4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

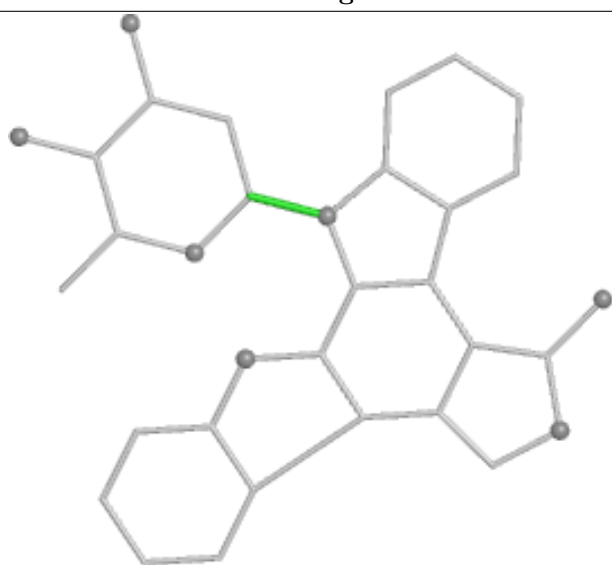
Ligand VI4 A 502



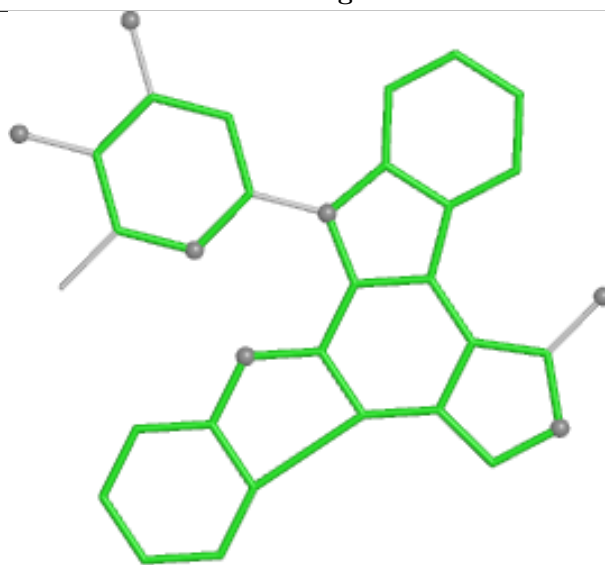
Bond lengths



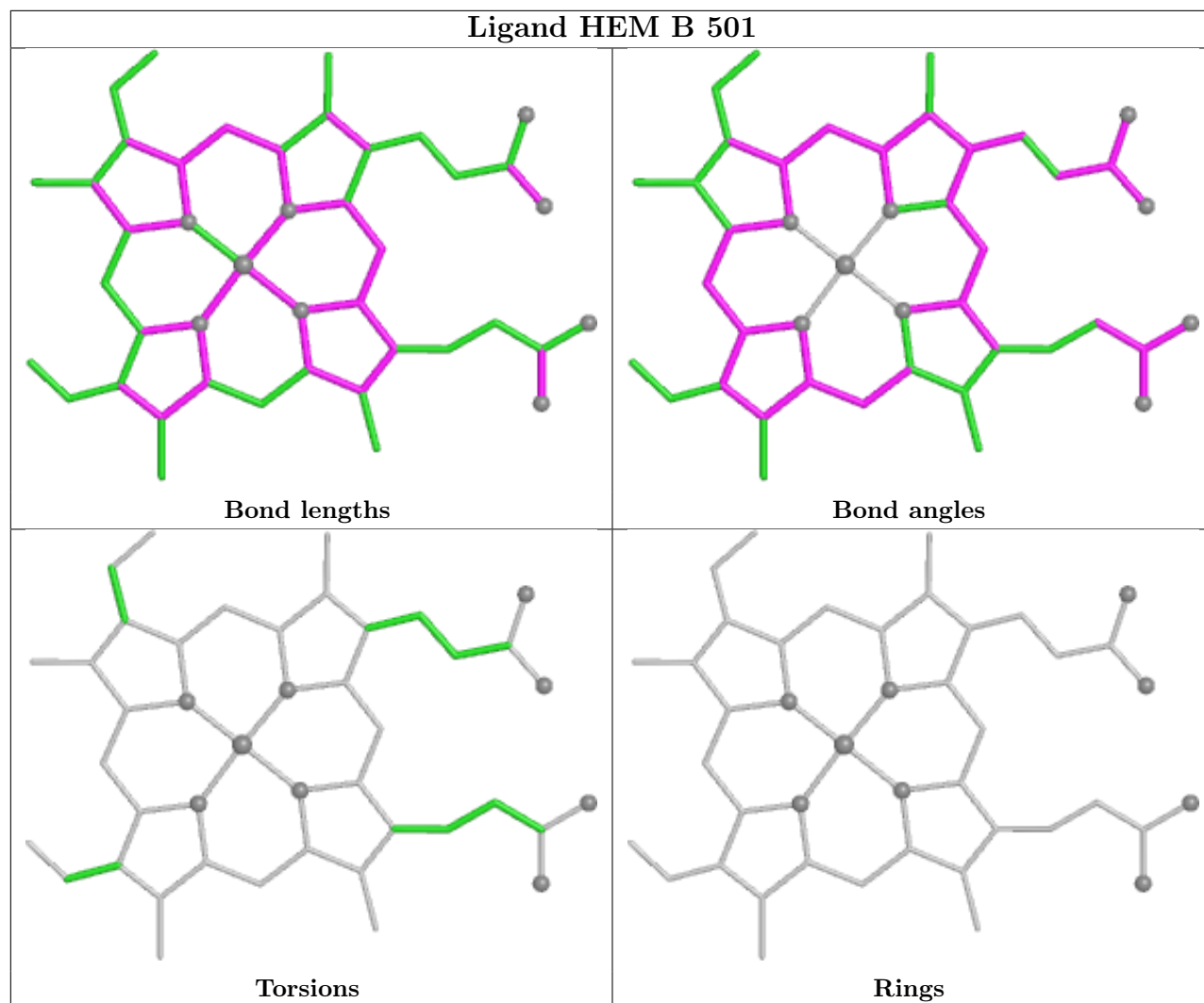
Bond angles

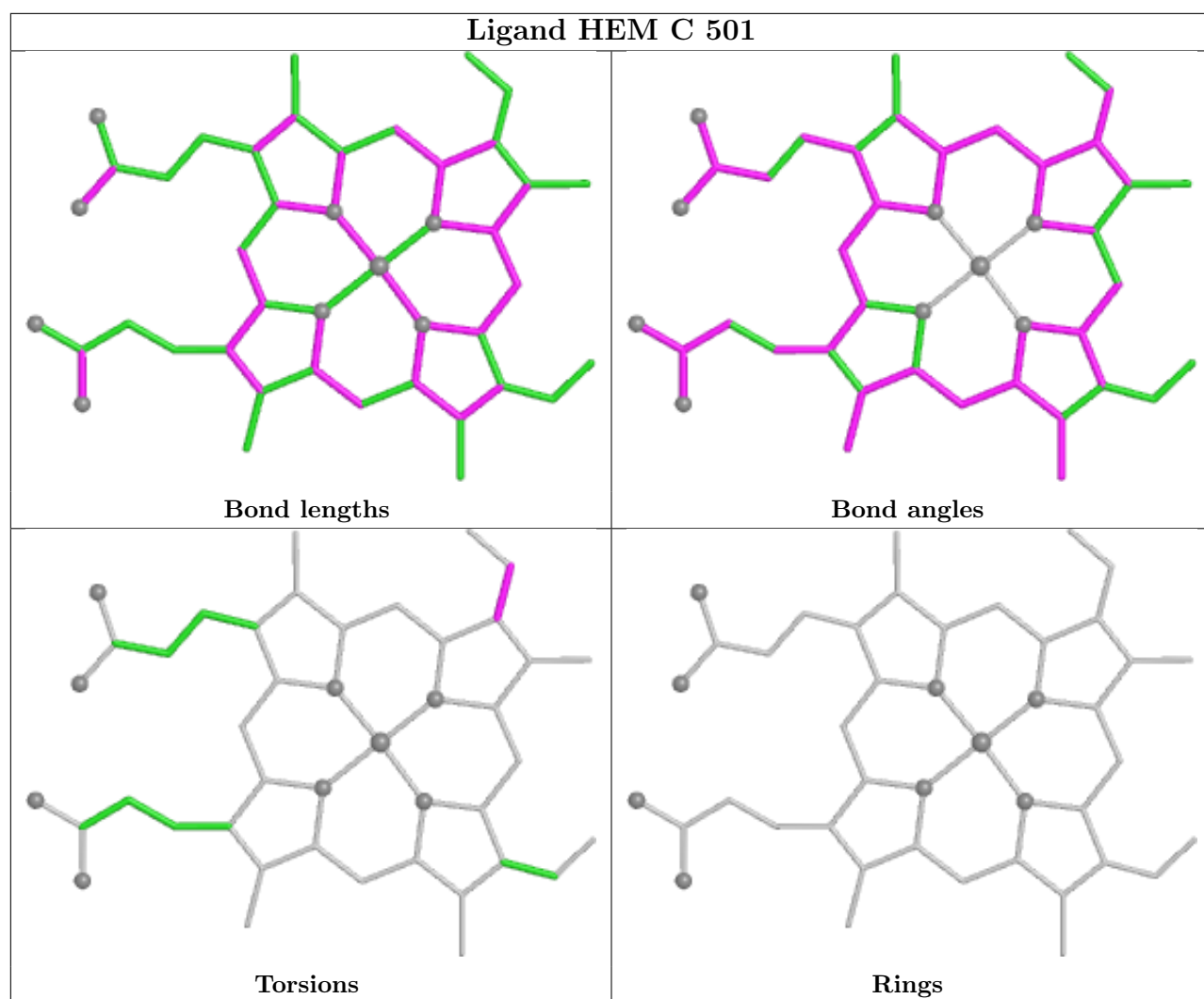


Torsions

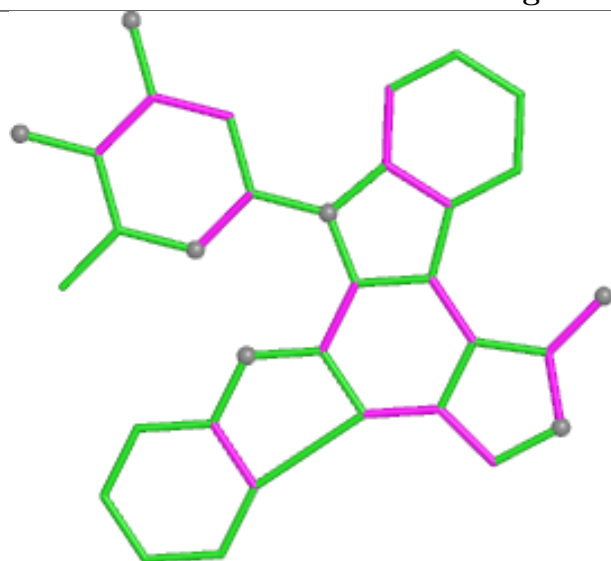


Rings

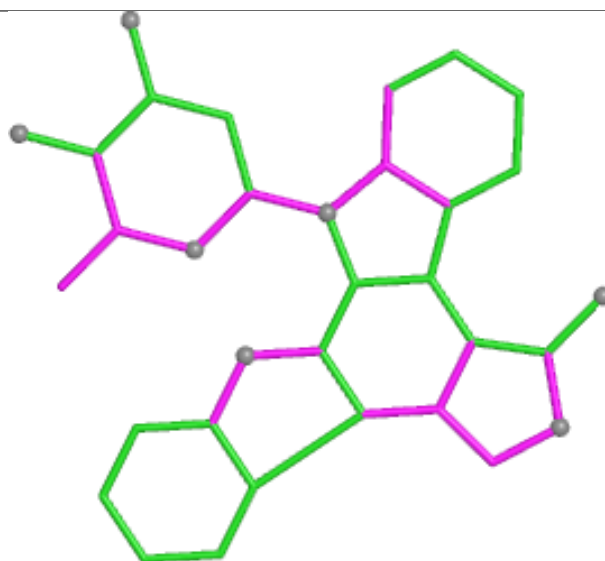




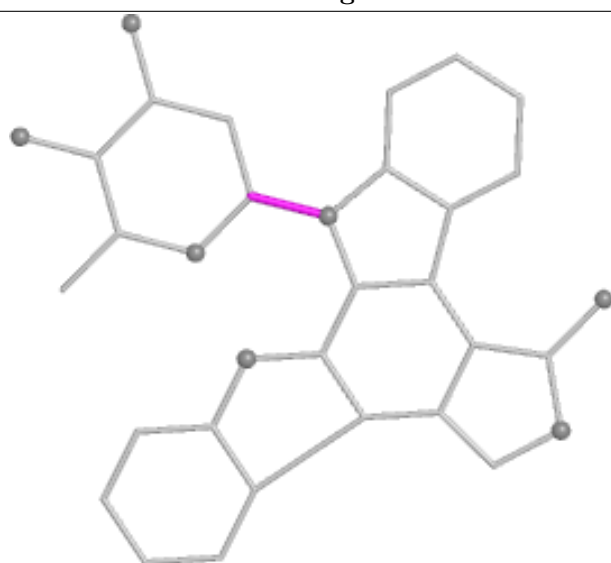
Ligand VI4 B 503



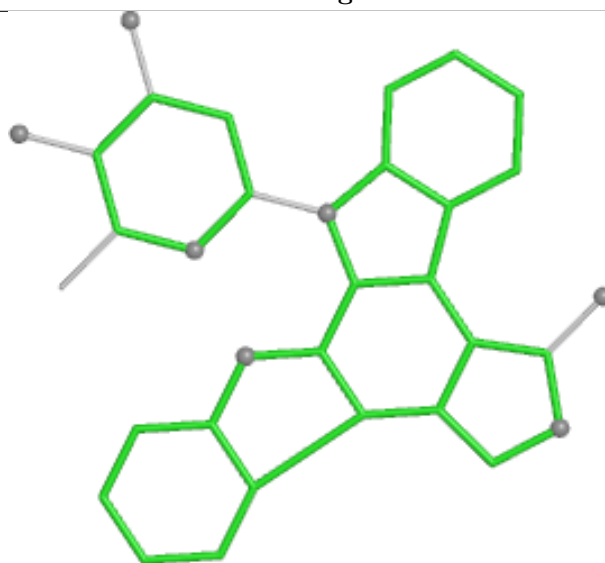
Bond lengths



Bond angles

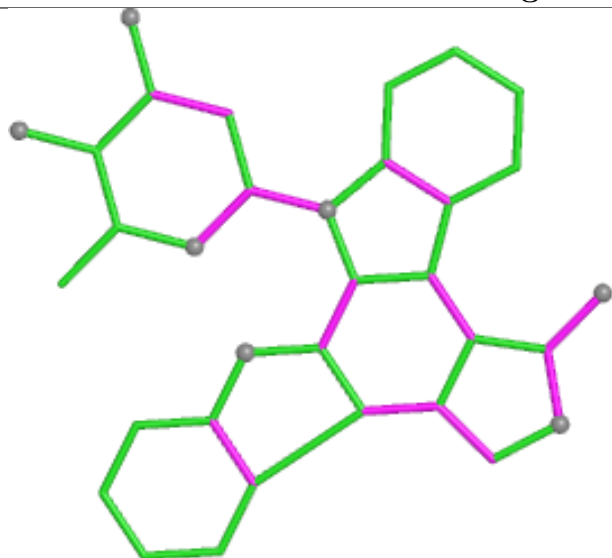


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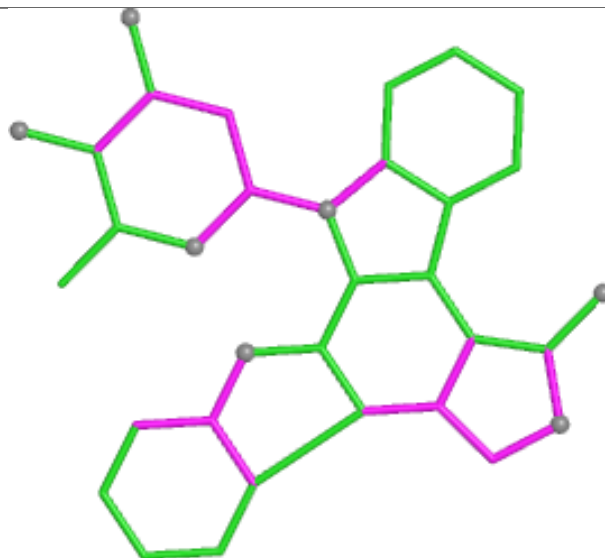


Rings

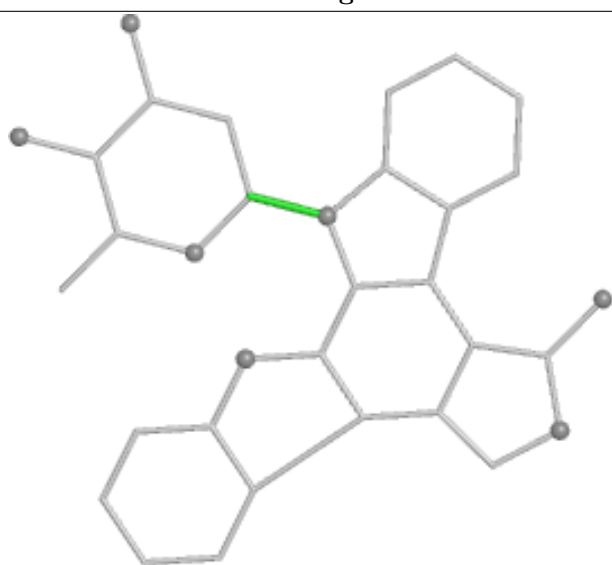
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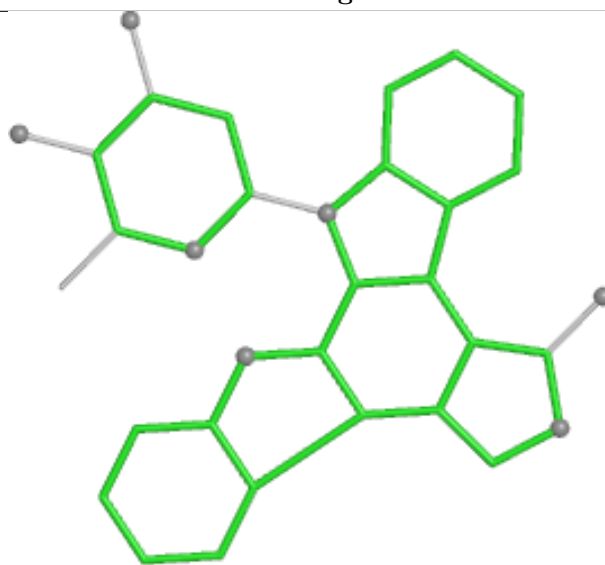
Bond lengths



Bond angles

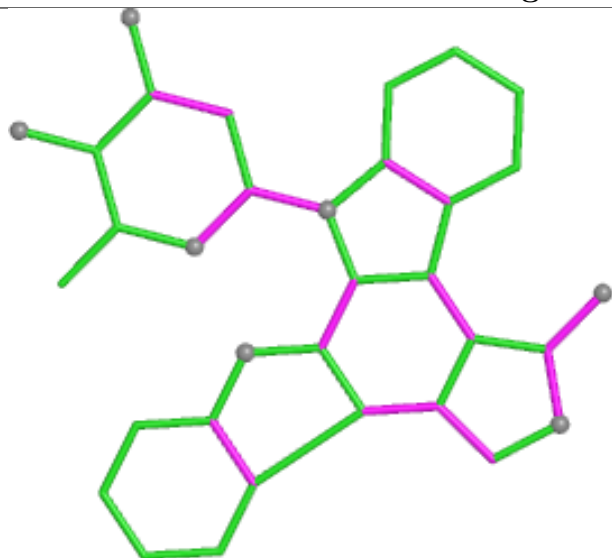


Torsions

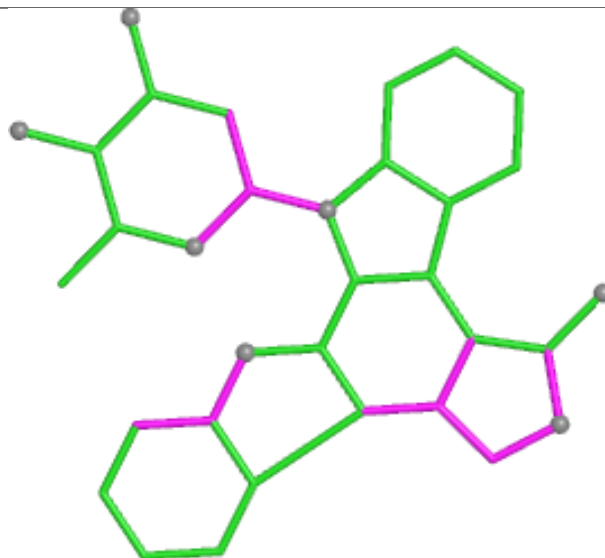


Rings

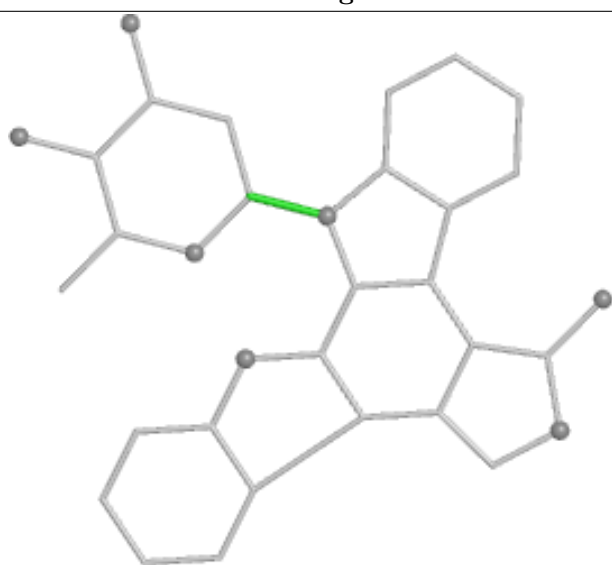
Ligand VI4 B 502



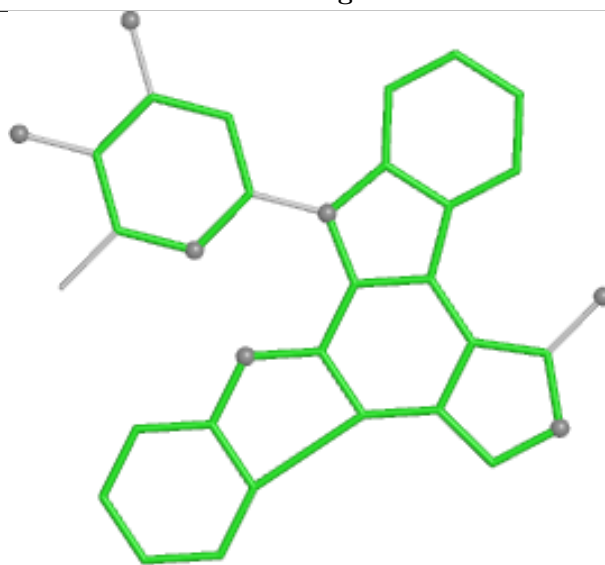
Bond lengths



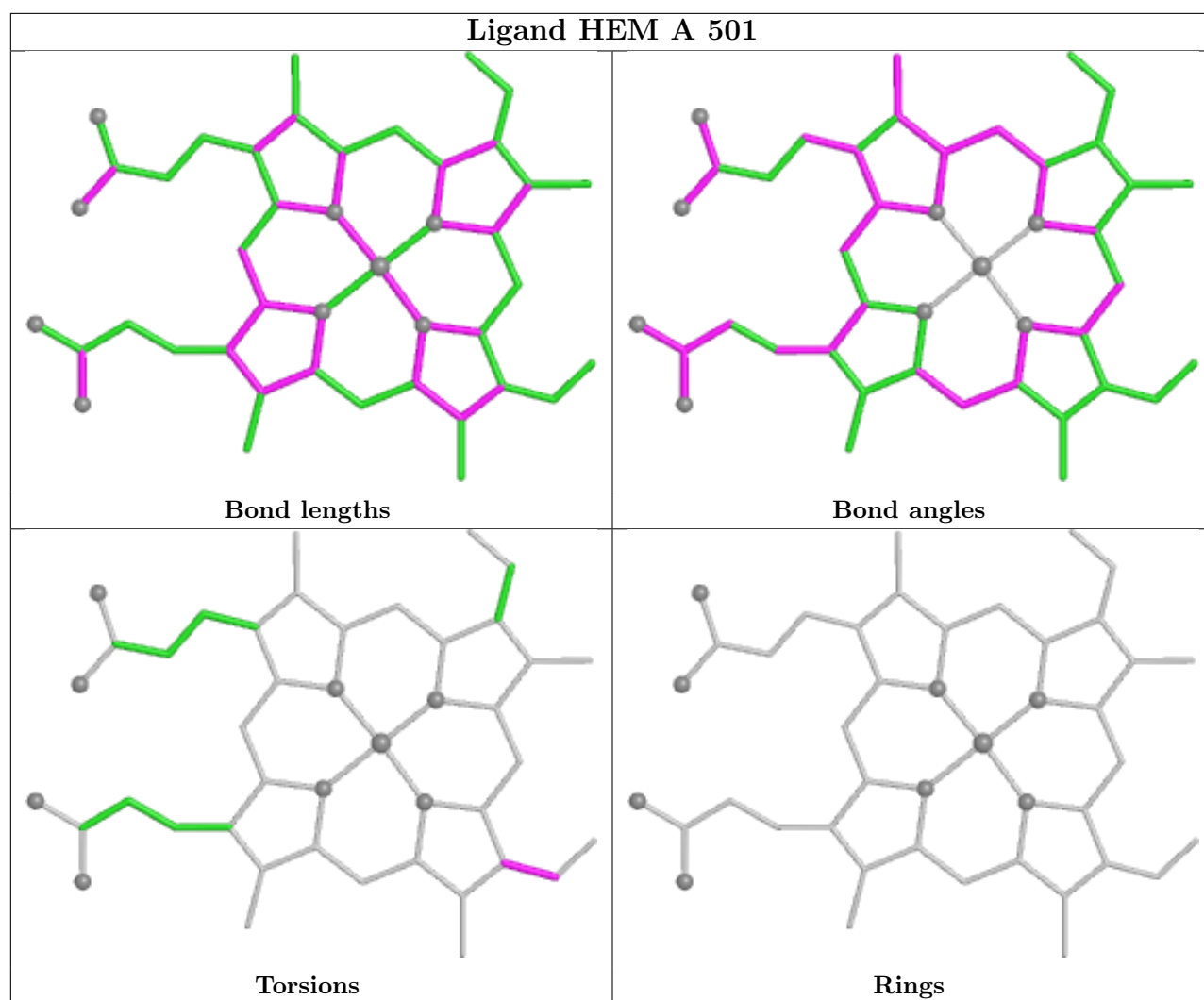
Bond angles



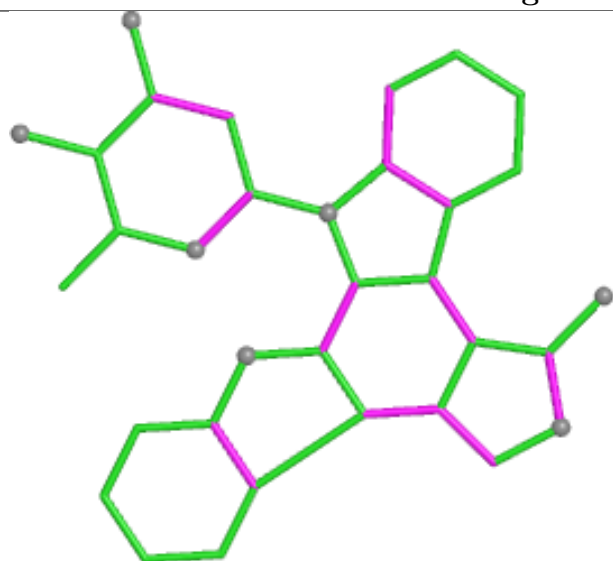
Torsions



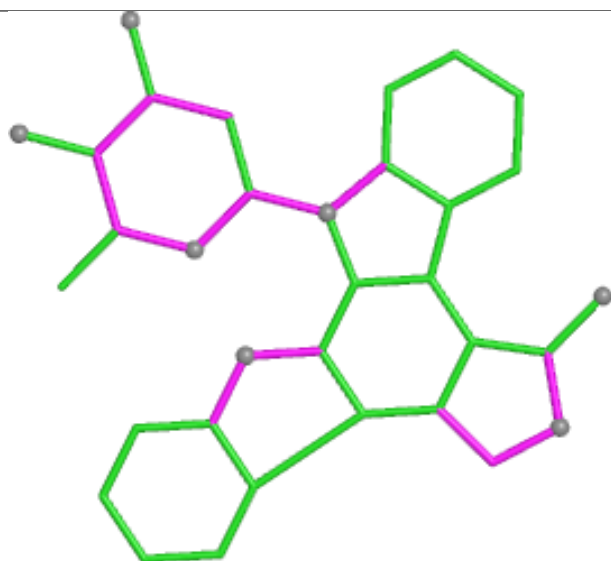
Rings



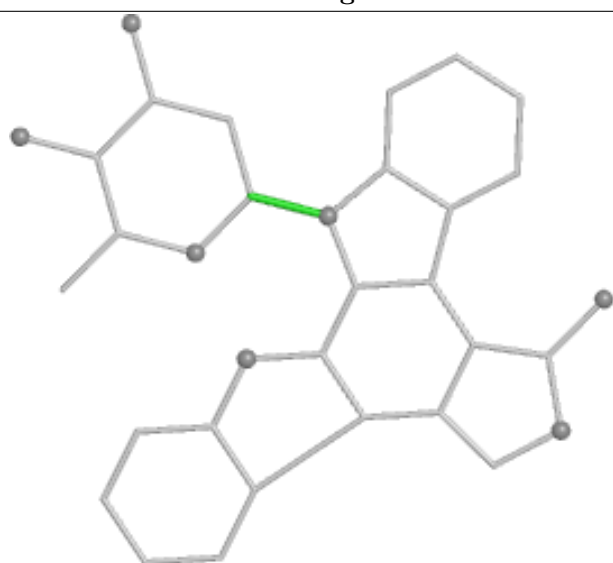
Ligand VI4 A 503



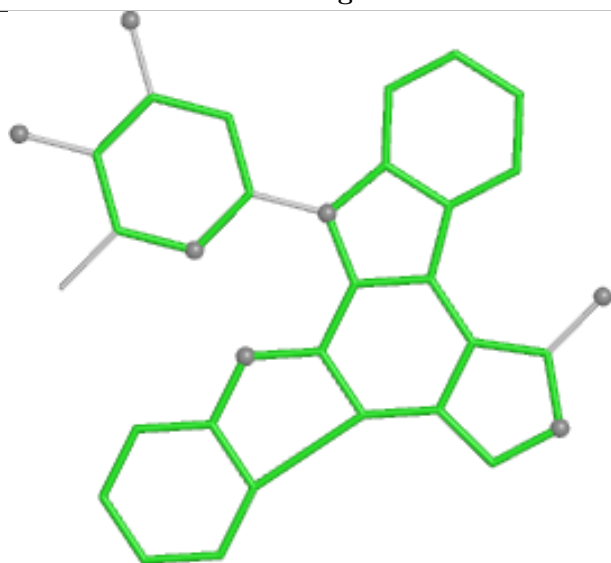
Bond lengths



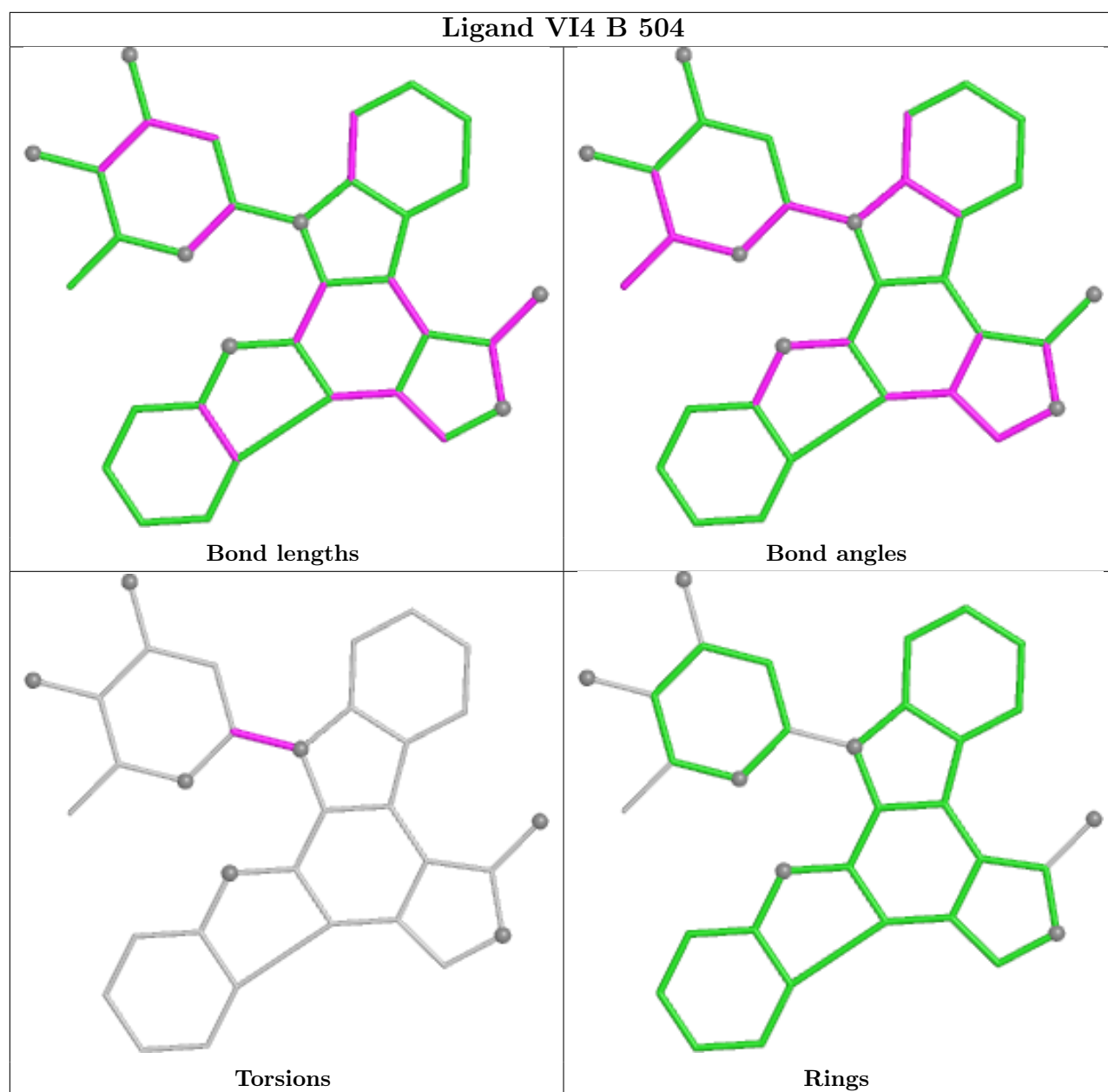
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/440 (88%)	-0.62	0 100 100	46, 73, 118, 156	0
1	B	387/440 (87%)	-0.53	0 100 100	49, 74, 113, 174	0
1	C	381/440 (86%)	-0.53	1 (0%) 90 90	46, 87, 125, 167	0
All	All	1158/1320 (87%)	-0.56	1 (0%) 92 92	46, 78, 120, 174	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	ASP	2.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	VI4	A	503	33/33	0.98	0.07	85,112,126,126	0
3	VI4	B	503	33/33	0.98	0.09	91,117,136,138	0

Continued on next page...

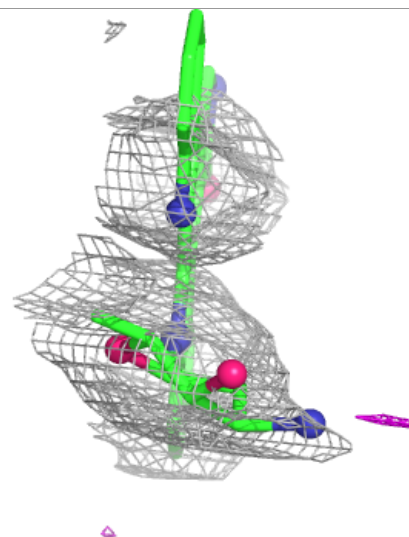
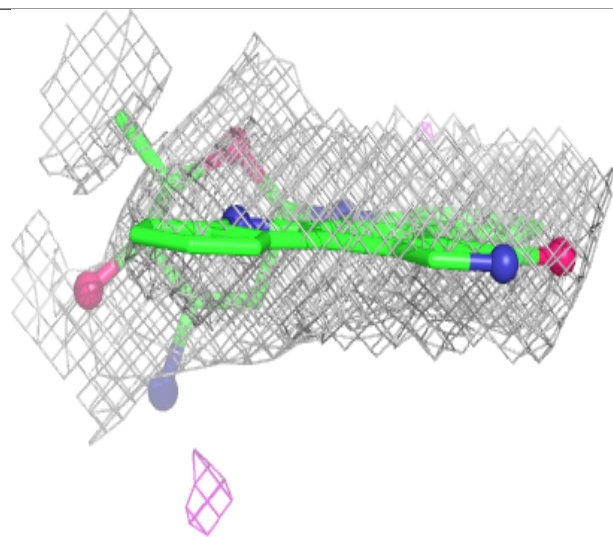
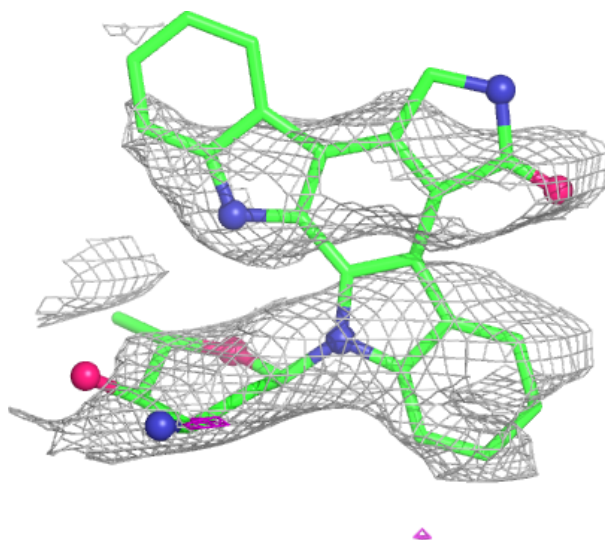
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VI4	B	504	33/33	0.98	0.07	84,108,115,130	0
3	VI4	B	502	33/33	0.99	0.05	52,63,71,72	0
3	VI4	A	502	33/33	0.99	0.05	39,49,57,61	0
2	HEM	A	501	43/43	0.99	0.05	36,47,57,62	0
3	VI4	C	502	33/33	0.99	0.06	48,54,67,67	0
2	HEM	B	501	43/43	1.00	0.04	42,51,59,63	0
2	HEM	C	501	43/43	1.00	0.04	40,50,66,70	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.

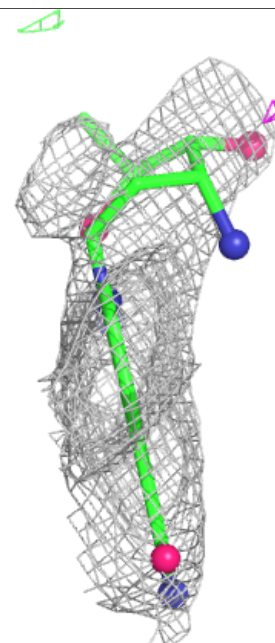
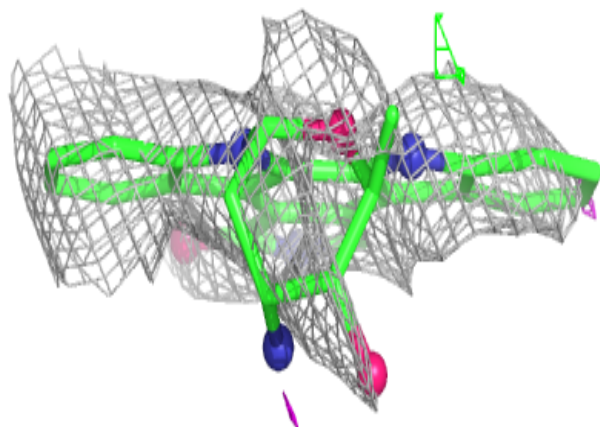
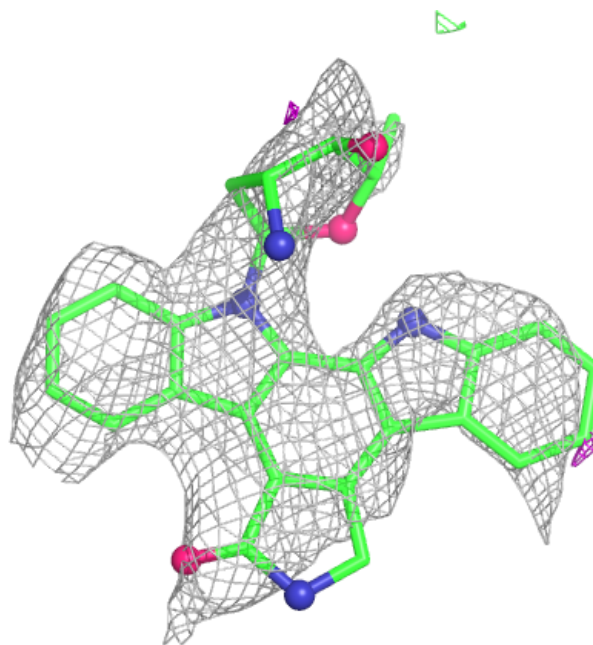
Electron density around VI4 A 503:

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



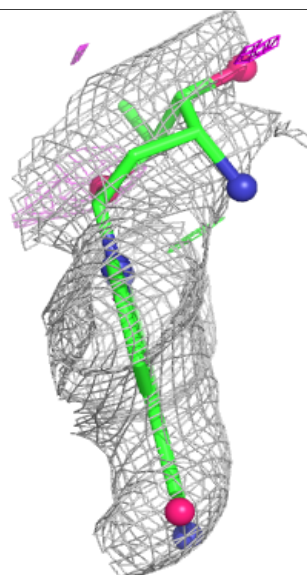
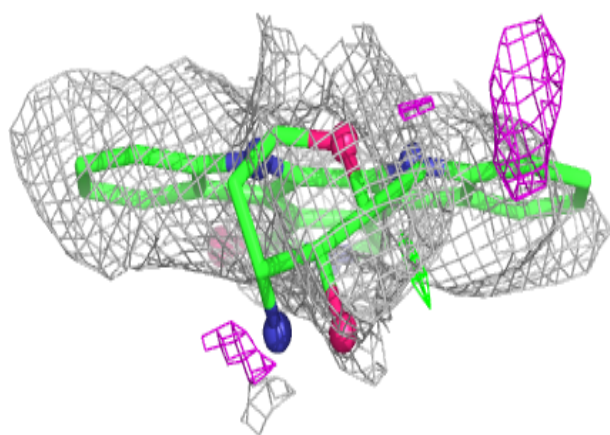
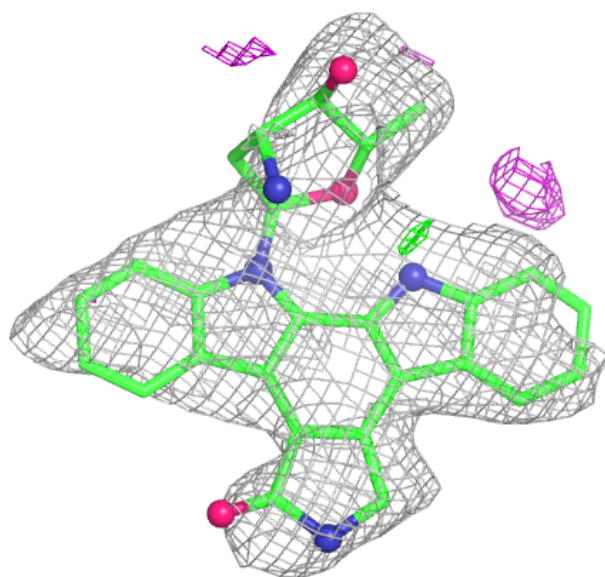
Electron density around VI4 B 503:

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



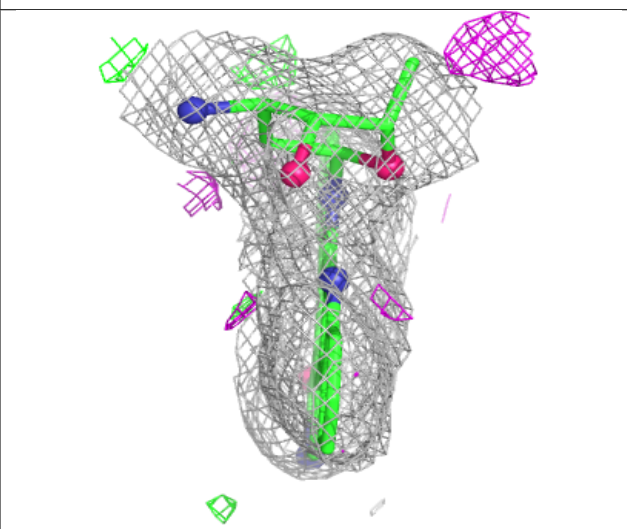
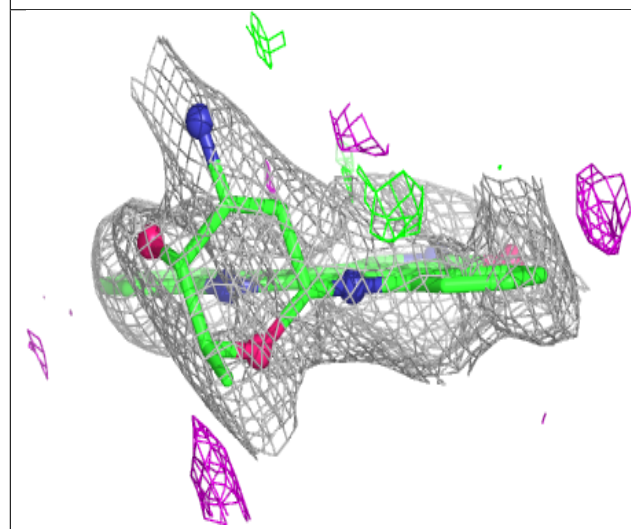
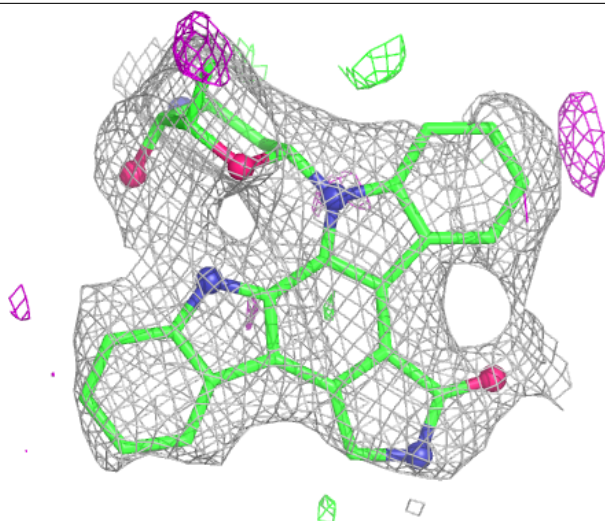
Electron density around VI4 B 504:

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and green (positive)



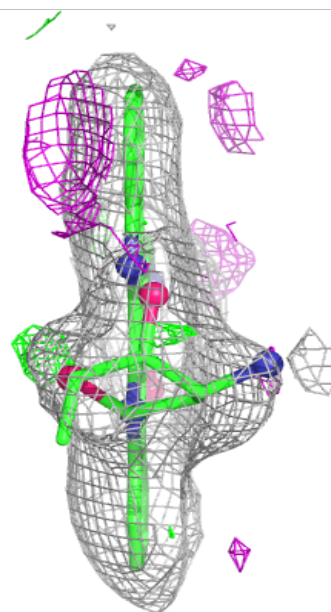
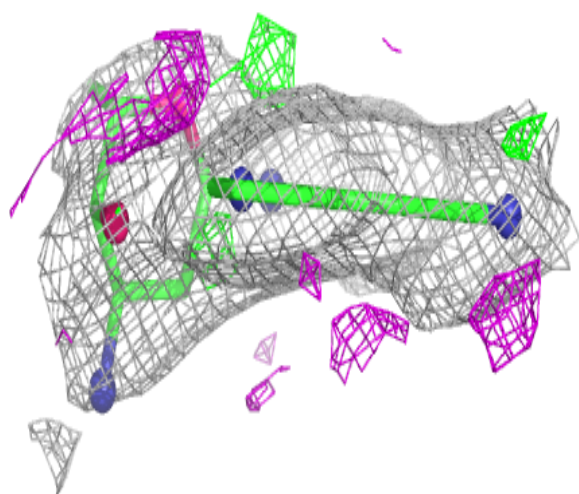
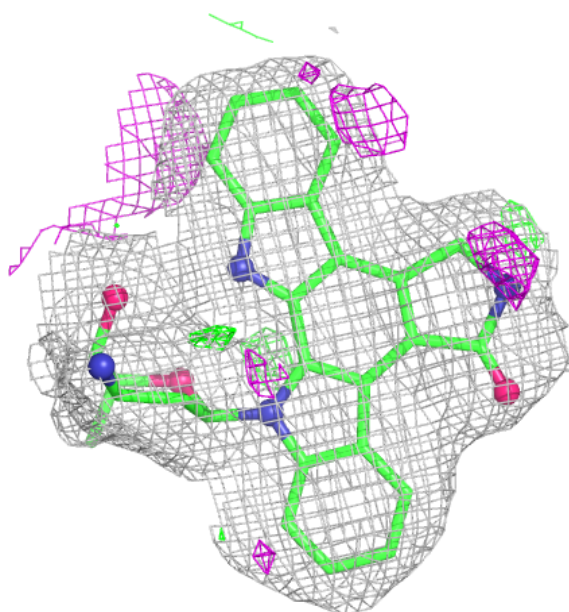
Electron density around VI4 B 502:

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



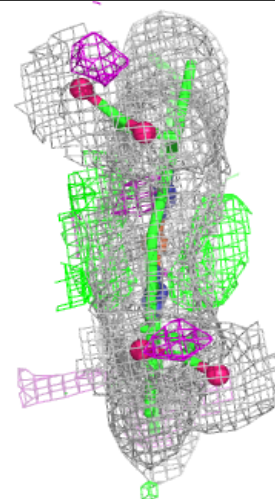
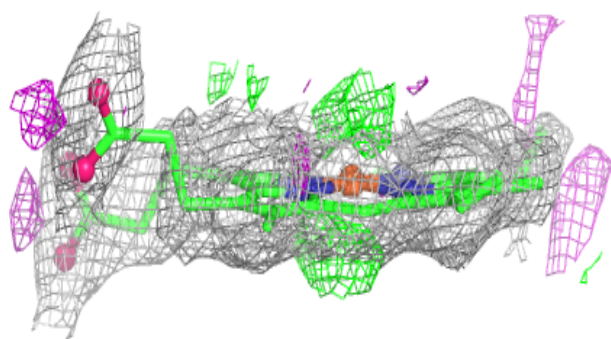
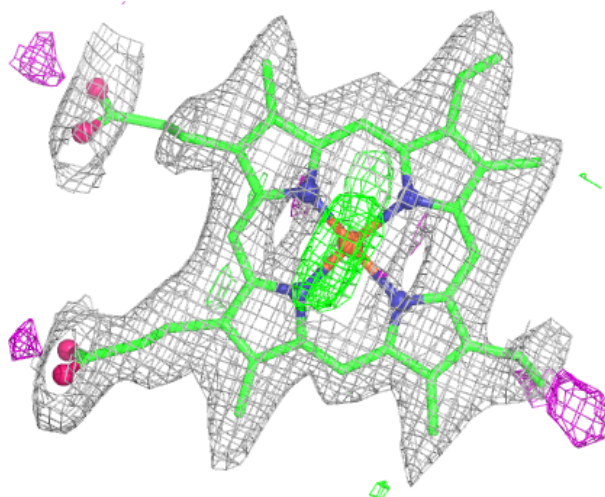
Electron density around VI4 A 502:

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



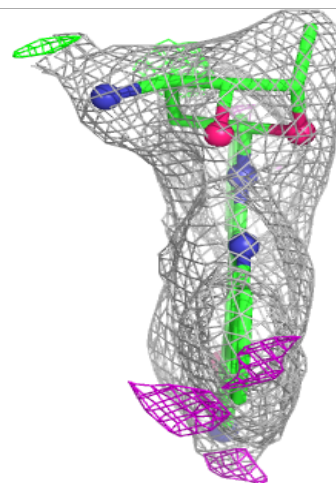
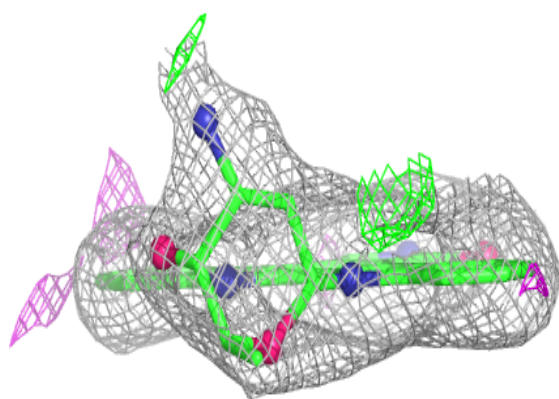
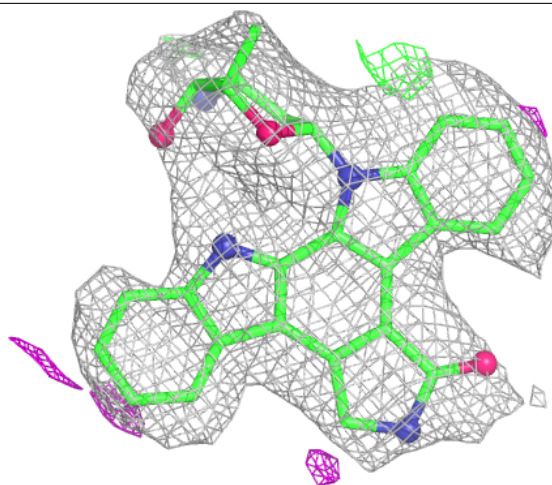
Electron density around HEM A 501:

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



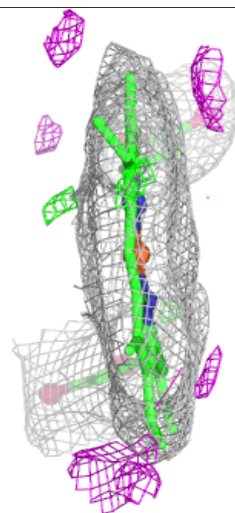
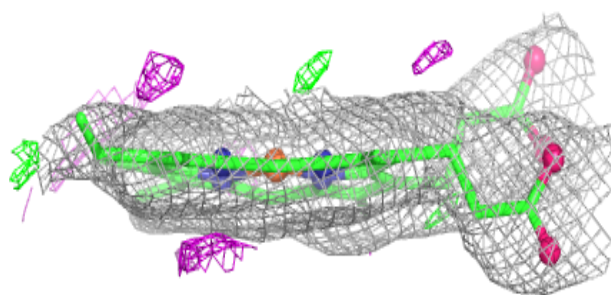
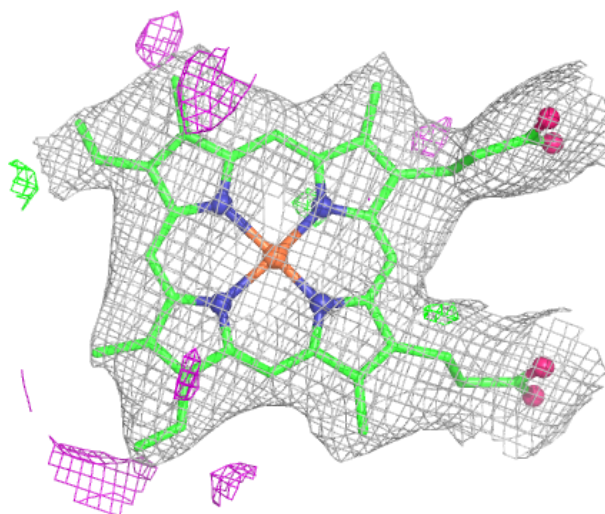
Electron density around VI4 C 502:

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



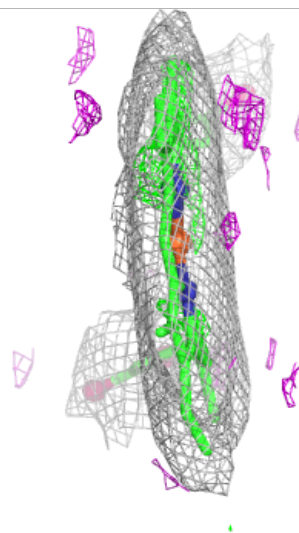
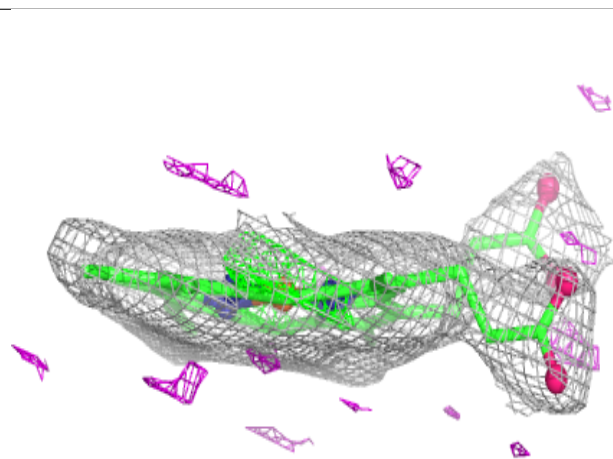
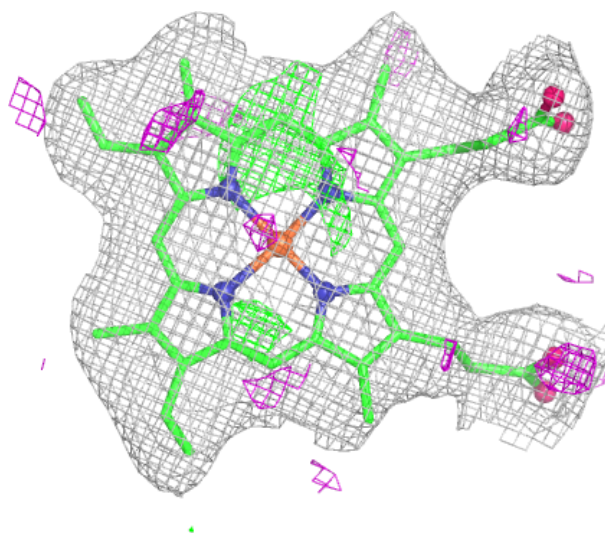
Electron density around HEM B 501:

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



Electron density around HEM C 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.