Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2026 – 12:25 AM JST

PDB ID	:	7WDD / pdb_00007wdd
Title	:	Crystal structure of the P450 BM3 heme domain mutant F87K in complex with N-imidazolyl-hexanoyl-L-phenylalanine, styrene and hydroxylamine
Authors	:	Jiang, Y.; Dong, S.; Feng, Y.; Cong, Z.
Deposited on	:	2021-12-21
Resolution	:	2.21 Å(reported)

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

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

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

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

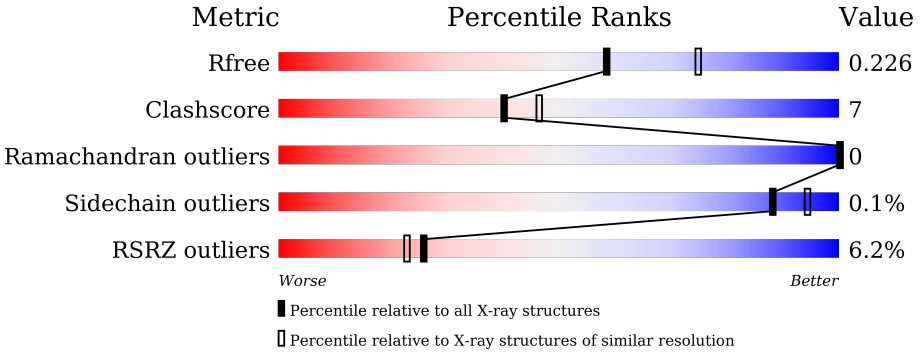
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 (i)

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

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	465	6% 81% 14% 5%
1	B	465	6% 84% 9% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SYN	B	505	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7367 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.

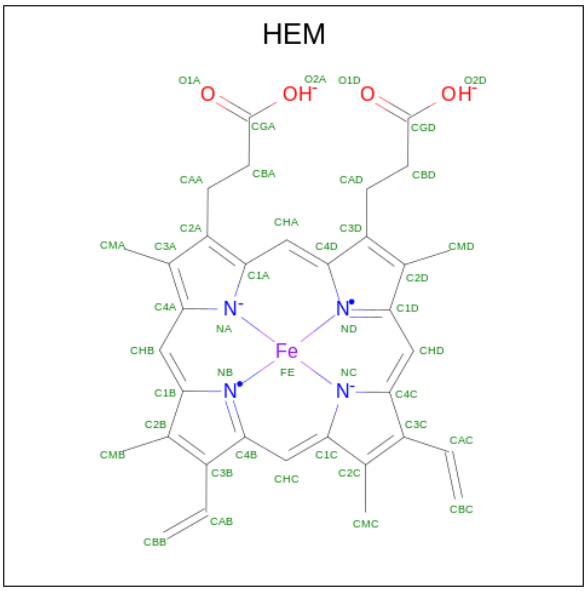
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH–P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	3492	2235	598	642	17	0	1	0
1	B	436	3417	2189	589	623	16	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

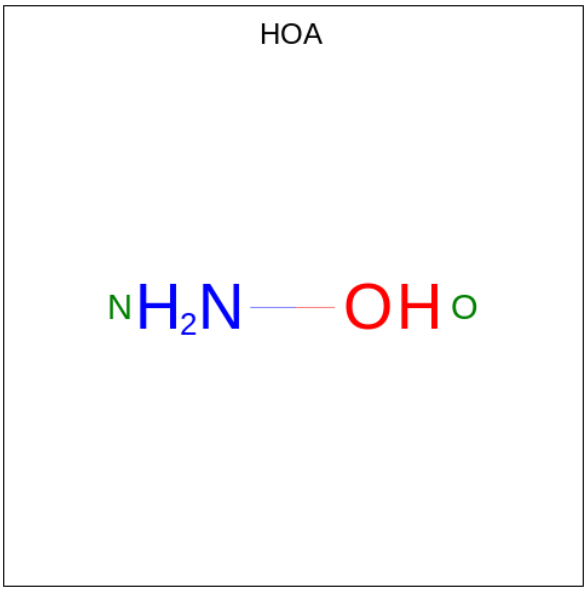
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A1Q8UP87
A	87	LYS	PHE	engineered mutation	UNP A0A1Q8UP87
A	456	LEU	-	expression tag	UNP A0A1Q8UP87
A	457	GLU	-	expression tag	UNP A0A1Q8UP87
A	458	HIS	-	expression tag	UNP A0A1Q8UP87
A	459	HIS	-	expression tag	UNP A0A1Q8UP87
A	460	HIS	-	expression tag	UNP A0A1Q8UP87
A	461	HIS	-	expression tag	UNP A0A1Q8UP87
A	462	HIS	-	expression tag	UNP A0A1Q8UP87
A	463	HIS	-	expression tag	UNP A0A1Q8UP87
B	-1	GLY	-	expression tag	UNP A0A1Q8UP87
B	87	LYS	PHE	engineered mutation	UNP A0A1Q8UP87
B	456	LEU	-	expression tag	UNP A0A1Q8UP87
B	457	GLU	-	expression tag	UNP A0A1Q8UP87
B	458	HIS	-	expression tag	UNP A0A1Q8UP87
B	459	HIS	-	expression tag	UNP A0A1Q8UP87
B	460	HIS	-	expression tag	UNP A0A1Q8UP87
B	461	HIS	-	expression tag	UNP A0A1Q8UP87
B	462	HIS	-	expression tag	UNP A0A1Q8UP87
B	463	HIS	-	expression tag	UNP A0A1Q8UP87

- 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is HYDROXYAMINE (CCD ID: HOA) (formula: H_3NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
3	A	1	2	1	1	0	0

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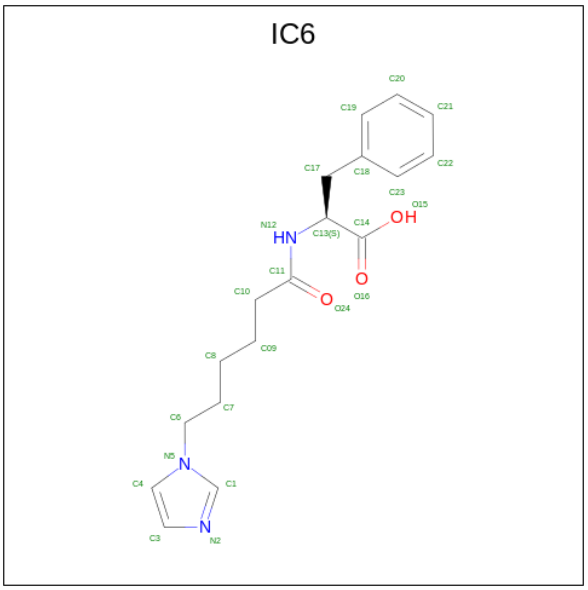
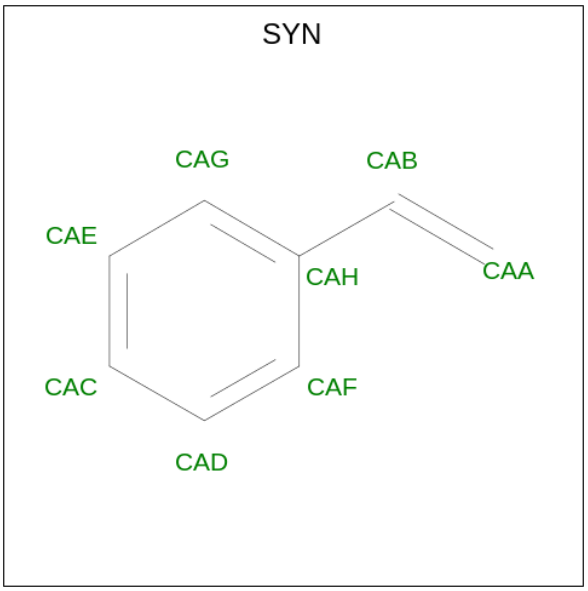
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
3	B	1	2	1	1	0	0

- Molecule 4 is (2S)-2-(6-imidazol-1-ylhexanoylamino)-3-phenyl-propanoic acid (CCD ID: IC6) (formula: $C_{18}H_{23}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	24	18	3	3	0	1
			Total	C	N	O		
4	A	1	24	18	3	3	0	1
			Total	C	N	O		
4	B	1	24	18	3	3	0	1
			Total	C	N	O		
4	B	1	24	18	3	3	0	1

- Molecule 5 is ethenylbenzene (CCD ID: SYN) (formula: C_8H_8) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0

- Molecule 6 is water.

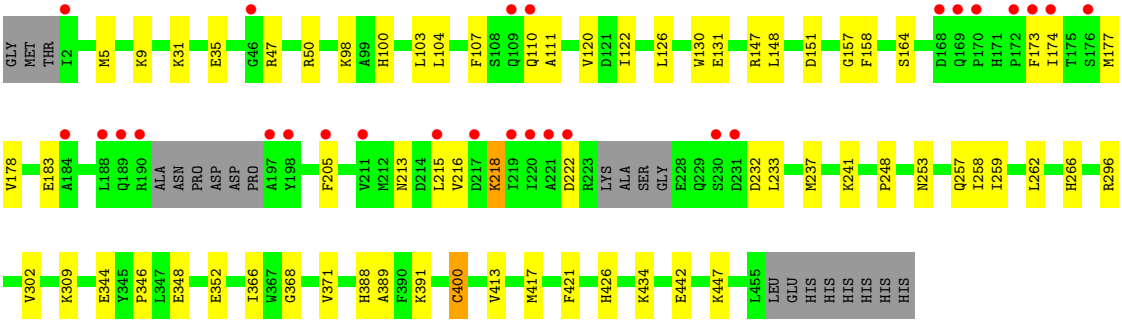
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	113	Total O 113 113	0	0
6	B	135	Total O 135 135	0	0

3 Residue-property plots (i)

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

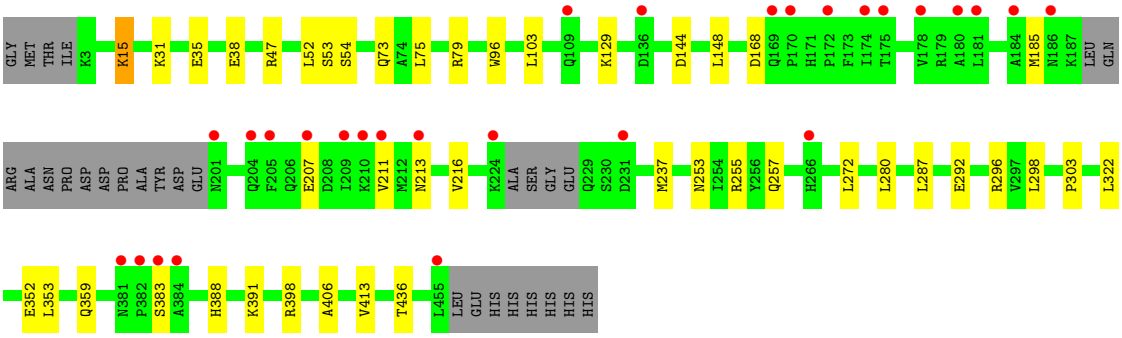
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain A:



• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.82Å 148.84Å 65.34Å 90.00° 100.09° 90.00°	Depositor
Resolution (Å)	39.72 – 2.21 39.72 – 2.21	Depositor EDS
% Data completeness (in resolution range)	89.2 (39.72-2.21) 87.1 (39.72-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.197 , 0.226 0.199 , 0.226	Depositor DCC
R_{free} test set	1893 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7367	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SYN, HOA, IC6, 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	0.43	2/3574 (0.1%)	0.58	1/4838 (0.0%)
1	B	0.27	1/3495 (0.0%)	0.46	0/4734
All	All	0.36	3/7069 (0.0%)	0.52	1/9572 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	LYS	C-O	-6.15	1.19	1.24
1	A	346	PRO	C-O	-5.89	1.17	1.23
1	A	400	CYS	C-O	-5.19	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	LYS	N-CA-C	-5.93	104.74	111.14

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	3492	0	3390	55	0
1	B	3417	0	3316	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	1	0
2	B	43	0	30	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	48	0	0	0	0
4	B	48	0	0	2	0
5	B	24	0	24	5	0
6	A	113	0	0	6	0
6	B	135	0	0	1	0
All	All	7367	0	6790	92	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 7.

All (92) 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:A:173:PHE:HB2	1:A:215:LEU:CD1	1.91	1.00
1:A:173:PHE:CD1	1:A:215:LEU:HD13	2.02	0.95
1:A:173:PHE:HB2	1:A:215:LEU:HD12	1.49	0.94
1:A:173:PHE:CG	1:A:215:LEU:HD13	2.14	0.81
1:A:173:PHE:CB	1:A:215:LEU:CD1	2.68	0.72
1:A:215:LEU:C	1:A:215:LEU:HD23	2.17	0.69
1:A:47:ARG:NH1	1:A:352:GLU:OE2	2.26	0.69
1:B:213:ASN:HA	1:B:216:VAL:HG22	1.73	0.69
1:A:173:PHE:HB2	1:A:215:LEU:HD13	1.77	0.66
1:B:292:GLU:HG3	1:B:296[A]:ARG:HH12	1.60	0.66
1:A:111:ALA:HA	6:A:601:HOH:O	1.94	0.66
1:A:241:LYS:HZ2	1:A:248:PRO:HD3	1.61	0.65
1:B:292:GLU:HG3	1:B:296[A]:ARG:NH1	2.11	0.65
1:A:103:LEU:HD21	1:A:237:MET:HG2	1.81	0.63
1:A:426:HIS:CD2	1:A:447:LYS:HE2	2.33	0.63
1:A:173:PHE:CB	1:A:215:LEU:HD13	2.29	0.62
1:A:107:PHE:CE2	1:A:233:LEU:HD21	2.36	0.60
1:B:280:LEU:HB3	1:B:287:LEU:HD13	1.81	0.60
1:A:98:LYS:NZ	1:A:248:PRO:O	2.33	0.60
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.83	0.60
1:B:168:ASP:OD1	5:B:505:SYN:H1	2.02	0.60
1:A:216:VAL:HG11	1:A:259:ILE:HG13	1.83	0.59
1:A:215:LEU:HD23	1:A:215:LEU:O	2.02	0.59
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD21	1:B:237:MET:HG2	1.85	0.58
1:B:213:ASN:HA	1:B:216:VAL:CG2	2.34	0.58
1:B:47:ARG:NH1	1:B:73:GLN:HB2	2.19	0.57
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.86	0.56
5:B:505:SYN:H5	6:B:642:HOH:O	2.06	0.55
1:A:262:LEU:O	1:A:266:HIS:HD2	1.89	0.55
1:B:213:ASN:O	1:B:216:VAL:HG22	2.07	0.54
1:A:174:ILE:HA	1:A:177:MET:HB3	1.89	0.54
1:A:47:ARG:NH1	6:A:608:HOH:O	2.39	0.54
1:A:174:ILE:O	1:A:178:VAL:HG12	2.08	0.54
1:B:15:LYS:HE2	1:B:15:LYS:HA	1.90	0.54
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.90	0.54
1:A:158:PHE:CE2	1:A:258:ILE:HG12	2.43	0.54
1:A:296[A]:ARG:NH1	6:A:610:HOH:O	2.41	0.53
1:B:213:ASN:CA	1:B:216:VAL:HG22	2.39	0.53
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.90	0.52
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.91	0.52
1:B:31:LYS:O	1:B:35:GLU:HG3	2.10	0.52
1:B:53:SER:HB2	1:B:359:GLN:HB3	1.93	0.51
1:B:213:ASN:C	1:B:216:VAL:HG22	2.35	0.51
1:B:52:LEU:HD11	1:B:353:LEU:HD13	1.94	0.50
1:A:177:MET:HE1	1:A:266:HIS:NE2	2.27	0.49
1:A:131:GLU:HG2	1:A:421:PHE:CE1	2.47	0.49
1:B:406:ALA:HB1	2:B:501:HEM:CBB	2.43	0.49
1:B:129:LYS:NZ	5:B:505:SYN:H4	2.27	0.48
1:A:426:HIS:CG	1:A:447:LYS:HE2	2.49	0.48
1:A:213:ASN:O	1:A:216:VAL:HG22	2.14	0.48
1:A:130:TRP:CZ3	1:A:417:MET:HG2	2.49	0.48
1:B:47:ARG:NH1	4:B:504[B]:IC6:O16	2.44	0.48
1:A:9:LYS:NZ	6:A:615:HOH:O	2.46	0.47
1:A:5:MET:SD	1:A:50:ARG:HG2	2.54	0.47
1:A:241:LYS:HD3	1:A:248:PRO:HB3	1.96	0.47
1:B:272:LEU:HD13	1:B:322:LEU:HG	1.96	0.47
1:A:122:ILE:HD12	1:A:151:ASP:HB3	1.96	0.47
1:A:147:ARG:HG2	1:A:164:SER:HB3	1.96	0.46
1:B:38:GLU:HB2	1:B:54:SER:HB3	1.96	0.46
1:A:400:CYS:HB2	2:A:501:HEM:NA	2.30	0.46
1:A:215:LEU:C	1:A:215:LEU:CD2	2.84	0.46
1:A:434:LYS:HD2	1:A:442:GLU:OE1	2.17	0.45
1:B:185:MET:SD	1:B:436:THR:HA	2.57	0.45
1:A:218:LYS:O	1:A:222:ASP:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASN:O	1:B:216:VAL:CG2	2.65	0.45
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.99	0.44
1:A:130:TRP:HZ3	1:A:417:MET:HG2	1.83	0.43
1:B:96:TRP:CZ2	1:B:398:ARG:HD2	2.54	0.43
1:A:126:LEU:HD22	1:A:148:LEU:HD13	2.01	0.43
1:B:79:ARG:HE	5:B:507:SYN:CAA	2.31	0.43
1:B:168:ASP:OD1	5:B:505:SYN:CAF	2.66	0.43
1:A:104:LEU:HD13	1:B:383:SER:HB3	2.01	0.42
1:A:253:ASN:O	1:A:257:GLN:HG2	2.18	0.42
1:A:31:LYS:O	1:A:35:GLU:HG3	2.19	0.42
1:B:216:VAL:HG21	1:B:255:ARG:HG3	2.00	0.42
1:A:100:HIS:NE2	1:A:104:LEU:HD11	2.35	0.42
1:A:110:GLN:O	6:A:601:HOH:O	2.21	0.41
1:A:157:GLY:O	1:A:232:ASP:HB2	2.21	0.41
1:A:366:ILE:HG21	1:A:389:ALA:HB1	2.02	0.41
1:A:158:PHE:HE2	1:A:258:ILE:HG12	1.83	0.41
1:A:368:GLY:O	1:A:371:VAL:HG13	2.19	0.41
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.92	0.41
1:B:352:GLU:O	1:B:353:LEU:HD23	2.21	0.41
1:A:47:ARG:HH12	1:A:352:GLU:CD	2.28	0.41
1:A:348:GLU:HG2	6:A:698:HOH:O	2.21	0.41
1:B:253:ASN:O	1:B:257:GLN:HG2	2.20	0.41
1:B:47:ARG:NH2	4:B:504[B]:IC6:O16	2.54	0.41
1:B:207:GLU:O	1:B:211:VAL:HG23	2.21	0.41
1:A:183:GLU:HG2	1:A:205:PHE:CD1	2.56	0.40
1:B:129:LYS:NZ	1:B:144:ASP:OD1	2.51	0.40
1:A:309:LYS:HD3	1:A:309:LYS:HA	1.92	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	439/465 (94%)	426 (97%)	13 (3%)	0	100	100
1	B	431/465 (93%)	417 (97%)	14 (3%)	0	100	100
All	All	870/930 (94%)	843 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/408 (89%)	362 (100%)	1 (0%)	86	93
1	B	352/408 (86%)	352 (100%)	0	100	100
All	All	715/816 (88%)	714 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	GLU

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

Mol	Chain	Res	Type
1	A	70	ASN
1	A	204	GLN
1	A	266	HIS
1	B	70	ASN
1	B	92	HIS
1	B	134	ASN
1	B	159	ASN
1	B	403	GLN
1	B	428	ASN

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)

11 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	$\#\|Z\| > 2$
5	SYN	B	506	-	8,8,8	0.18	0	9,9,9	0.17	0
5	SYN	B	507	-	8,8,8	0.44	0	9,9,9	0.69	0
4	IC6	A	504[B]	-	25,25,25	1.53	2 (8%)	31,31,31	1.25	3 (9%)
4	IC6	B	503[A]	-	25,25,25	1.43	2 (8%)	31,31,31	0.99	0
2	HEM	A	501	1,3	50,50,50	1.32	8 (16%)	66,82,82	1.25	9 (13%)
3	HOA	B	502	2	0,1,1	-	-	-		
5	SYN	B	505	-	8,8,8	0.18	0	9,9,9	0.17	0
2	HEM	B	501	3	50,50,50	1.36	7 (14%)	66,82,82	1.39	10 (15%)
4	IC6	A	503[A]	-	25,25,25	1.44	2 (8%)	31,31,31	0.99	0
4	IC6	B	504[B]	-	25,25,25	1.50	5 (20%)	31,31,31	1.69	8 (25%)
3	HOA	A	502	2	0,1,1	-	-	-		

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
5	SYN	B	506	-	-	0/2/2/2	0/1/1/1
5	SYN	B	507	-	-	0/2/2/2	0/1/1/1
4	IC6	A	504[B]	-	-	9/20/20/20	0/2/2/2
4	IC6	B	503[A]	-	-	1/20/20/20	0/2/2/2
2	HEM	A	501	1,3	-	0/14/54/54	-
5	SYN	B	505	-	-	0/2/2/2	0/1/1/1
2	HEM	B	501	3	-	1/14/54/54	-
4	IC6	A	503[A]	-	-	1/20/20/20	0/2/2/2
4	IC6	B	504[B]	-	-	4/20/20/20	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504[B]	IC6	C11-N12	6.06	1.47	1.34
4	A	503[A]	IC6	C11-N12	5.60	1.46	1.34
4	B	503[A]	IC6	C11-N12	5.56	1.45	1.34
4	B	504[B]	IC6	C11-N12	4.12	1.42	1.34
2	B	501	HEM	FE-ND	3.11	2.04	1.94
2	B	501	HEM	FE-NB	3.00	2.04	1.94
2	A	501	HEM	FE-NC	2.95	2.05	1.95
2	A	501	HEM	CAB-C3B	2.92	1.55	1.47
2	B	501	HEM	CAC-C3C	2.91	1.55	1.47
2	A	501	HEM	CAC-C3C	2.82	1.55	1.47
2	B	501	HEM	FE-NA	2.74	2.04	1.95
2	B	501	HEM	FE-NC	2.73	2.04	1.95
2	B	501	HEM	CAB-C3B	2.71	1.54	1.47
2	A	501	HEM	FE-NB	2.66	2.03	1.94
2	A	501	HEM	FE-ND	2.57	2.02	1.94
2	A	501	HEM	FE-NA	2.49	2.03	1.95
4	B	504[B]	IC6	O15-C14	-2.38	1.22	1.30
4	B	504[B]	IC6	C4-N5	-2.28	1.31	1.37
4	B	504[B]	IC6	O24-C11	-2.26	1.18	1.23
4	B	504[B]	IC6	C10-C11	2.16	1.55	1.51
4	A	503[A]	IC6	O24-C11	-2.15	1.18	1.23
4	A	504[B]	IC6	O24-C11	-2.13	1.18	1.23
4	B	503[A]	IC6	O24-C11	-2.12	1.19	1.23
2	A	501	HEM	CMC-C2C	2.05	1.55	1.50
2	B	501	HEM	C3B-C2B	-2.02	1.33	1.37
2	A	501	HEM	CMB-C2B	2.02	1.55	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504[B]	IC6	O24-C11-N12	-3.86	116.44	122.95
4	B	504[B]	IC6	O15-C14-O16	-3.49	116.17	124.09
4	A	504[B]	IC6	C13-N12-C11	3.46	130.54	121.65
2	B	501	HEM	C1B-NB-C4B	3.40	108.58	105.07
2	B	501	HEM	C4C-NC-C1C	3.25	108.53	105.35
4	A	504[B]	IC6	C17-C13-N12	3.10	117.33	110.79
4	B	504[B]	IC6	C7-C6-N5	3.09	122.18	112.31
2	A	501	HEM	C4A-NA-C1A	3.04	108.33	105.35
4	B	504[B]	IC6	O24-C11-C10	3.00	127.51	122.02
4	B	504[B]	IC6	C14-C13-N12	-2.96	103.54	110.55
2	B	501	HEM	C4D-ND-C1D	2.90	108.07	105.07
2	A	501	HEM	C4D-ND-C1D	2.84	108.00	105.07
2	A	501	HEM	C1B-NB-C4B	2.83	108.00	105.07
2	B	501	HEM	C3B-C2B-C1B	2.78	108.55	106.49
4	B	504[B]	IC6	C4-N5-C1	-2.73	103.22	106.66
2	B	501	HEM	C4A-NA-C1A	2.52	107.82	105.35
2	A	501	HEM	CBD-CAD-C3D	-2.44	105.86	112.63
4	B	504[B]	IC6	O15-C14-C13	2.36	121.23	113.40
2	B	501	HEM	CAB-C3B-C2B	-2.35	120.87	128.60
2	A	501	HEM	C2A-C1A-NA	-2.33	107.55	110.15
2	A	501	HEM	C3D-C4D-ND	-2.30	107.60	110.17
2	A	501	HEM	CBA-CAA-C2A	-2.30	106.24	112.63
2	A	501	HEM	C4C-NC-C1C	2.29	107.59	105.35
4	B	504[B]	IC6	C3-C4-N5	2.24	110.28	106.59
2	B	501	HEM	CAD-CBD-CGD	-2.17	108.93	113.60
2	B	501	HEM	CHB-C1B-NB	2.17	127.04	124.37
2	A	501	HEM	CHC-C4B-NB	2.16	126.76	124.42
4	A	504[B]	IC6	O24-C11-C10	-2.14	118.10	122.02
2	B	501	HEM	C3D-C4D-ND	-2.14	107.78	110.17
2	B	501	HEM	C2A-C1A-NA	-2.04	107.87	110.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504[B]	IC6	C17-C13-N12-C11
4	A	504[B]	IC6	C8-C09-C10-C11
4	B	504[B]	IC6	C8-C09-C10-C11
4	A	504[B]	IC6	C09-C10-C11-O24
4	A	504[B]	IC6	C09-C10-C11-N12
4	A	503[A]	IC6	C10-C09-C8-C7
4	A	504[B]	IC6	C6-C7-C8-C09
4	A	504[B]	IC6	N5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	B	504[B]	IC6	C10-C09-C8-C7
4	A	504[B]	IC6	C10-C09-C8-C7
2	B	501	HEM	C4B-C3B-CAB-CBB
4	B	504[B]	IC6	C09-C10-C11-O24
4	A	504[B]	IC6	C7-C6-N5-C1
4	B	504[B]	IC6	C09-C10-C11-N12
4	A	504[B]	IC6	C7-C6-N5-C4
4	B	503[A]	IC6	C10-C09-C8-C7

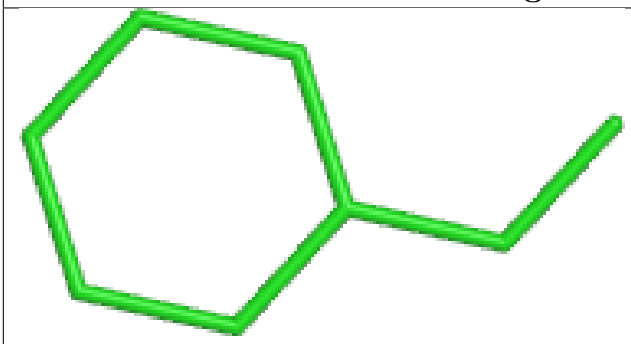
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	507	SYN	1	0
2	A	501	HEM	1	0
5	B	505	SYN	4	0
2	B	501	HEM	2	0
4	B	504[B]	IC6	2	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 SYN B 506



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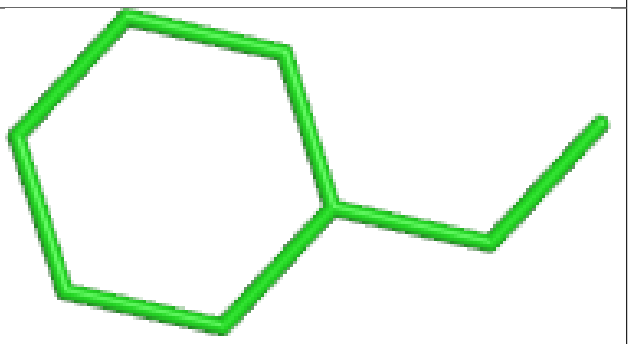

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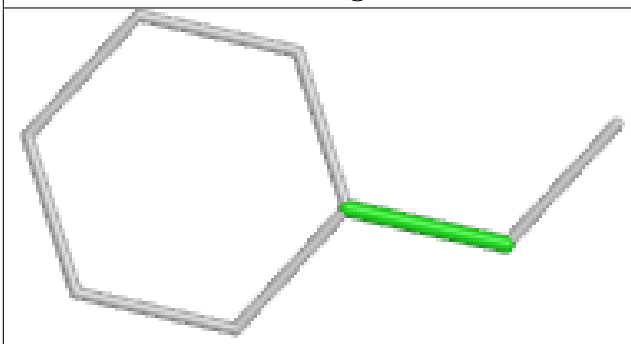
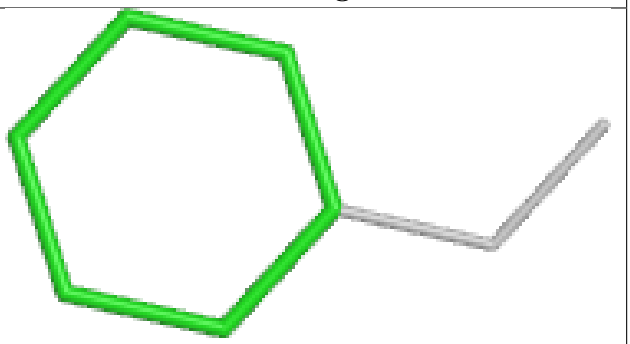
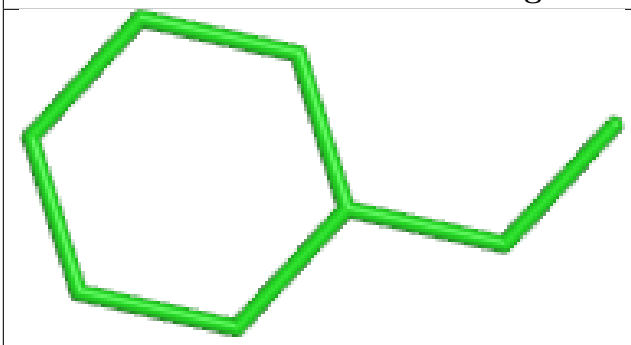


Torsions



Rings

Ligand SYN B 507



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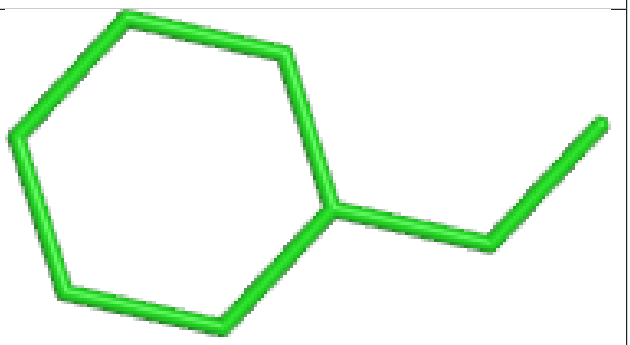

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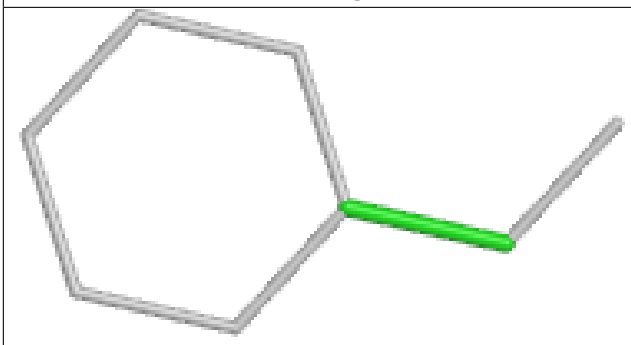

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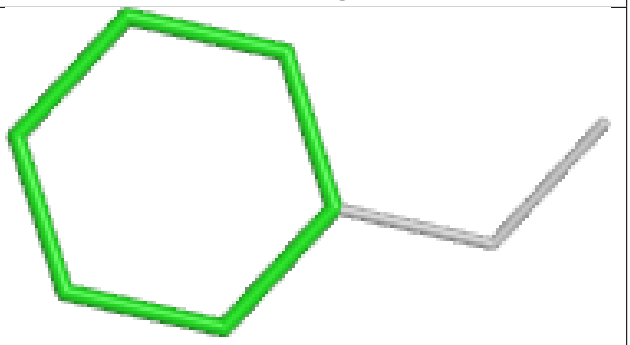
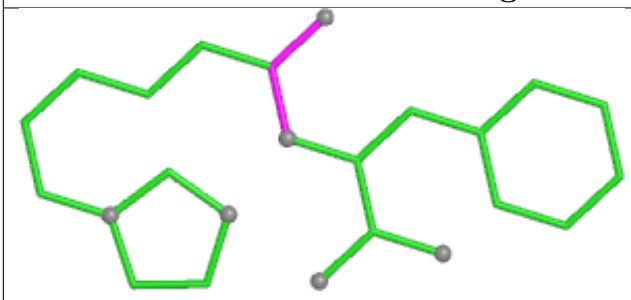


Rings

Ligand IC6 A 504 (B)



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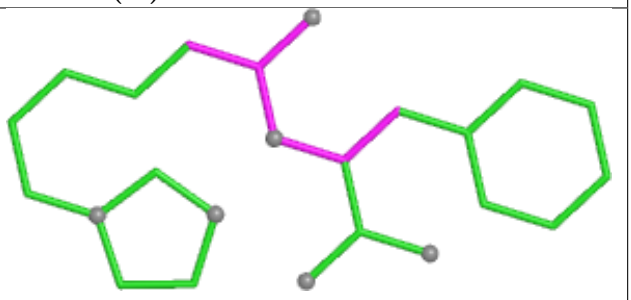

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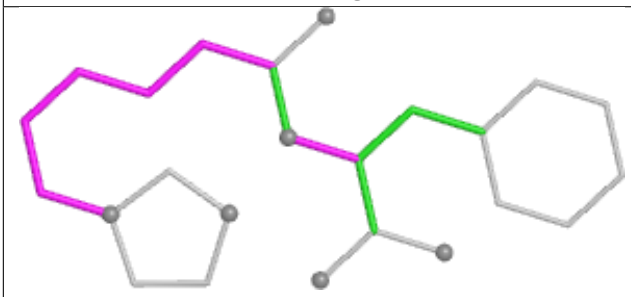

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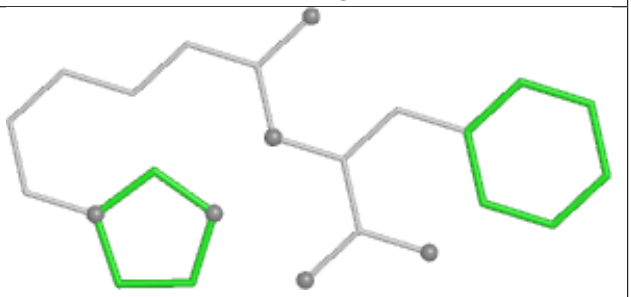

Rings

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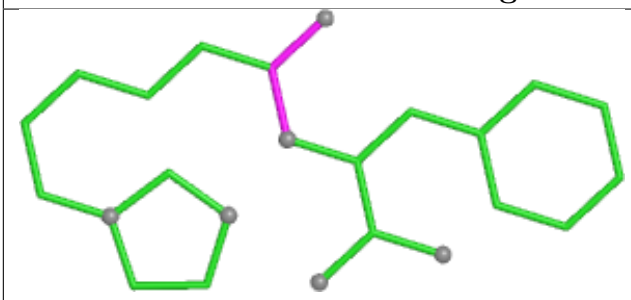

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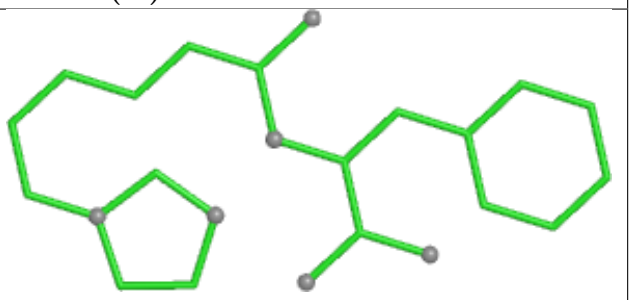

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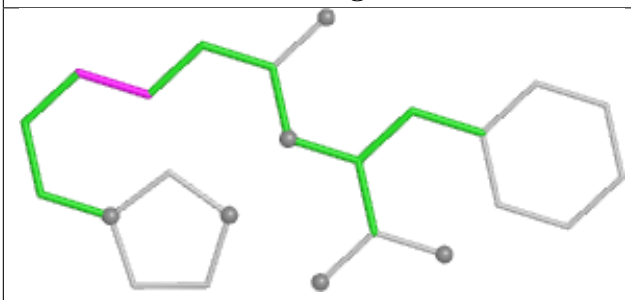

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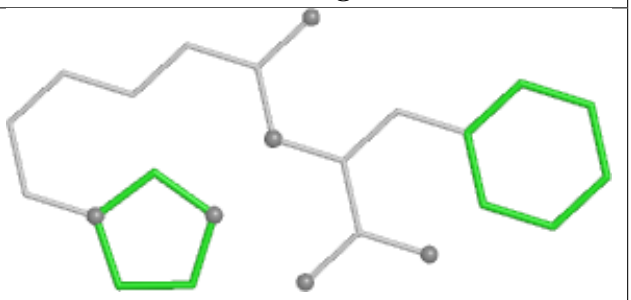
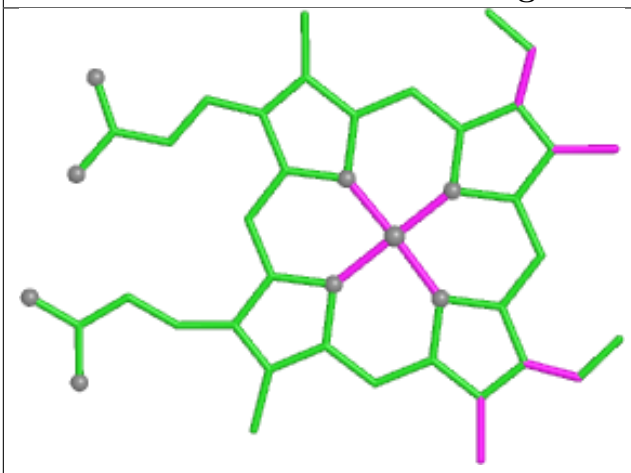


Rings

Ligand HEM A 501



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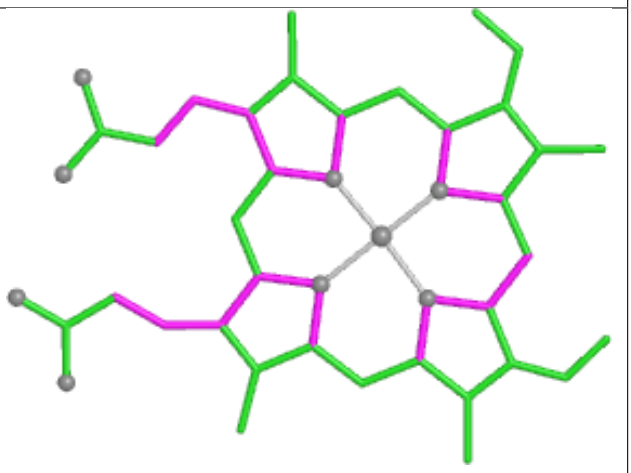

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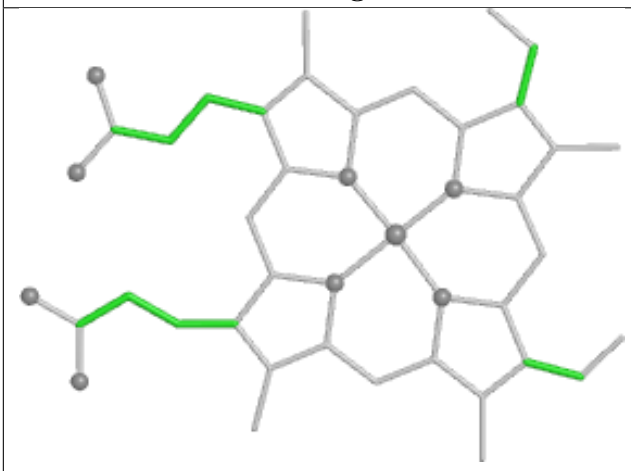

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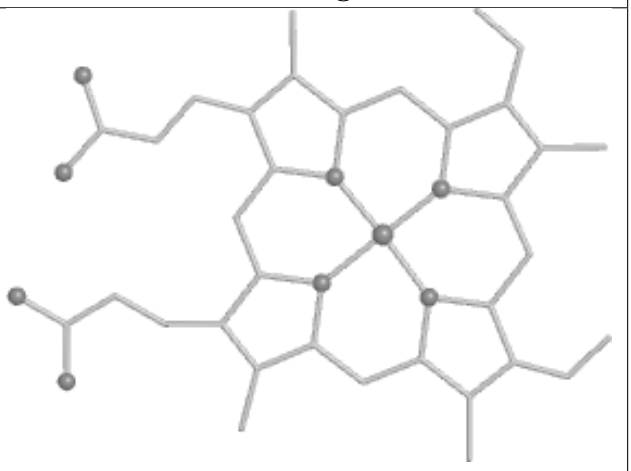
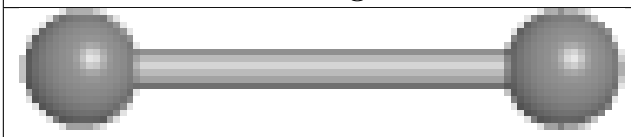


Rings

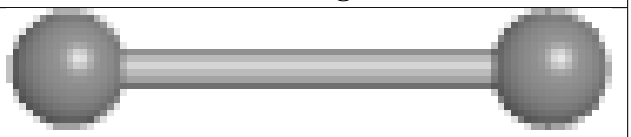
Ligand HOA B 502

Bond lengths

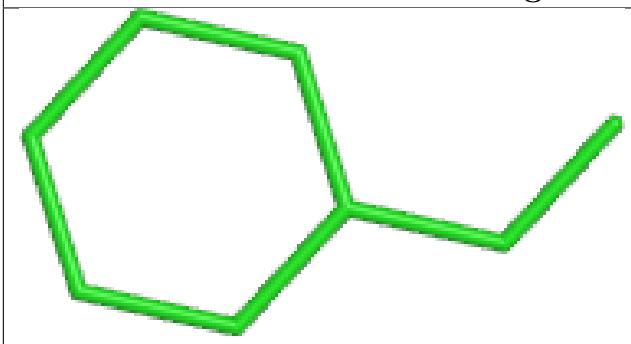
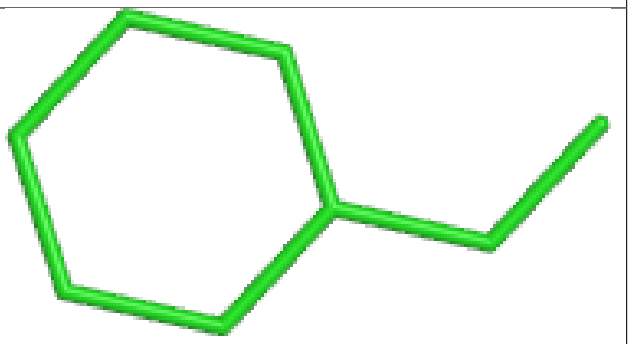
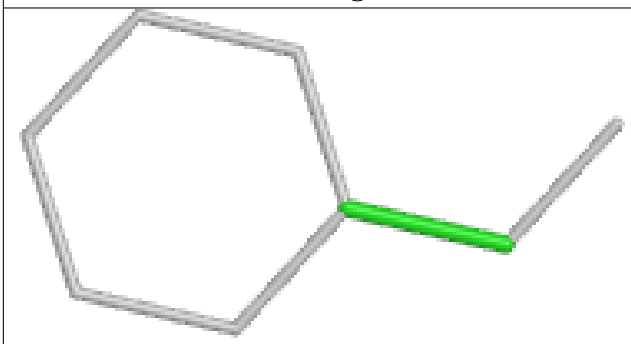
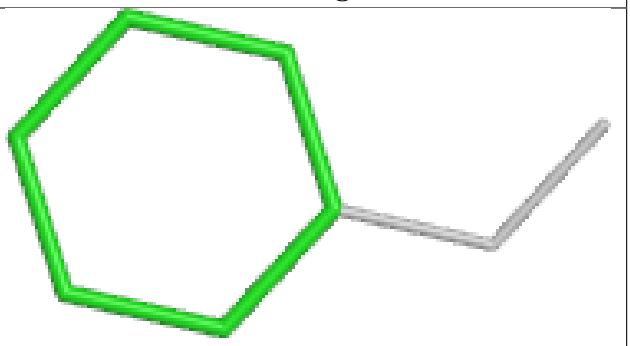
Bond angles



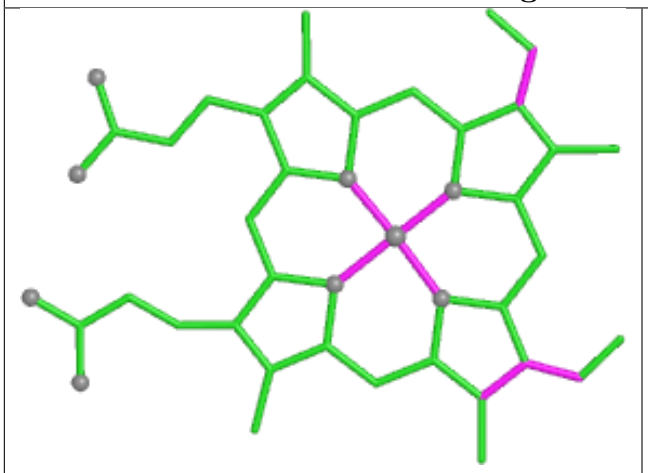
Torsions



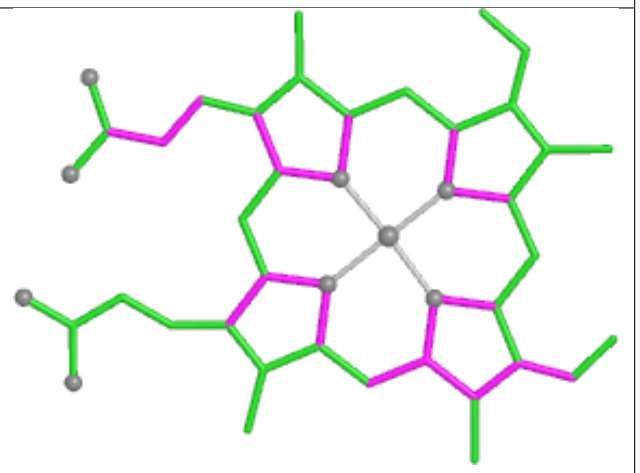
Rings

Ligand SYN B 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

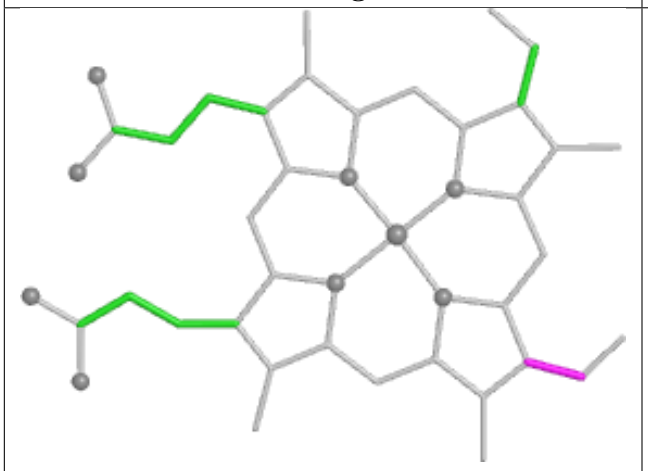
Ligand HEM B 501



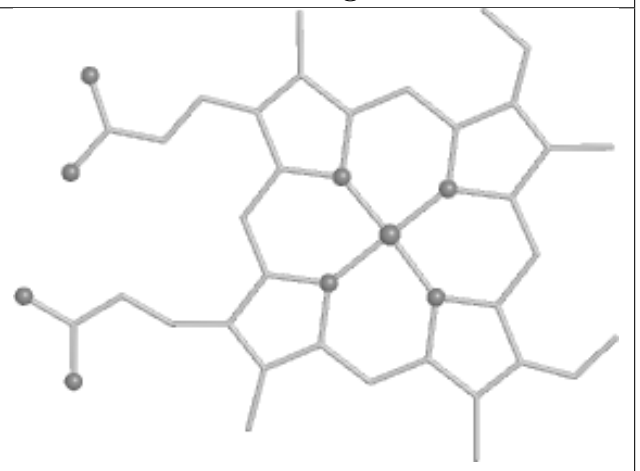
Bond lengths



Bond angles

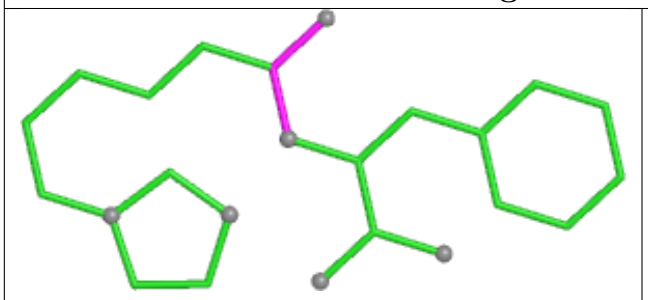


Torsions

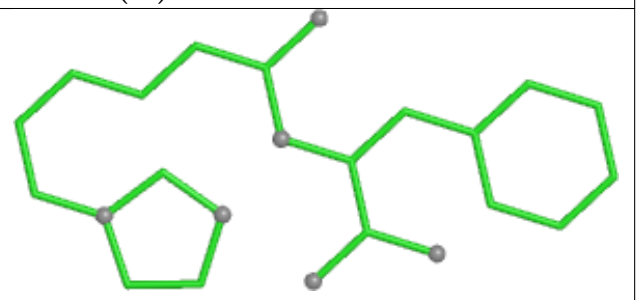


Rings

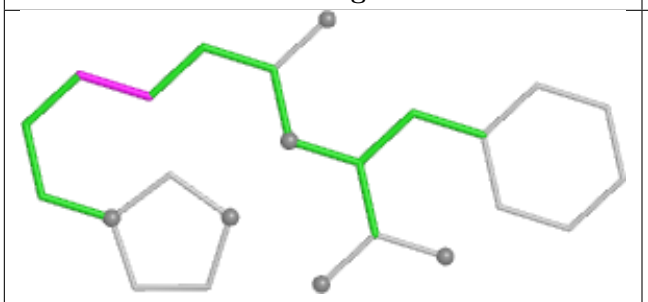
Ligand IC6 A 503 (A)



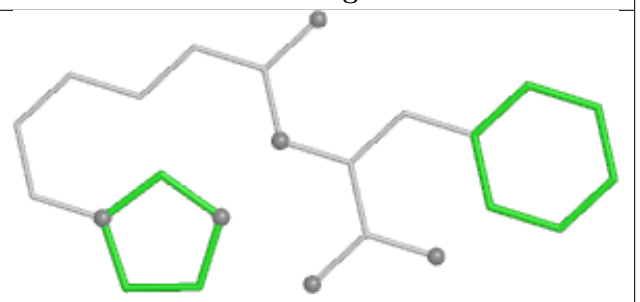
Bond lengths



Bond angles

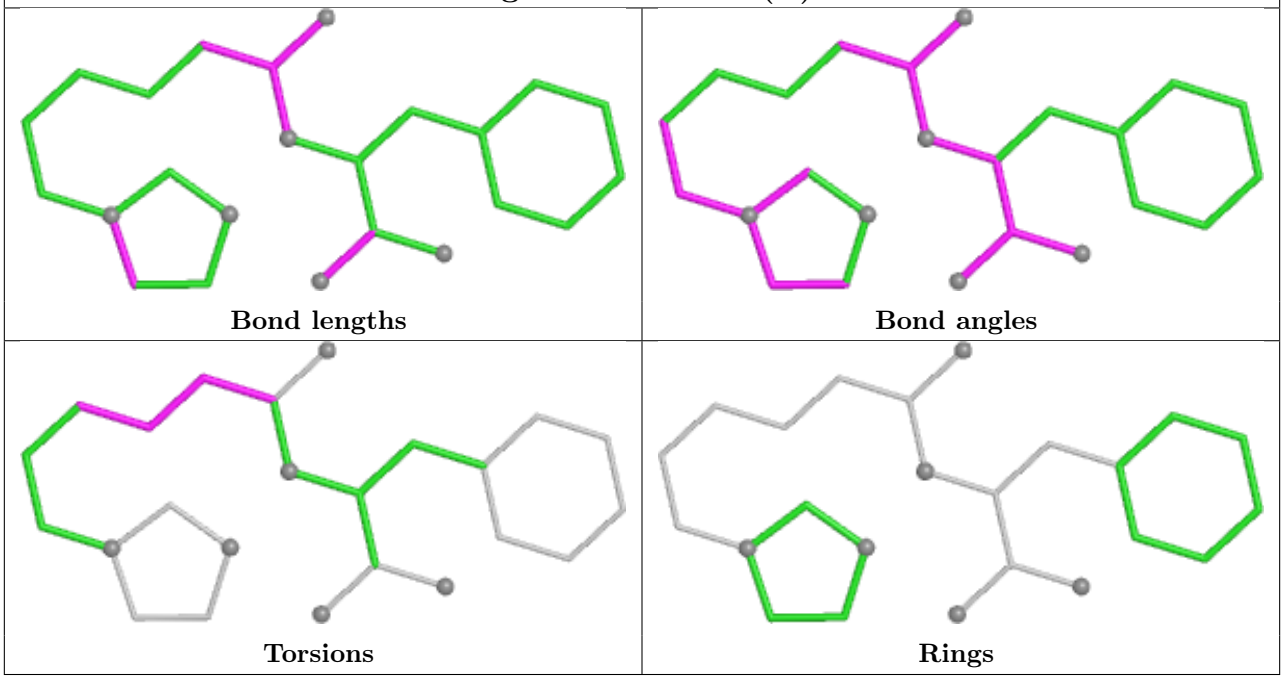


Torsions

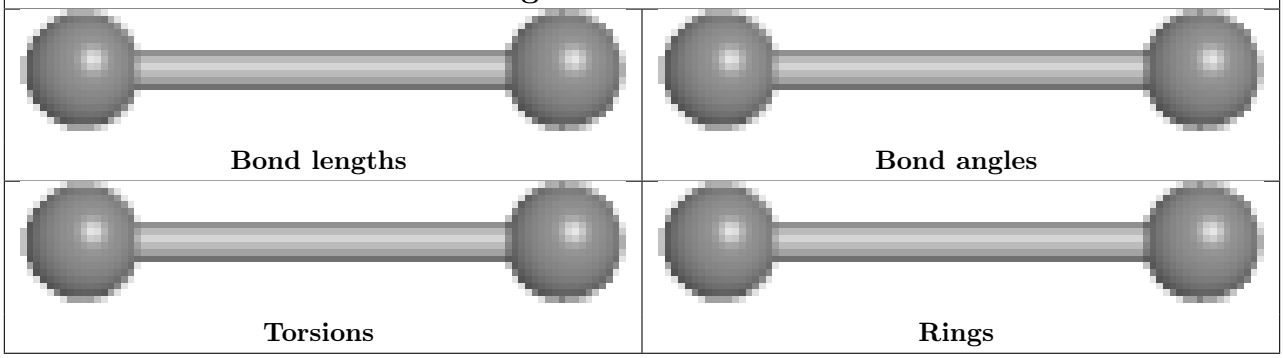


Rings

Ligand IC6 B 504 (B)



Ligand HOA A 502



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	444/465 (95%)	0.45	27 (6%)	27	24	30, 47, 83, 107	1 (0%)
1	B	436/465 (93%)	0.44	28 (6%)	25	22	23, 47, 86, 105	1 (0%)
All	All	880/930 (94%)	0.45	55 (6%)	26	23	23, 47, 85, 107	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	ALA	6.4
1	B	231	ASP	5.5
1	A	174	ILE	4.6
1	A	220	ILE	4.5
1	B	184	ALA	4.5
1	B	175	THR	4.4
1	B	174	ILE	4.4
1	A	231	ASP	4.3
1	A	221	ALA	4.1
1	A	173	PHE	4.0
1	B	205	PHE	4.0
1	A	198	TYR	3.9
1	A	219	ILE	3.8
1	B	211	VAL	3.8
1	A	217	ASP	3.7
1	A	197	ALA	3.7
1	A	188	LEU	3.6
1	B	383	SER	3.4
1	B	169	GLN	3.4
1	A	109	GLN	3.3
1	B	381	ASN	3.1
1	B	186	ASN	3.0
1	A	189	GLN	2.9
1	A	222	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	204	GLN	2.9
1	B	224	LYS	2.9
1	B	384	ALA	2.9
1	B	180	ALA	2.8
1	B	207	GLU	2.6
1	A	215	LEU	2.6
1	A	2	ILE	2.6
1	A	176	SER	2.5
1	A	168	ASP	2.4
1	B	201	ASN	2.4
1	B	382	PRO	2.4
1	A	110	GLN	2.3
1	A	211	VAL	2.3
1	B	181	LEU	2.2
1	A	205	PHE	2.2
1	A	172	PRO	2.2
1	A	46	GLY	2.2
1	B	455	LEU	2.2
1	B	210	LYS	2.2
1	B	178	VAL	2.2
1	A	169	GLN	2.2
1	B	209	ILE	2.1
1	B	170	PRO	2.1
1	B	136	ASP	2.1
1	B	172	PRO	2.1
1	B	213	ASN	2.1
1	A	170	PRO	2.1
1	B	109	GLN	2.0
1	A	190	ARG	2.0
1	A	230	SER	2.0
1	B	266	HIS	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 oligosaccharides in this entry.

6.4 Ligands (i)

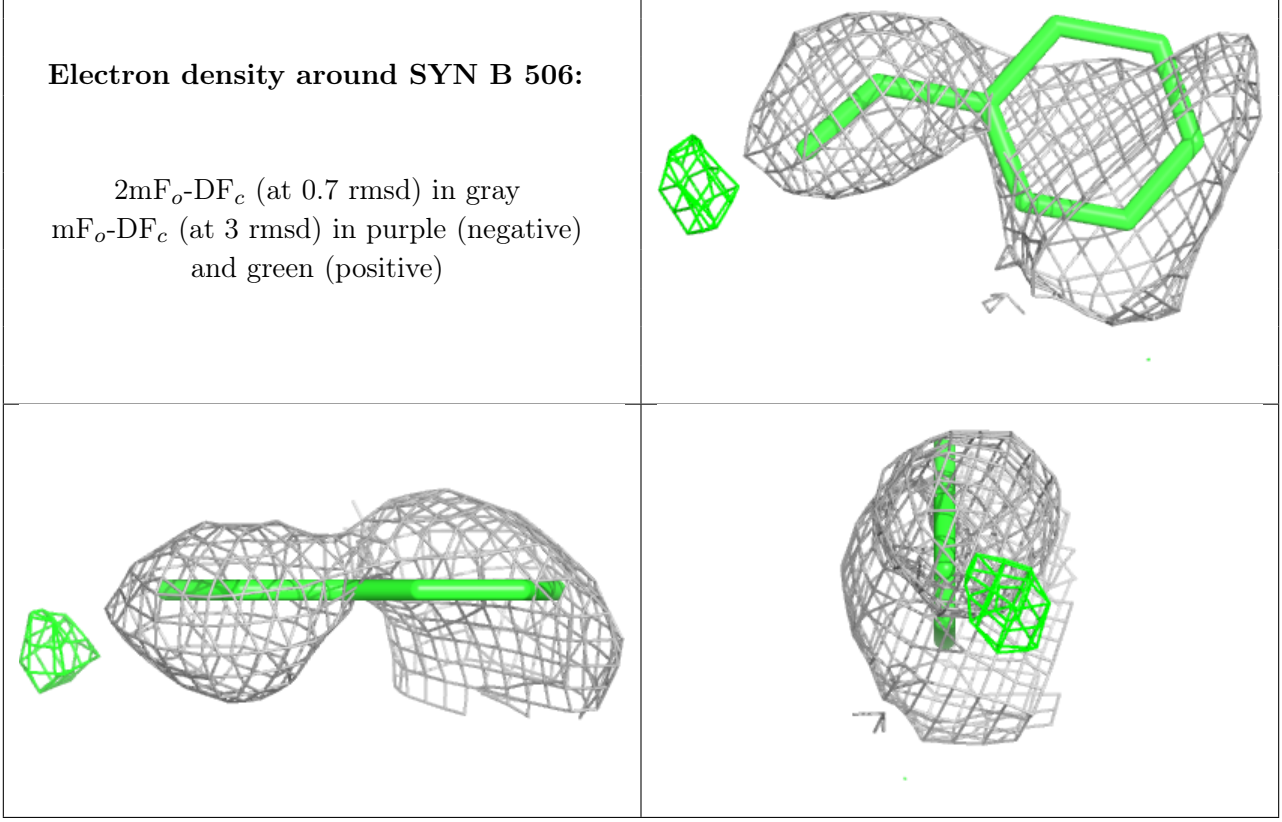
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SYN	B	506	8/8	0.65	0.20	51,71,79,83	0
5	SYN	B	507	8/8	0.81	0.20	61,67,75,75	0
5	SYN	B	505	8/8	0.86	0.17	59,63,69,69	0
4	IC6	A	504[B]	24/24	0.89	0.13	40,48,53,55	24
4	IC6	B	504[B]	24/24	0.90	0.13	41,47,55,59	24
4	IC6	B	503[A]	24/24	0.91	0.14	43,47,51,54	24
4	IC6	A	503[A]	24/24	0.92	0.14	36,45,51,52	24
3	HOA	A	502	2/2	0.93	0.18	44,44,44,46	0
3	HOA	B	502	2/2	0.96	0.15	44,44,44,47	0
2	HEM	B	501	43/43	0.96	0.09	27,37,45,74	0
2	HEM	A	501	43/43	0.97	0.08	29,38,42,47	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.

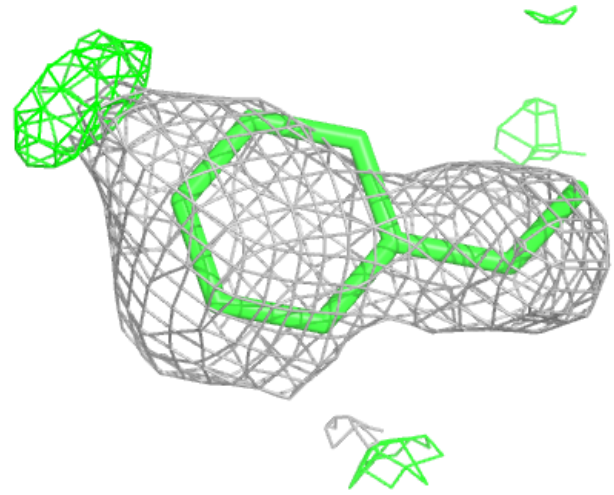
Electron density around SYN B 506:

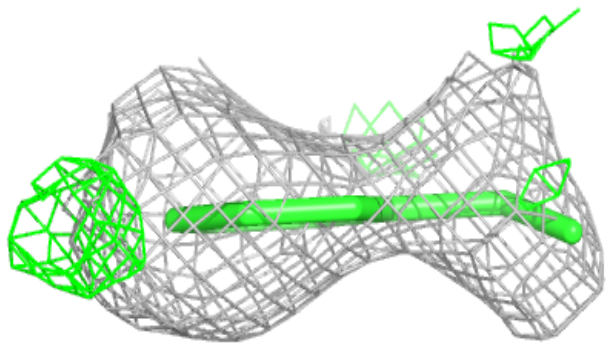
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

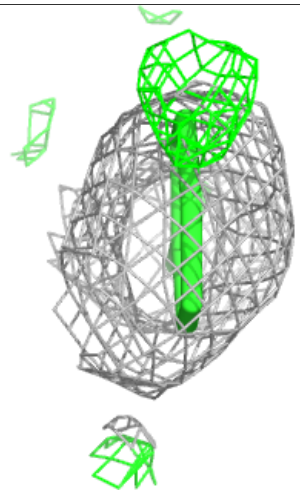


Electron density around SYN B 507:

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

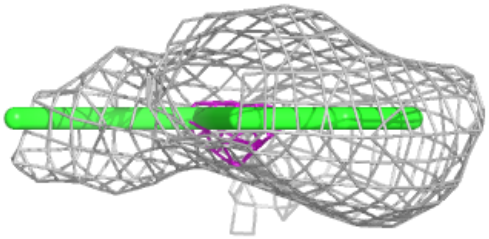


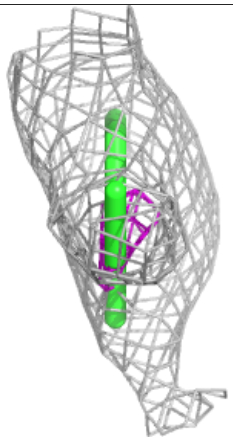




Electron density around SYN B 505:

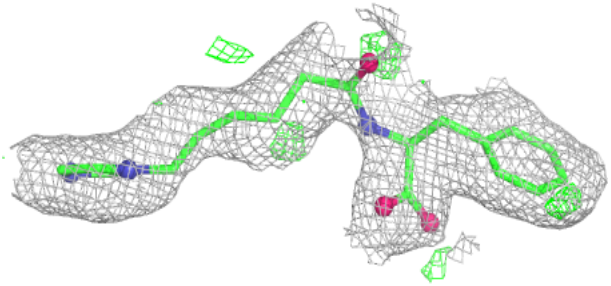
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

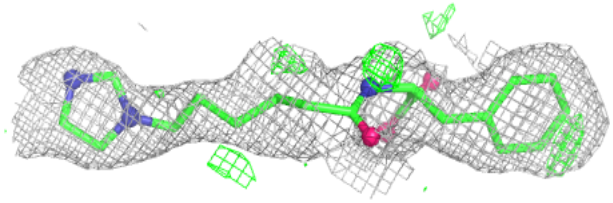


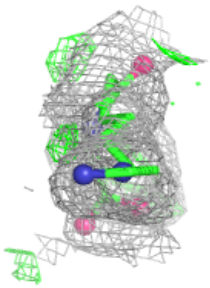


Electron density around IC6 A 504 (B):

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







Electron density around IC6 B 504 (B):

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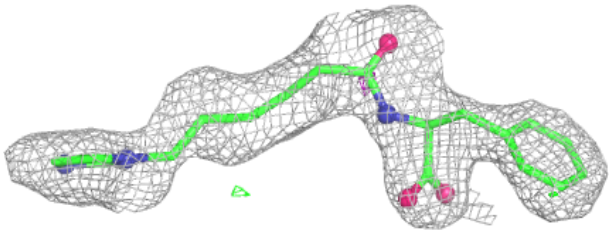
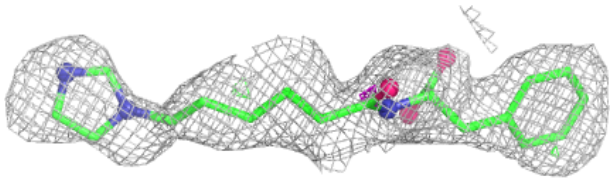
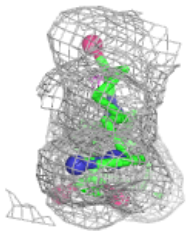
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around IC6 B 503 (A):

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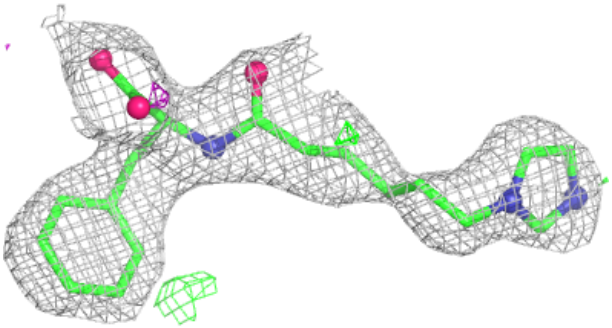
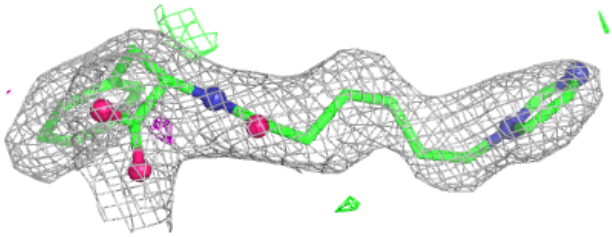
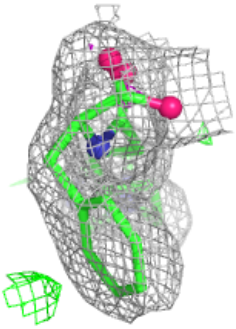
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

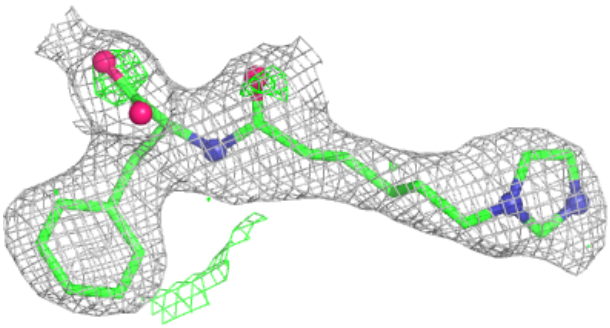


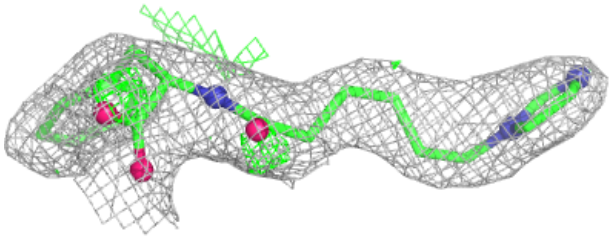


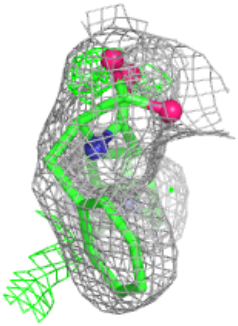


Electron density around IC6 A 503 (A):

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

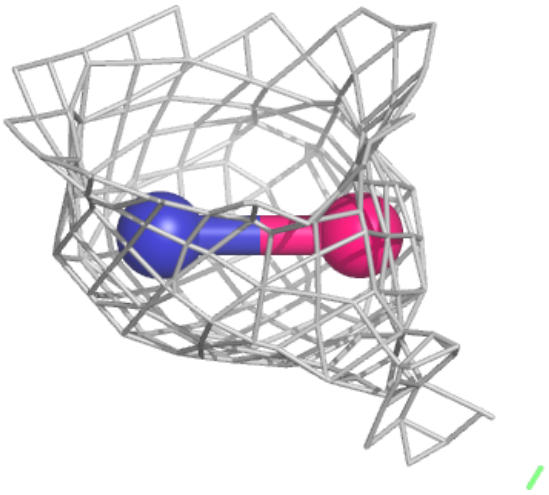


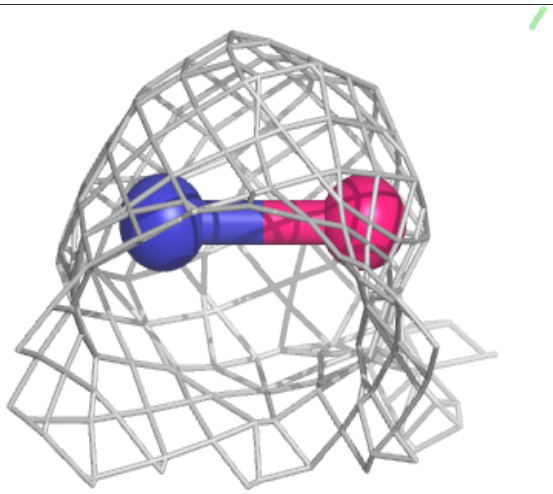


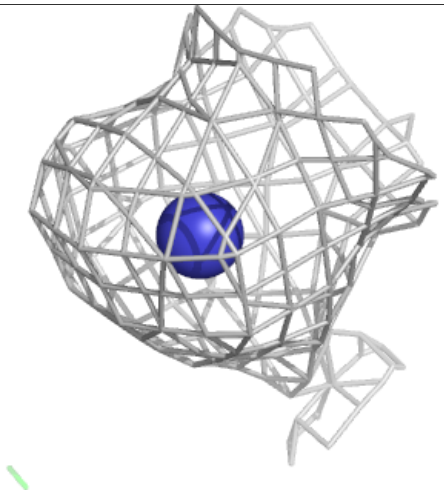


Electron density around HOA A 502:

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

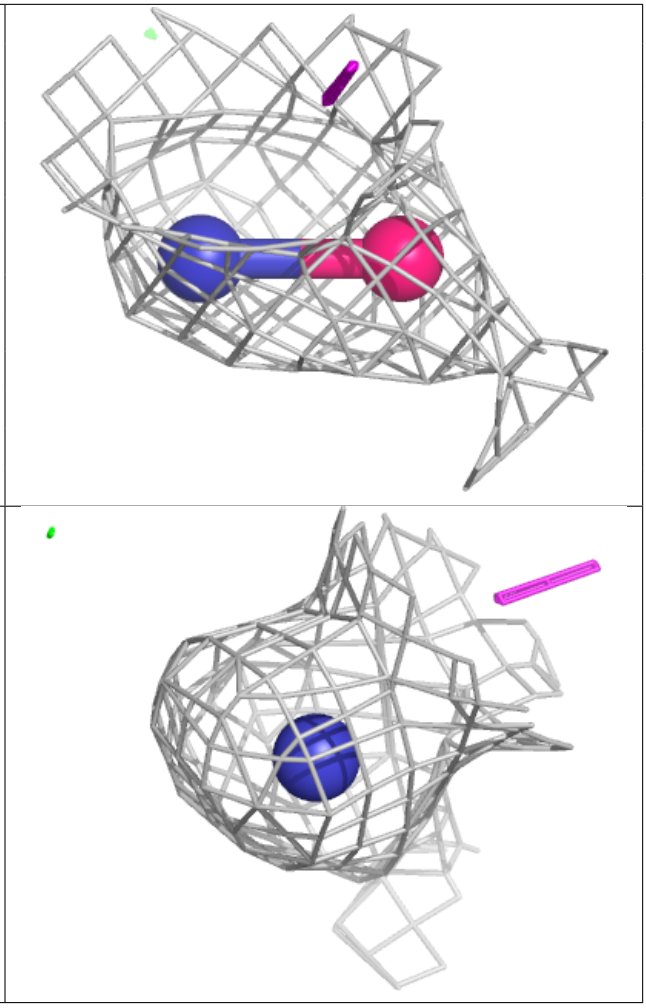






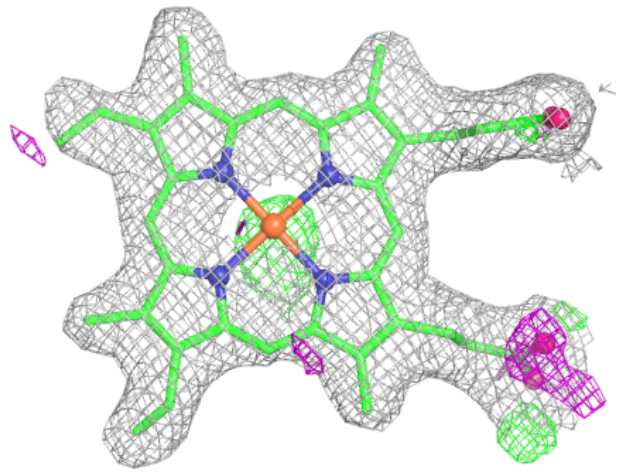
Electron density around HOA B 502:

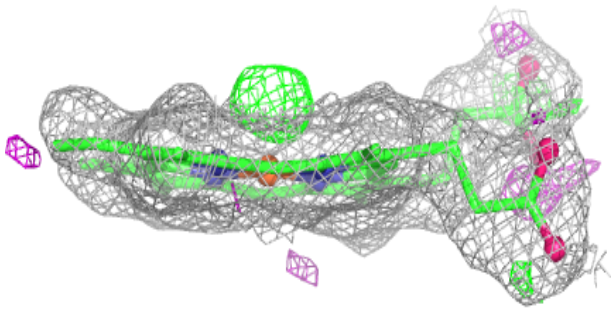
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

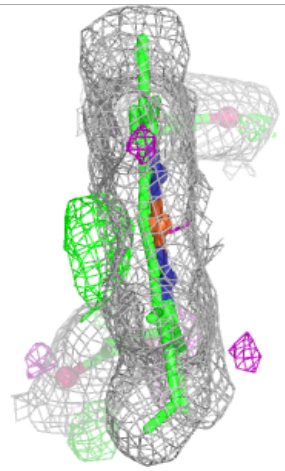


Electron density around HEM B 501:

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

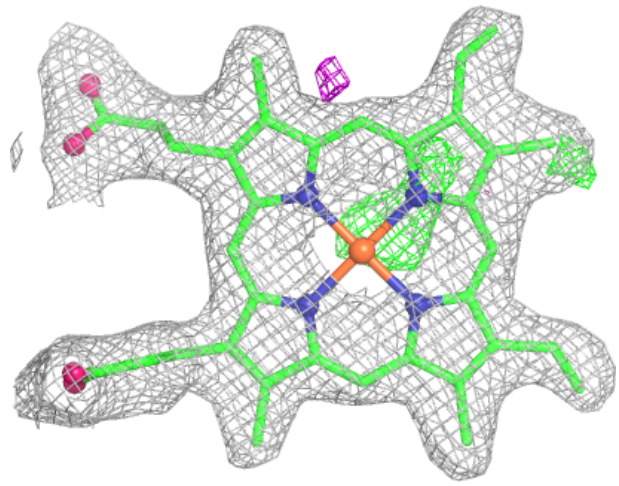


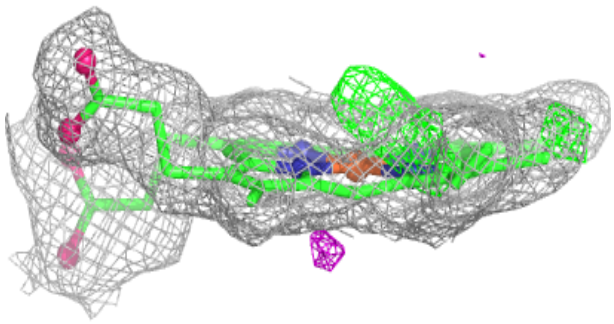


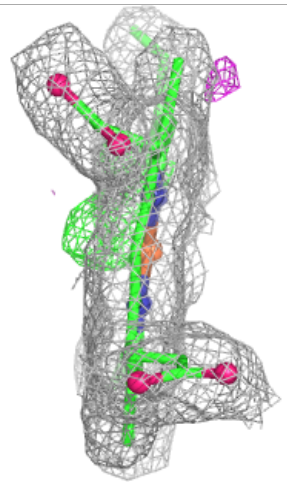


Electron density around HEM A 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.