Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 11:47 PM JST

PDB ID	:	7WDE / pdb_00007wde
Title	:	Crystal structure of the P450 BM3 heme domain mutant F87L 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	:	2.11 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:

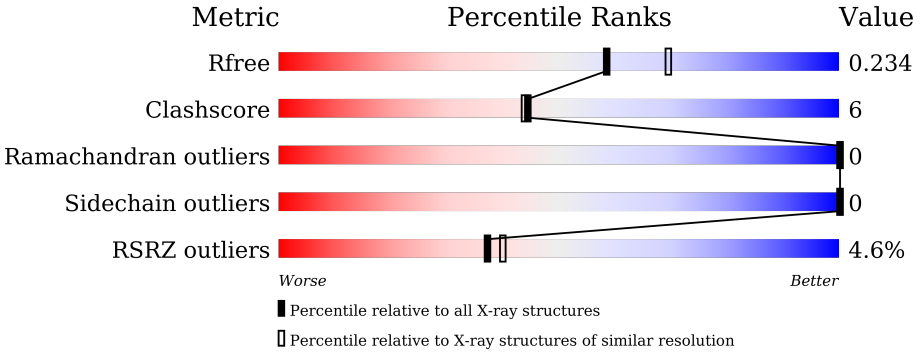
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	465	4% 83% 13% •
1	B	465	5% 84% 12% •

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	A	507	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7654 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.

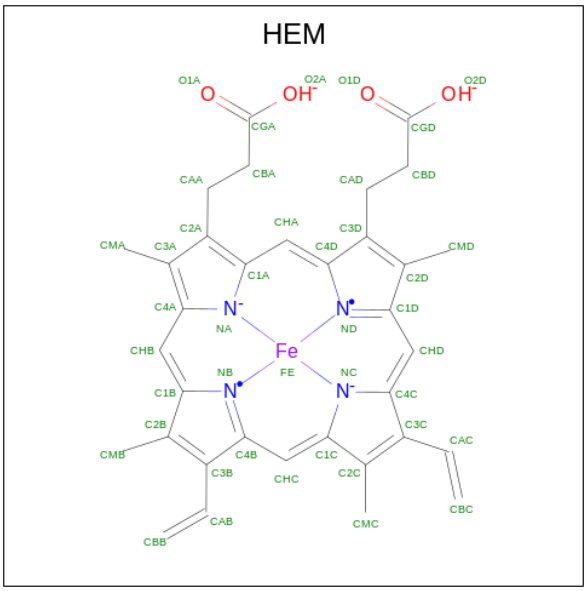
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH–P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	449	3554	2278	605	654	17	0	0	0
1	B	449	3549	2275	603	654	17	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

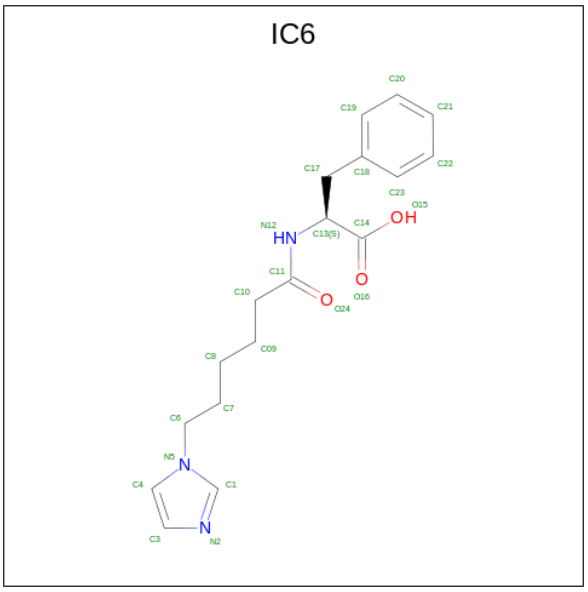
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A1Q8UP87
A	87	LEU	PHE	engineered mutation	UNP A0A1Q8UP87
A	456	LEU	-	expression tag	UNP A0A1Q8UP87
A	457	GLU	-	expression tag	UNP A0A1Q8UP87
A	458	HIS	-	expression tag	UNP A0A1Q8UP87
A	459	HIS	-	expression tag	UNP A0A1Q8UP87
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	LEU	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 (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		
3	A	1	24	18	3	3	0	1

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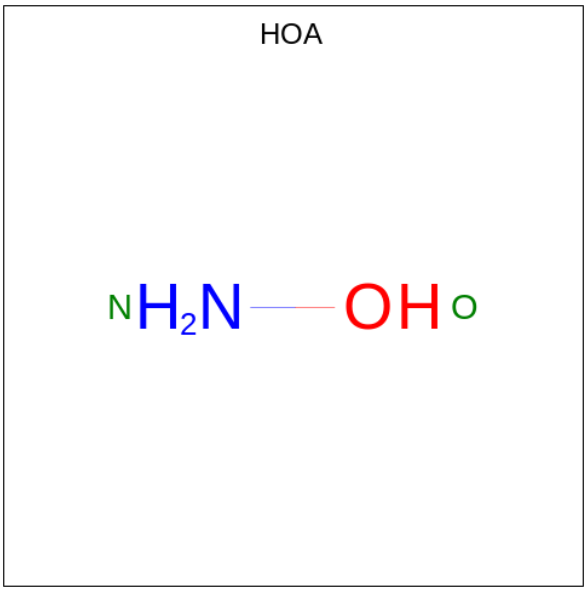
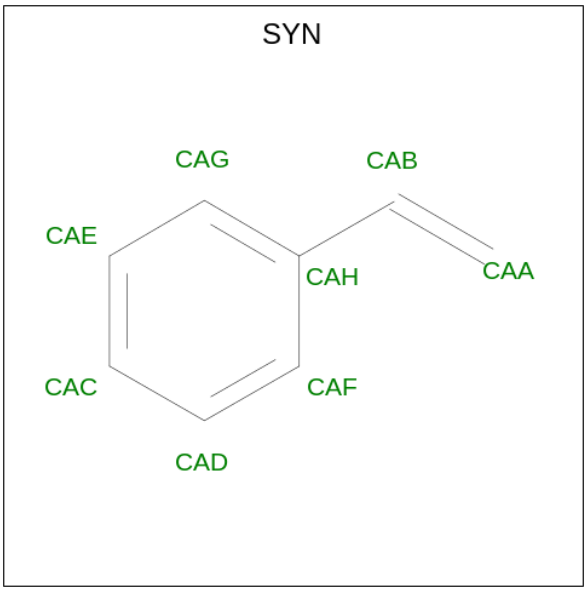
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	24	18	3	3	0	1
			Total	C	N	O		
3	B	1	24	18	3	3	0	1
			Total	C	N	O		
3	B	1	24	18	3	3	0	1

- Molecule 4 is HYDROXYAMINE (CCD ID: HOA) (formula: H_3NO) (labeled as "Ligand of Interest" by depositor).



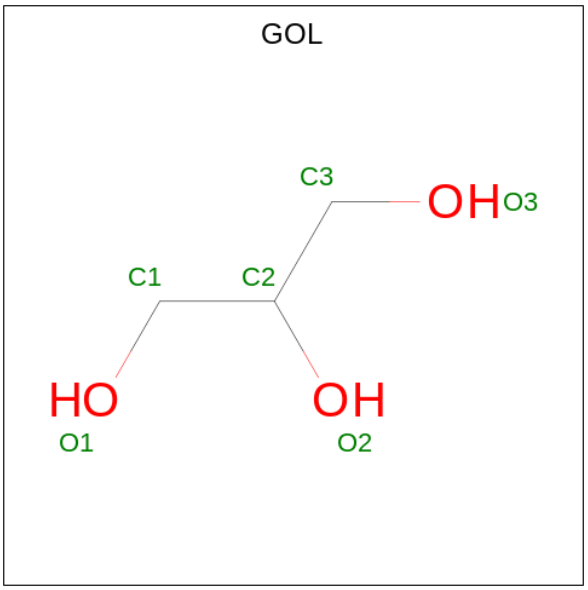
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
4	A	1	2	1	1	0	0
			Total	N	O		
4	B	1	2	1	1	0	0

- 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	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0

- Molecule 7 is water.

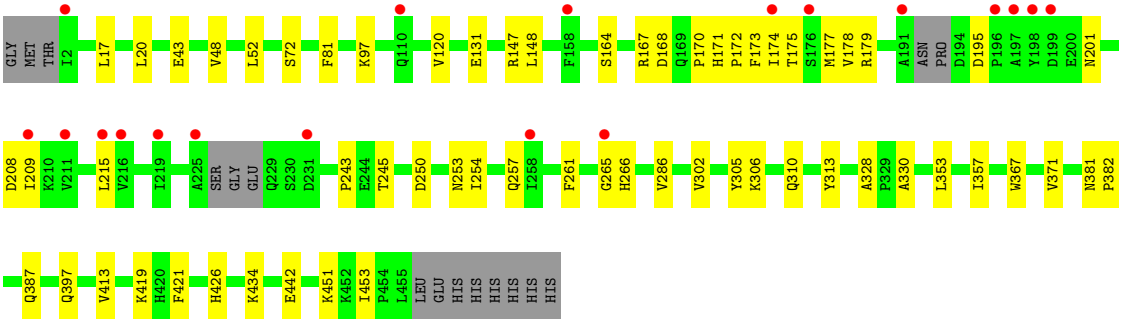
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	172	172	172	0	0
			Total	O		
7	B	155	155	155	0	0

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.

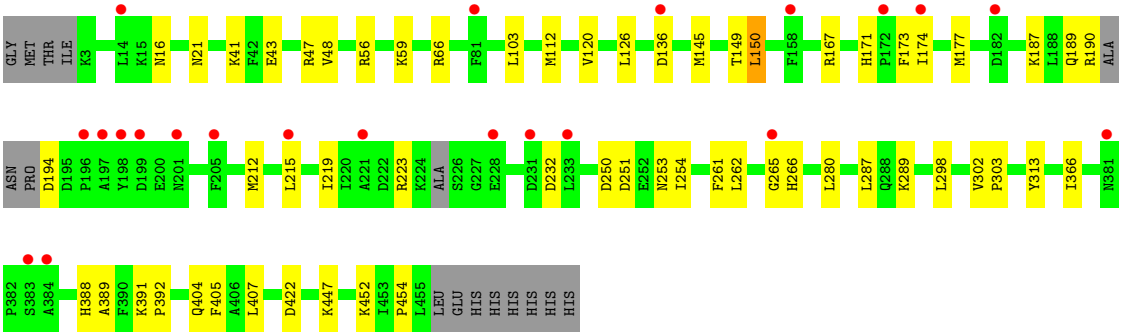
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

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	58.89Å 147.96Å 64.58Å 90.00° 99.67° 90.00°	Depositor
Resolution (Å)	47.01 – 2.11 47.01 – 2.11	Depositor EDS
% Data completeness (in resolution range)	90.2 (47.01-2.11) 88.6 (47.01-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.196 , 0.235 0.199 , 0.234	Depositor DCC
R_{free} test set	1944 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7654	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% 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: HEM, HOA, SYN, IC6, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.62	5/3634 (0.1%)	0.69	2/4920 (0.0%)
1	B	0.65	5/3629 (0.1%)	0.71	1/4912 (0.0%)
All	All	0.63	10/7263 (0.1%)	0.70	3/9832 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	PRO	C-O	-8.04	1.14	1.24
1	A	453	ILE	C-O	-7.08	1.15	1.24
1	A	243	PRO	C-O	-6.94	1.15	1.24
1	B	253	ASN	C-O	-6.67	1.16	1.24
1	B	454	PRO	C-O	-6.03	1.16	1.23
1	A	382	PRO	C-O	-5.89	1.16	1.24
1	B	150	LEU	C-O	-5.77	1.17	1.24
1	A	381	ASN	C-O	-5.28	1.18	1.25
1	A	426	HIS	C-O	-5.27	1.17	1.24
1	B	149	THR	C-O	-5.14	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	452	LYS	CB-CA-C	5.95	120.34	111.89
1	A	168	ASP	N-CA-C	-5.49	105.39	112.68
1	A	245	THR	N-CA-C	-5.01	107.01	113.23

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	3554	0	3486	38	0
1	B	3549	0	3470	43	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	48	0	0	2	0
3	B	48	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	1	0
5	A	32	0	32	6	0
6	A	6	0	8	0	0
7	A	172	0	0	5	0
7	B	155	0	0	7	0
All	All	7654	0	7056	86	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 6.

All (86) 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:72:SER:HB2	3:A:504[B]:IC6:O15	1.80	0.81
1:B:150:LEU:HD21	1:B:174:ILE:HD13	1.63	0.79
1:A:43:GLU:HG2	1:A:48:VAL:HG22	1.64	0.79
1:B:150:LEU:CD2	1:B:174:ILE:HD13	2.15	0.76
1:B:66:ARG:NH1	7:B:601:HOH:O	2.20	0.73
1:B:251:ASP:HA	1:B:254:ILE:HD13	1.72	0.70
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.74	0.70
1:A:173:PHE:HB2	1:A:215:LEU:HD13	1.73	0.69
1:B:173:PHE:HB2	1:B:215:LEU:HD13	1.79	0.65
1:A:177:MET:HE1	1:A:266:HIS:CE1	2.33	0.64
1:A:174:ILE:O	1:A:178:VAL:HG12	1.99	0.62
1:A:170:PRO:HB3	1:A:174:ILE:HD11	1.82	0.60
1:A:17:LEU:HD12	1:A:20:LEU:HD12	1.84	0.60
1:B:194:ASP:N	7:B:607:HOH:O	2.34	0.60
1:B:254:ILE:H	1:B:254:ILE:HD12	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:HA	1:B:190:ARG:HD2	1.84	0.59
1:B:250:ASP:O	1:B:254:ILE:CD1	2.51	0.58
1:B:150:LEU:HD21	1:B:174:ILE:HG21	1.85	0.58
1:A:397:GLN:NE2	5:A:507:SYN:H3	2.19	0.57
1:B:41:LYS:NZ	7:B:611:HOH:O	2.37	0.57
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.87	0.56
1:B:136:ASP:HA	1:B:447:LYS:HE2	1.87	0.56
1:B:250:ASP:O	1:B:254:ILE:HD12	2.04	0.56
1:A:201:ASN:ND2	7:A:617:HOH:O	2.38	0.56
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.89	0.55
1:B:404:GLN:NE2	7:B:609:HOH:O	2.35	0.55
1:A:419:LYS:O	1:A:451:LYS:HD2	2.07	0.55
1:B:173:PHE:HD2	1:B:174:ILE:HG23	1.73	0.54
1:B:254:ILE:HD12	1:B:254:ILE:N	2.23	0.53
1:B:171:HIS:HB3	1:B:174:ILE:HG12	1.91	0.53
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.34	0.51
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.92	0.51
1:A:330:ALA:HB3	3:A:504[B]:IC6:C09	2.41	0.50
1:B:47:ARG:NH2	3:B:504[B]:IC6:O15	2.37	0.50
1:B:289:LYS:HD2	1:B:313:TYR:CE1	2.46	0.49
1:A:397:GLN:HE22	5:A:507:SYN:H3	1.76	0.48
1:A:171:HIS:CG	1:A:172:PRO:HD2	2.49	0.48
1:A:195:ASP:CA	7:A:620:HOH:O	2.62	0.48
1:A:52:LEU:HD11	1:A:353:LEU:HD13	1.95	0.48
1:A:434:LYS:HD2	1:A:442:GLU:OE1	2.15	0.47
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.96	0.47
1:B:103:LEU:HD13	1:B:261:PHE:HZ	1.80	0.47
1:A:131:GLU:HG3	1:A:421:PHE:CZ	2.50	0.47
1:A:286:VAL:HG13	1:A:313:TYR:OH	2.14	0.46
1:B:190:ARG:NH1	7:B:604:HOH:O	2.25	0.46
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.98	0.46
1:A:179:ARG:NH1	1:A:208:ASP:OD1	2.48	0.46
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.97	0.46
1:B:422:ASP:OD2	7:B:602:HOH:O	2.21	0.45
1:A:167:ARG:HB2	5:A:505:SYN:H3	1.98	0.45
1:B:167:ARG:NH2	7:B:613:HOH:O	2.41	0.45
1:B:171:HIS:H	1:B:174:ILE:HD11	1.82	0.45
1:A:310:GLN:HG3	7:A:706:HOH:O	2.16	0.45
1:A:179:ARG:HD2	1:A:208:ASP:OD2	2.17	0.45
5:A:509:SYN:H4	7:A:663:HOH:O	2.17	0.44
1:B:56:ARG:O	1:B:59:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:PHE:O	1:B:265:GLY:N	2.50	0.44
1:B:280:LEU:HB3	1:B:287:LEU:HD12	1.99	0.44
1:A:97:LYS:HD3	5:A:507:SYN:H4	2.00	0.44
1:A:250:ASP:O	1:A:254:ILE:HG13	2.17	0.44
1:A:397:GLN:CD	5:A:507:SYN:H3	2.43	0.44
1:A:261:PHE:O	1:A:265:GLY:N	2.51	0.43
1:B:126:LEU:HD21	1:B:145:MET:HE1	1.99	0.43
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.99	0.43
1:A:306:LYS:N	1:A:306:LYS:HD3	2.33	0.43
1:A:328:ALA:O	1:A:357:ILE:HD12	2.19	0.43
1:B:173:PHE:CE1	1:B:212:MET:HG2	2.53	0.43
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	2.00	0.43
1:B:262:LEU:O	1:B:266:HIS:CD2	2.71	0.43
1:B:43:GLU:HG2	1:B:48:VAL:HG22	2.01	0.42
1:B:112:MET:SD	1:B:405:PHE:HA	2.60	0.42
1:A:147:ARG:HG2	1:A:164:SER:HB3	2.01	0.41
1:A:175:THR:HG22	1:A:179:ARG:HH21	1.84	0.41
1:A:387:GLN:NE2	7:A:601:HOH:O	2.24	0.41
1:A:253:ASN:O	1:A:257:GLN:HG2	2.21	0.41
1:B:177:MET:HE1	1:B:266:HIS:NE2	2.35	0.41
1:A:43:GLU:CG	1:A:48:VAL:HG22	2.43	0.41
1:A:305:TYR:HD2	1:A:306:LYS:HD3	1.86	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.51	0.41
1:B:21:ASN:HA	1:B:189:GLN:HB2	2.02	0.41
1:B:215:LEU:O	1:B:219:ILE:HG12	2.20	0.41
1:B:254:ILE:H	1:B:254:ILE:CD1	2.32	0.41
3:B:502[A]:IC6:N2	4:B:503:HOA:N	2.69	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.87	0.40
1:A:120:VAL:HG11	1:A:302:VAL:HG23	2.03	0.40
1:B:16:ASN:HB2	1:B:43:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/465 (95%)	427 (96%)	16 (4%)	0	100	100
1	B	443/465 (95%)	432 (98%)	11 (2%)	0	100	100
All	All	886/930 (95%)	859 (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	375/408 (92%)	375 (100%)	0	100	100
1	B	373/408 (91%)	373 (100%)	0	100	100
All	All	748/816 (92%)	748 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	73	GLN
1	B	70	ASN
1	B	134	ASN
1	B	201	ASN
1	B	359	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)

13 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	IC6	A	504[B]	-	25,25,25	1.43	2 (8%)	31,31,31	0.99	2 (6%)
5	SYN	A	507	-	8,8,8	0.43	0	9,9,9	1.18	1 (11%)
3	IC6	B	504[B]	-	25,25,25	1.43	2 (8%)	31,31,31	0.99	1 (3%)
4	HOA	B	503	2	0,1,1	-	-	-		
3	IC6	A	502[A]	-	25,25,25	1.43	2 (8%)	31,31,31	0.99	1 (3%)
6	GOL	A	508	-	5,5,5	1.07	0	5,5,5	1.08	0
4	HOA	A	503	2	0,1,1	-	-	-		
5	SYN	A	509	-	8,8,8	0.51	0	9,9,9	0.72	0
5	SYN	A	505	-	8,8,8	0.46	0	9,9,9	1.10	1 (11%)
2	HEM	B	501	1,4	50,50,50	1.67	9 (18%)	66,82,82	1.52	11 (16%)
5	SYN	A	506	-	8,8,8	0.57	0	9,9,9	0.67	0
2	HEM	A	501	1,4	50,50,50	1.77	10 (20%)	66,82,82	1.69	14 (21%)
3	IC6	B	502[A]	-	25,25,25	1.42	2 (8%)	31,31,31	0.99	1 (3%)

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	IC6	A	504[B]	-	-	7/20/20/20	0/2/2/2
5	SYN	A	507	-	-	2/2/2/2	0/1/1/1
3	IC6	B	504[B]	-	-	6/20/20/20	0/2/2/2
3	IC6	A	502[A]	-	-	5/20/20/20	0/2/2/2
6	GOL	A	508	-	-	2/4/4/4	-
5	SYN	A	509	-	-	0/2/2/2	0/1/1/1
5	SYN	A	505	-	-	2/2/2/2	0/1/1/1
2	HEM	B	501	1,4	-	2/14/54/54	-
5	SYN	A	506	-	-	2/2/2/2	0/1/1/1
2	HEM	A	501	1,4	-	2/14/54/54	-
3	IC6	B	502[A]	-	-	4/20/20/20	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-ND	6.01	2.13	1.94
2	A	501	HEM	FE-NB	5.84	2.13	1.94
3	A	504[B]	IC6	C11-N12	5.55	1.45	1.34
3	A	502[A]	IC6	C11-N12	5.54	1.45	1.34
3	B	504[B]	IC6	C11-N12	5.54	1.45	1.34
3	B	502[A]	IC6	C11-N12	5.54	1.45	1.34
2	B	501	HEM	FE-ND	4.96	2.10	1.94
2	B	501	HEM	FE-NB	4.73	2.09	1.94
2	B	501	HEM	FE-NA	4.33	2.09	1.95
2	A	501	HEM	CAB-C3B	2.92	1.55	1.47
2	B	501	HEM	CAB-C3B	2.92	1.55	1.47
2	B	501	HEM	CAC-C3C	2.75	1.54	1.47
2	A	501	HEM	FE-NC	2.63	2.04	1.95
2	A	501	HEM	CMA-C3A	2.43	1.55	1.50
2	A	501	HEM	C1B-NB	-2.39	1.36	1.40
2	A	501	HEM	CAC-C3C	2.38	1.53	1.47
2	B	501	HEM	CMA-C3A	2.30	1.55	1.50
2	B	501	HEM	C4D-ND	-2.29	1.36	1.40
2	A	501	HEM	FE-NA	2.18	2.02	1.95
2	A	501	HEM	CMC-C2C	2.16	1.55	1.50
3	B	504[B]	IC6	O24-C11	-2.14	1.18	1.23
3	A	502[A]	IC6	O24-C11	-2.14	1.18	1.23
3	A	504[B]	IC6	O24-C11	-2.13	1.18	1.23
2	A	501	HEM	CMB-C2B	2.11	1.55	1.50
3	B	502[A]	IC6	O24-C11	-2.10	1.19	1.23
2	B	501	HEM	C2A-C3A	-2.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CMB-C2B	2.02	1.55	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C1B-NB-C4B	5.82	111.09	105.07
2	A	501	HEM	C4D-ND-C1D	4.49	109.71	105.07
2	B	501	HEM	C1B-NB-C4B	4.09	109.30	105.07
2	B	501	HEM	C4D-ND-C1D	3.94	109.15	105.07
2	A	501	HEM	CHD-C4C-NC	3.80	128.55	124.44
2	A	501	HEM	C4C-NC-C1C	3.53	108.80	105.35
2	B	501	HEM	C4C-NC-C1C	3.24	108.52	105.35
2	A	501	HEM	C4C-C3C-C2C	3.19	109.37	106.75
2	B	501	HEM	C4A-NA-C1A	3.12	108.40	105.35
2	B	501	HEM	CHC-C4B-NB	3.02	127.70	124.42
2	A	501	HEM	C2B-C1B-NB	-2.97	106.32	109.84
2	B	501	HEM	C3D-C4D-ND	-2.77	107.08	110.17
2	B	501	HEM	CAC-C3C-C4C	-2.67	118.44	124.90
2	B	501	HEM	C2A-C1A-NA	-2.67	107.16	110.15
2	B	501	HEM	CHD-C4C-NC	2.62	127.27	124.44
2	A	501	HEM	C4A-NA-C1A	2.52	107.82	105.35
2	A	501	HEM	C2D-C1D-ND	-2.49	106.90	109.88
2	A	501	HEM	O2A-CGA-CBA	2.48	121.98	114.03
2	A	501	HEM	CAC-C3C-C4C	-2.46	118.96	124.90
3	B	502[A]	IC6	C10-C11-N12	2.43	120.05	115.83
3	B	504[B]	IC6	C10-C11-N12	2.42	120.03	115.83
2	A	501	HEM	CBD-CAD-C3D	-2.42	105.91	112.63
3	A	502[A]	IC6	C10-C11-N12	2.41	120.02	115.83
3	A	504[B]	IC6	C10-C11-N12	2.41	120.01	115.83
2	B	501	HEM	C4C-C3C-C2C	2.36	108.69	106.75
5	A	505	SYN	CAG-CAH-CAF	2.35	121.12	117.64
2	A	501	HEM	CHD-C1D-C2D	2.34	128.63	124.98
2	A	501	HEM	O1A-CGA-CBA	-2.29	115.71	123.08
5	A	507	SYN	CAG-CAH-CAF	2.29	121.03	117.64
2	A	501	HEM	C3D-C4D-ND	-2.24	107.68	110.17
2	B	501	HEM	CBA-CAA-C2A	-2.07	106.87	112.63
3	A	504[B]	IC6	O15-C14-C13	2.00	120.06	113.40

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504[B]	IC6	C8-C09-C10-C11
3	B	504[B]	IC6	C8-C09-C10-C11
5	A	506	SYN	CAA-CAB-CAH-CAF
5	A	506	SYN	CAA-CAB-CAH-CAG
5	A	507	SYN	CAA-CAB-CAH-CAG
5	A	507	SYN	CAA-CAB-CAH-CAF
6	A	508	GOL	O2-C2-C3-O3
3	A	502[A]	IC6	N5-C6-C7-C8
6	A	508	GOL	C1-C2-C3-O3
3	A	504[B]	IC6	C7-C6-N5-C4
3	A	502[A]	IC6	C10-C09-C8-C7
3	A	504[B]	IC6	C7-C6-N5-C1
3	B	502[A]	IC6	N5-C6-C7-C8
3	A	504[B]	IC6	N12-C13-C14-O16
3	A	502[A]	IC6	C7-C6-N5-C4
3	A	502[A]	IC6	C7-C6-N5-C1
3	B	504[B]	IC6	C6-C7-C8-C09
3	A	504[B]	IC6	N12-C13-C14-O15
3	B	504[B]	IC6	C7-C6-N5-C4
3	B	502[A]	IC6	C7-C6-N5-C4
5	A	505	SYN	CAA-CAB-CAH-CAG
5	A	505	SYN	CAA-CAB-CAH-CAF
3	B	504[B]	IC6	C7-C6-N5-C1
3	B	504[B]	IC6	C09-C10-C11-O24
3	B	502[A]	IC6	C7-C6-N5-C1
3	A	504[B]	IC6	C09-C10-C11-O24
3	B	504[B]	IC6	C09-C10-C11-N12
2	A	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A
3	B	502[A]	IC6	C10-C09-C8-C7
3	A	504[B]	IC6	C09-C10-C11-N12
2	A	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
3	A	502[A]	IC6	C8-C09-C10-C11

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504[B]	IC6	2	0
5	A	507	SYN	4	0
3	B	504[B]	IC6	1	0
4	B	503	HOA	1	0

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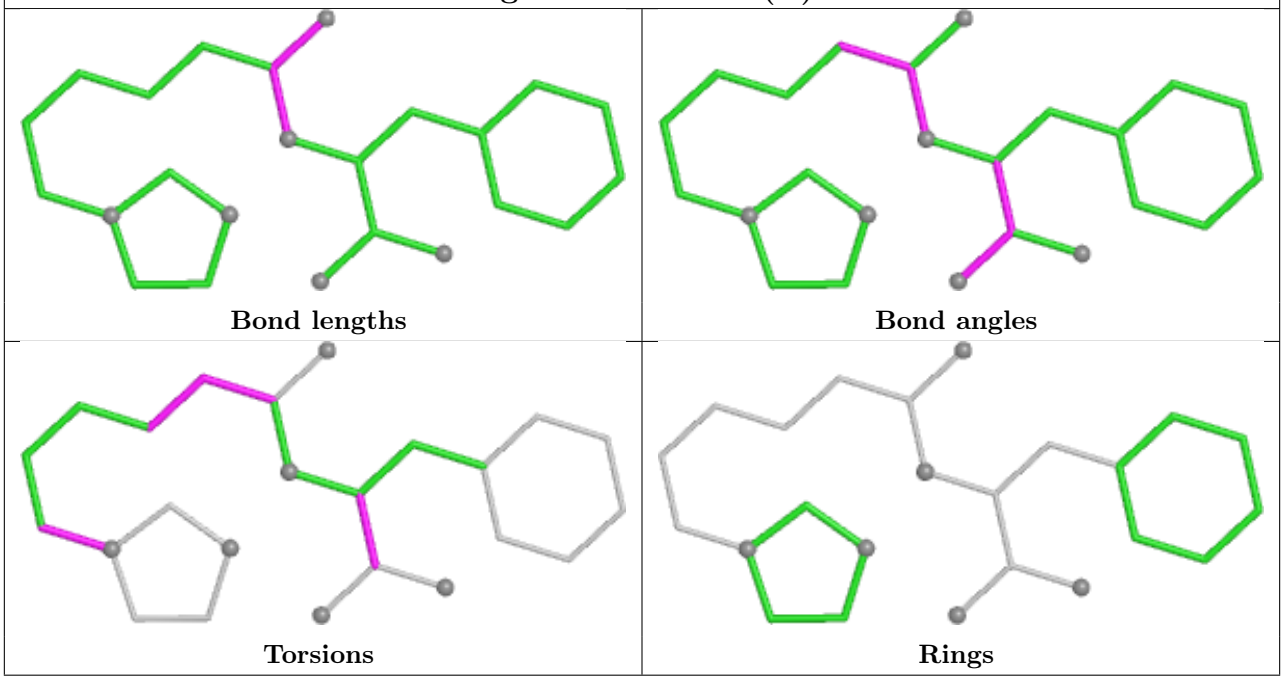
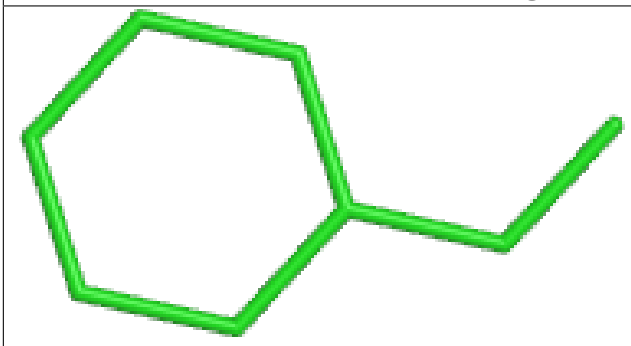
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	SYN	1	0
5	A	505	SYN	1	0
2	B	501	HEM	1	0
2	A	501	HEM	2	0
3	B	502[A]	IC6	1	0

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 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.

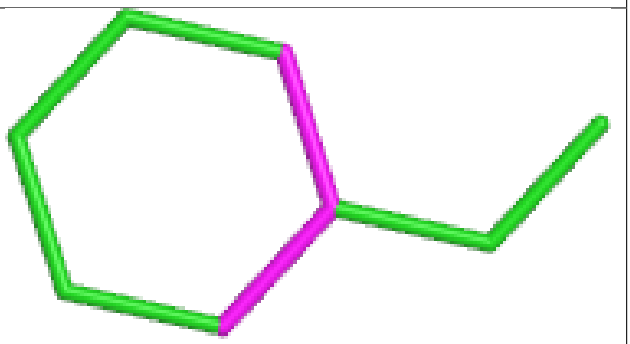
Ligand IC6 A 504 (B)



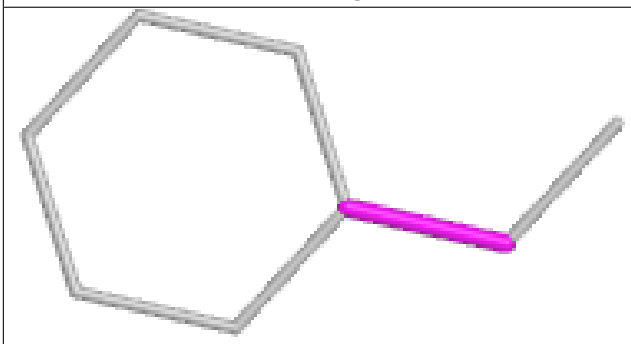
Ligand SYN A 507



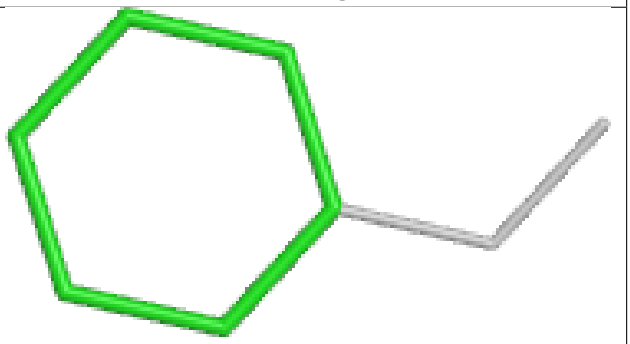
Bond lengths



Bond angles

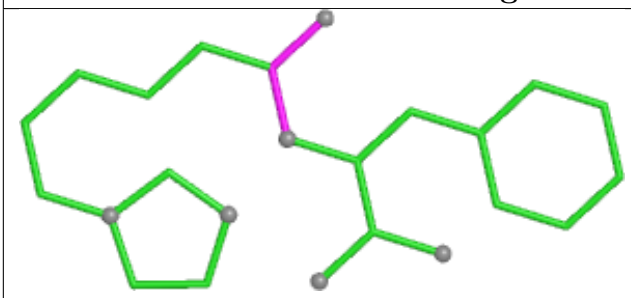


Torsions



Rings

Ligand IC6 B 504 (B)



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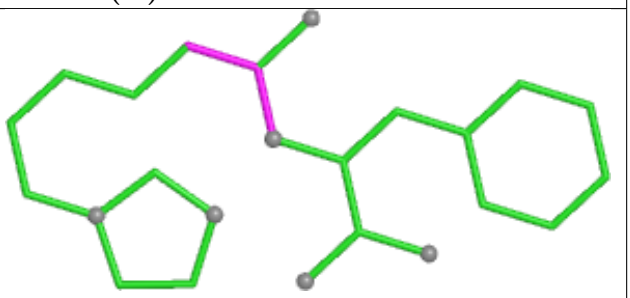
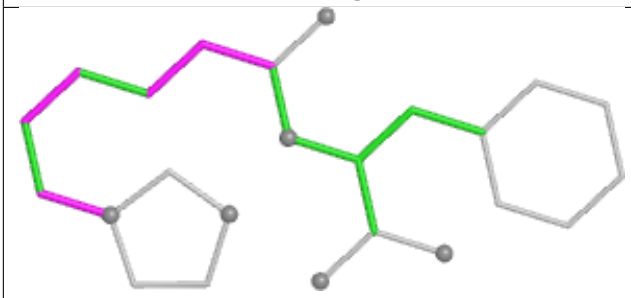
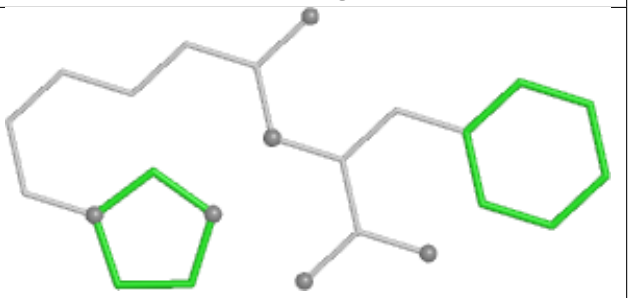


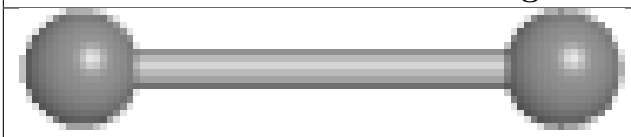
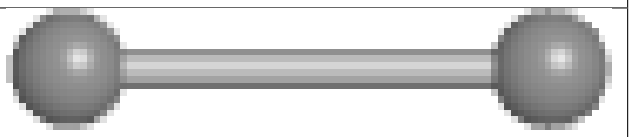
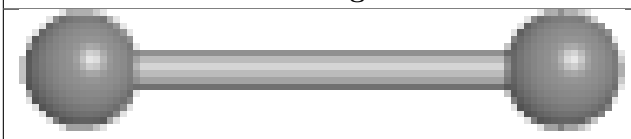
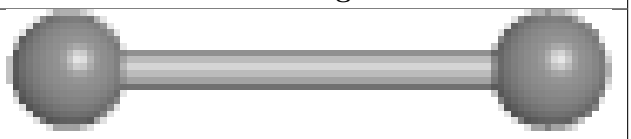
Bond angles

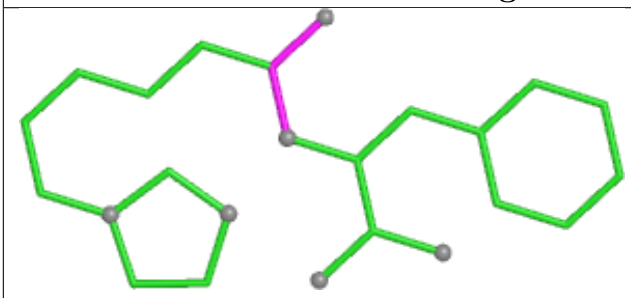
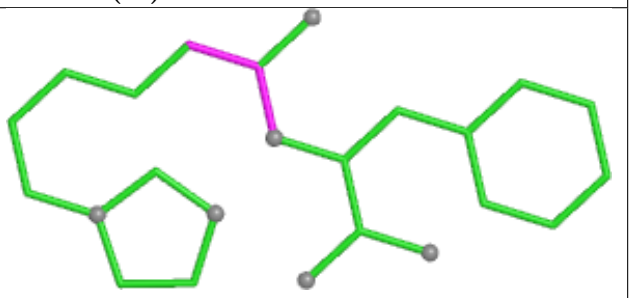
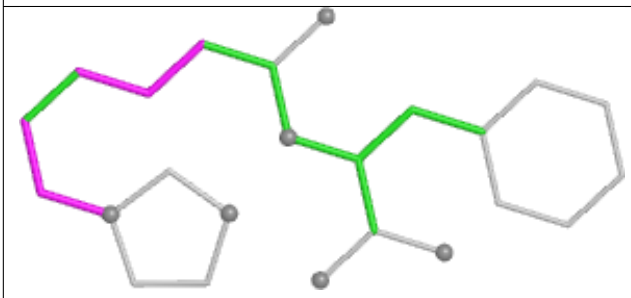
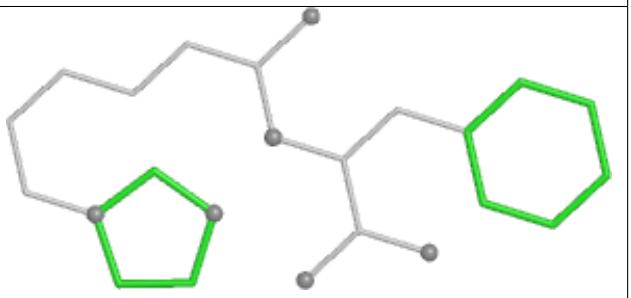


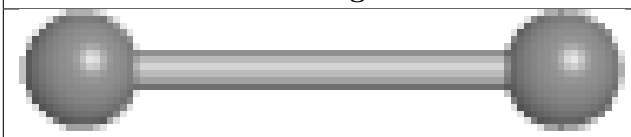
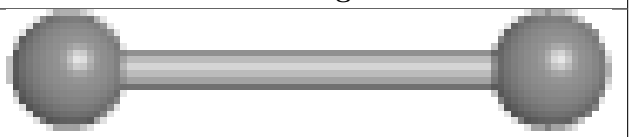
Torsions



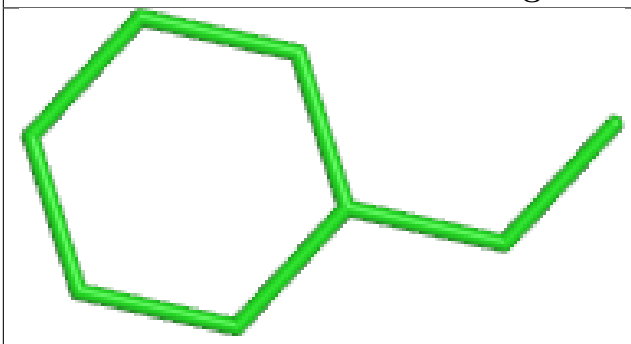
Rings

Ligand HOA B 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

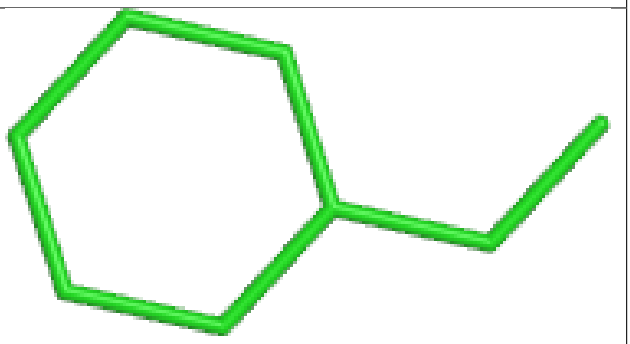
Ligand IC6 A 502 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HOA A 503	
Bond lengths	Bond angles
 Torsions	 Rings

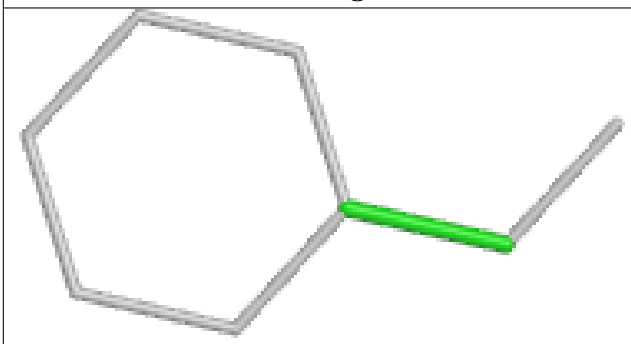
Ligand SYN A 509



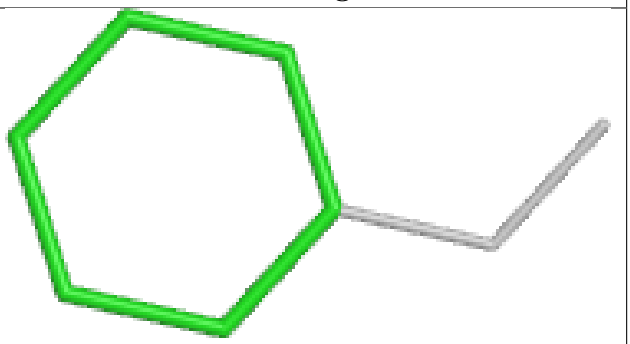
Bond lengths



Bond angles

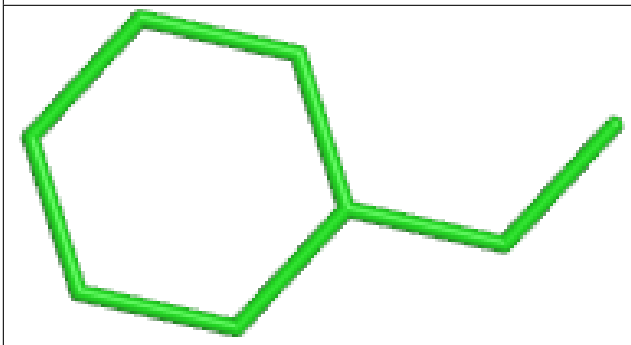


Torsions

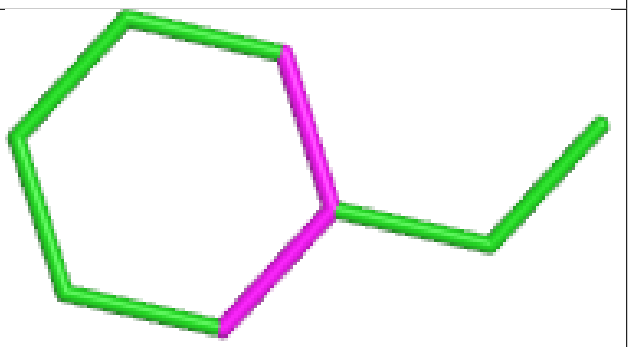


Rings

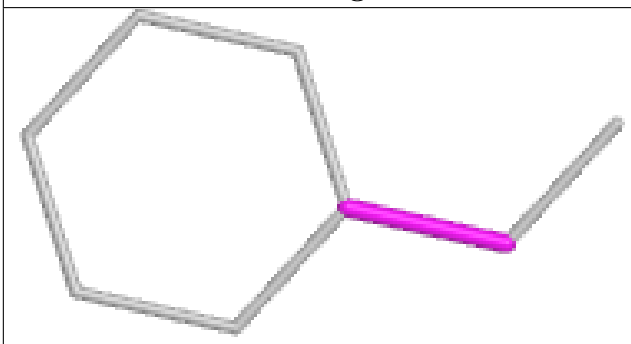
Ligand SYN A 505



Bond lengths



Bond angles



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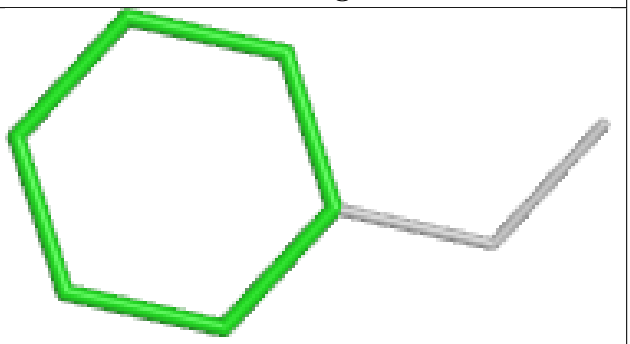
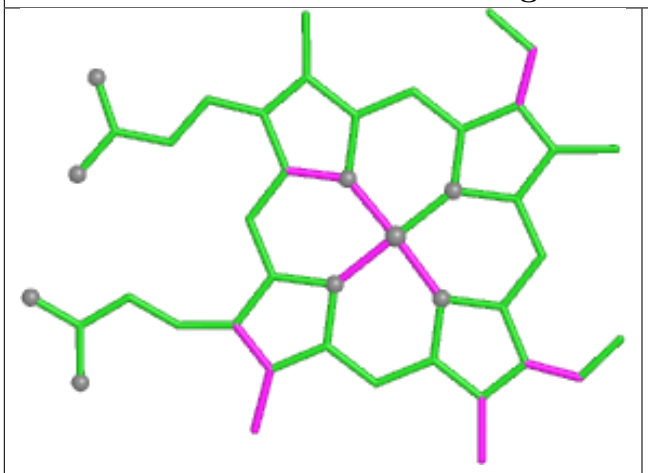
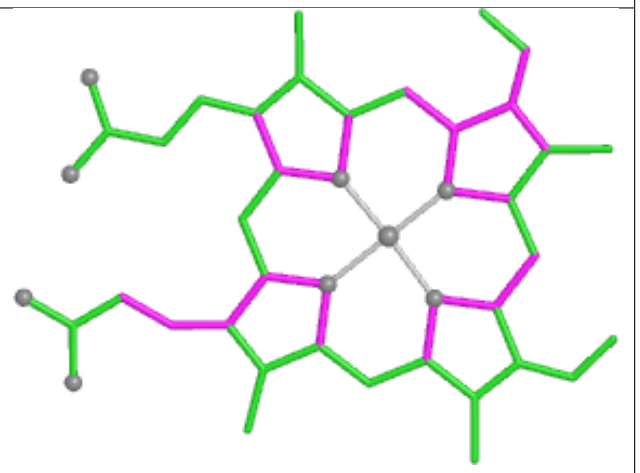


Rings

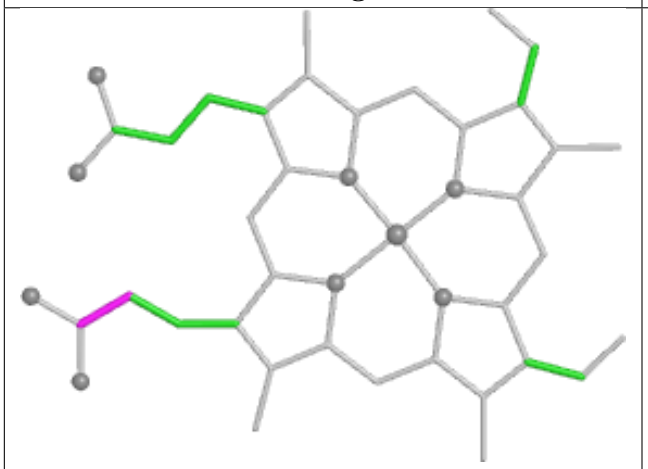
Ligand HEM B 501



Bond lengths



Bond angles



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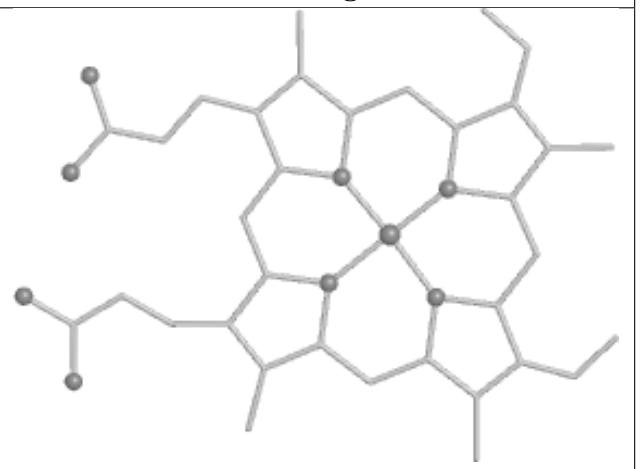
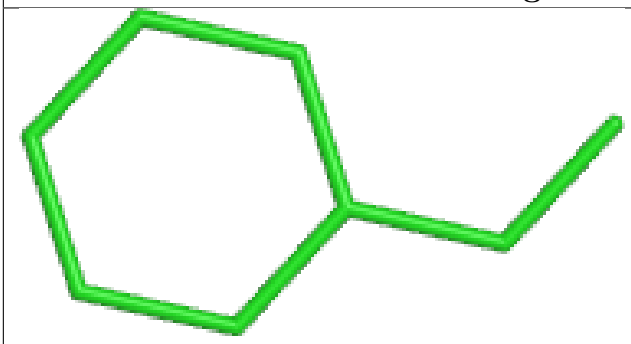
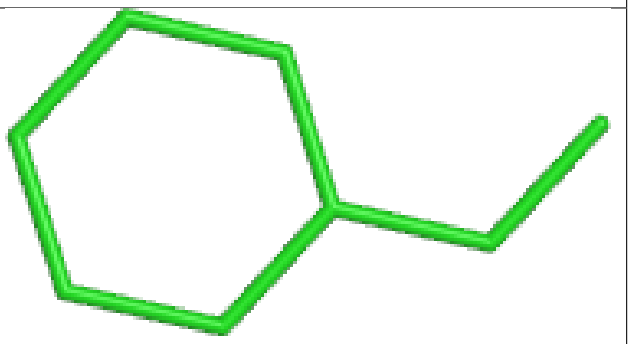


Rings

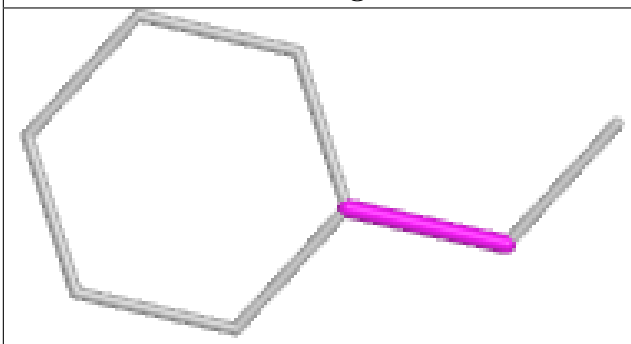
Ligand SYN A 506



Bond lengths



Bond angles



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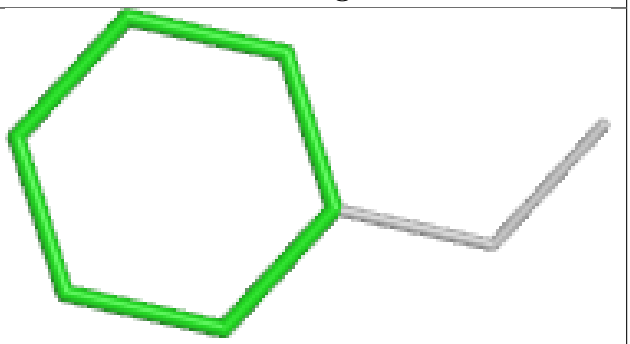
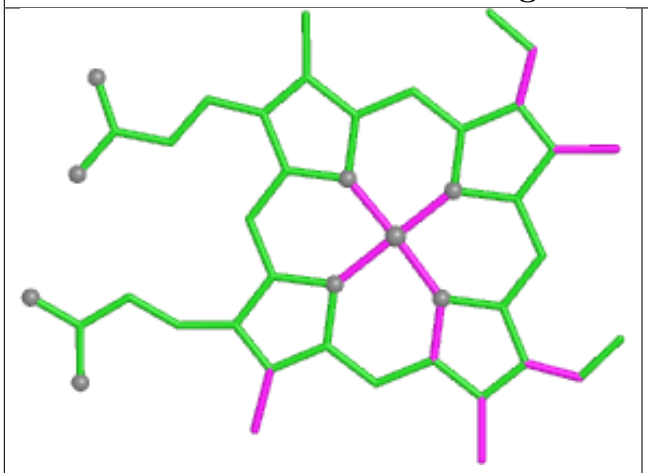
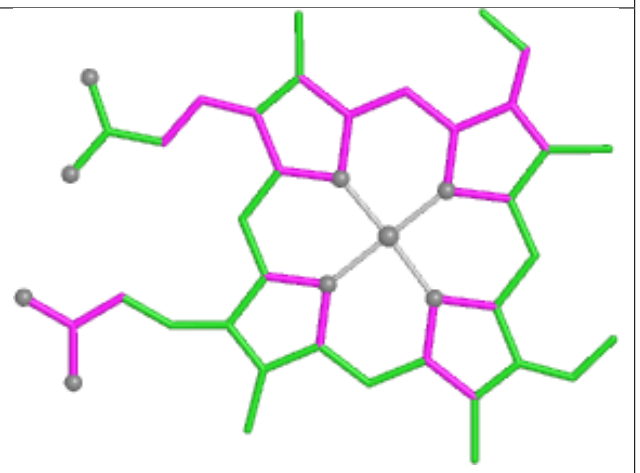


Rings

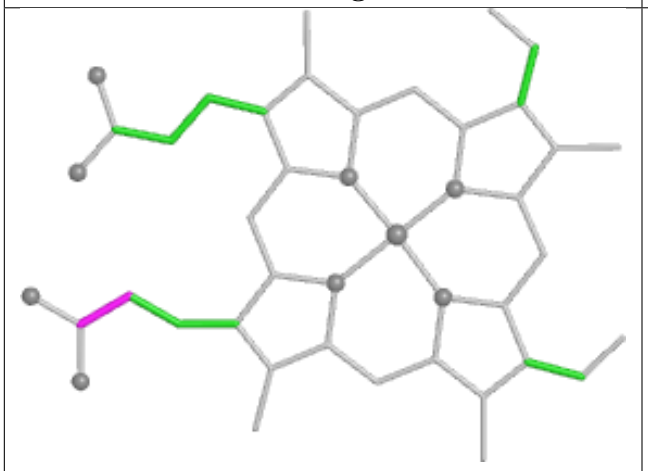
Ligand HEM A 501



Bond lengths



Bond angles



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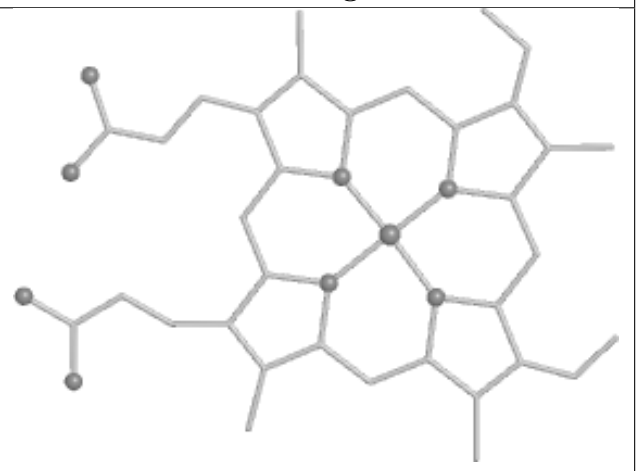
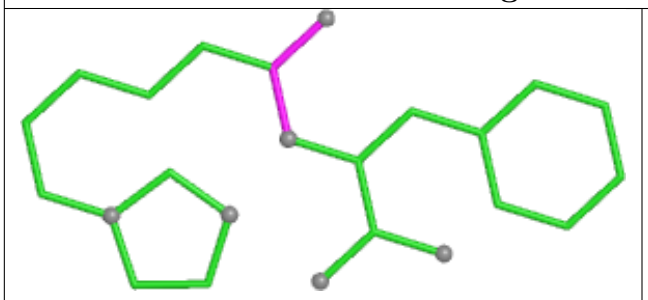


Rings

Ligand IC6 B 502 (A)



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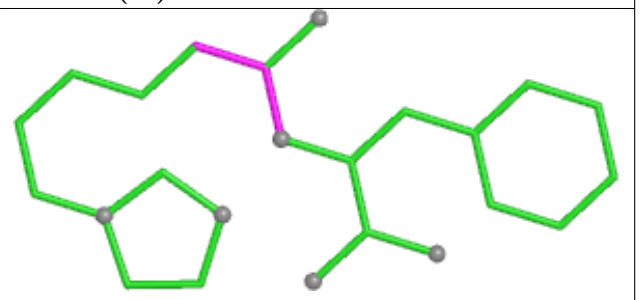
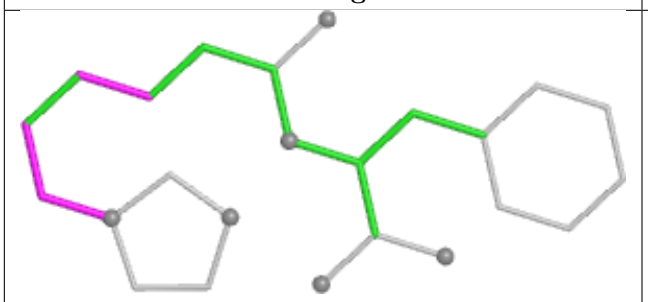
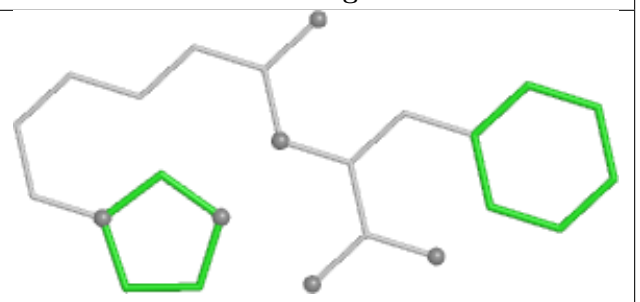


Bond angles



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	449/465 (96%)	0.52	19 (4%)	40	43	29, 43, 70, 92	0
1	B	449/465 (96%)	0.58	22 (4%)	35	37	30, 45, 70, 90	0
All	All	898/930 (96%)	0.55	41 (4%)	37	40	29, 44, 70, 92	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	PHE	4.1
1	A	158	PHE	3.8
1	B	383	SER	3.7
1	A	215	LEU	3.6
1	B	196	PRO	3.4
1	A	197	ALA	3.3
1	B	381	ASN	3.2
1	B	174	ILE	3.1
1	A	191	ALA	3.1
1	A	176	SER	3.0
1	A	216	VAL	3.0
1	B	172	PRO	3.0
1	B	231	ASP	3.0
1	A	174	ILE	2.9
1	B	384	ALA	2.9
1	B	215	LEU	2.8
1	A	199	ASP	2.7
1	A	2	ILE	2.7
1	A	225	ALA	2.6
1	A	231	ASP	2.6
1	A	258	ILE	2.6
1	A	209	ILE	2.5
1	A	198	TYR	2.5
1	B	228	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	2.4
1	B	201	ASN	2.4
1	B	199	ASP	2.3
1	B	233	LEU	2.3
1	B	205	PHE	2.3
1	A	196	PRO	2.3
1	B	197	ALA	2.2
1	B	221	ALA	2.2
1	B	14	LEU	2.2
1	A	219	ILE	2.1
1	B	265	GLY	2.1
1	B	81	PHE	2.1
1	A	110	GLN	2.1
1	B	136	ASP	2.0
1	A	211	VAL	2.0
1	B	182	ASP	2.0
1	B	198	TYR	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	A	507	8/8	0.72	0.20	61,72,76,77	0
5	SYN	A	509	8/8	0.76	0.20	55,69,72,73	0
5	SYN	A	505	8/8	0.80	0.18	54,59,62,62	0
5	SYN	A	506	8/8	0.86	0.14	53,60,66,71	0
3	IC6	B	504[B]	24/24	0.87	0.13	32,37,41,43	24
3	IC6	A	504[B]	24/24	0.90	0.14	33,37,44,47	24

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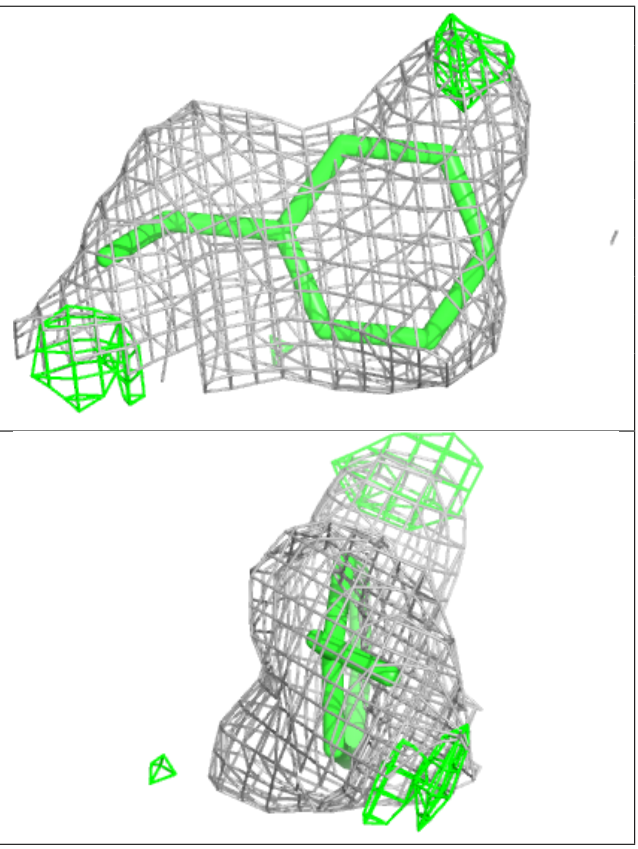
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IC6	B	502[A]	24/24	0.92	0.12	28,33,38,40	24
4	HOA	A	503	2/2	0.92	0.13	36,36,36,51	0
6	GOL	A	508	6/6	0.92	0.10	30,54,61,75	0
3	IC6	A	502[A]	24/24	0.93	0.11	25,33,42,48	24
4	HOA	B	503	2/2	0.95	0.24	38,38,38,51	0
2	HEM	B	501	43/43	0.97	0.08	25,33,37,43	0
2	HEM	A	501	43/43	0.97	0.07	24,32,37,46	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 A 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 A 509:

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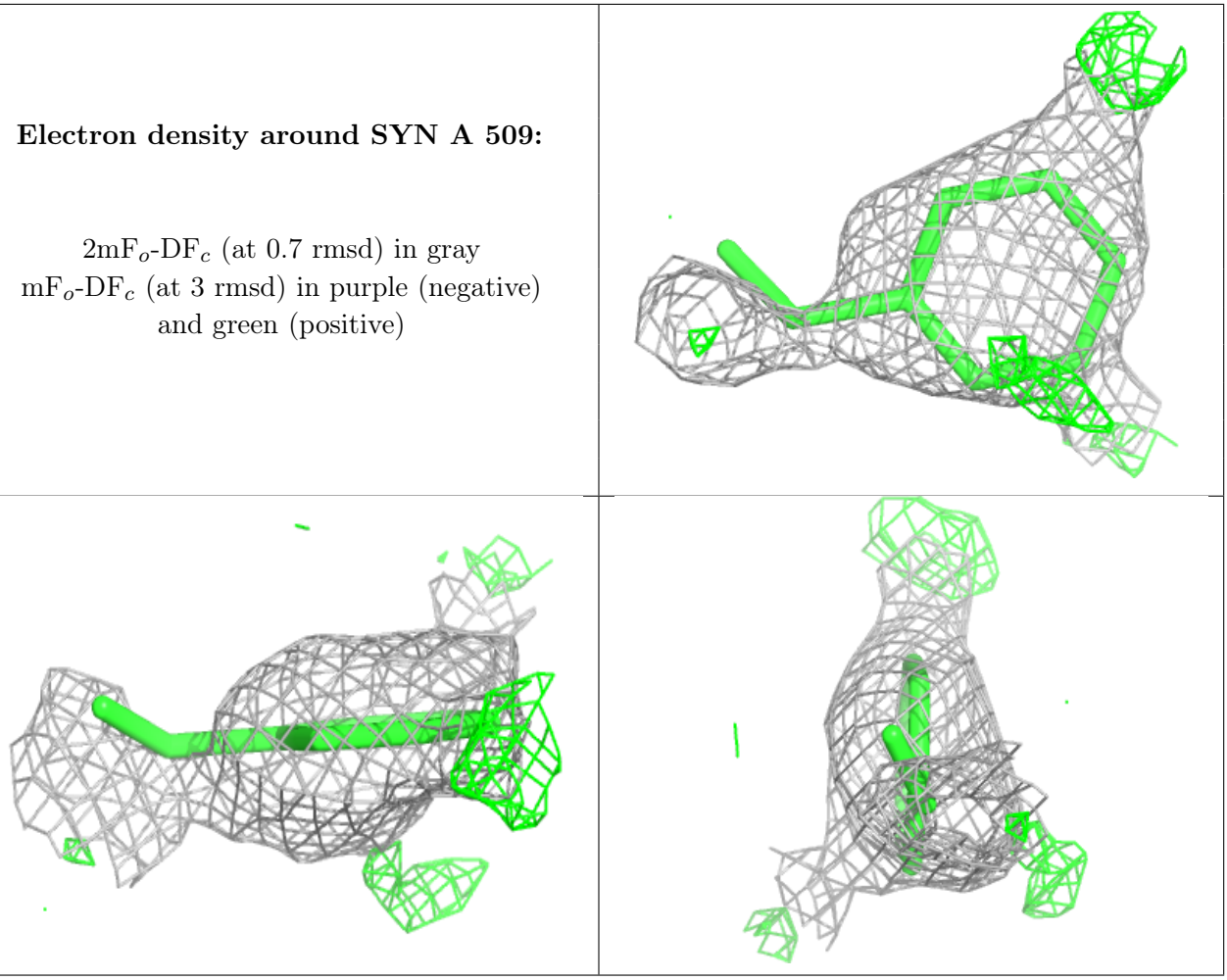
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SYN A 505:

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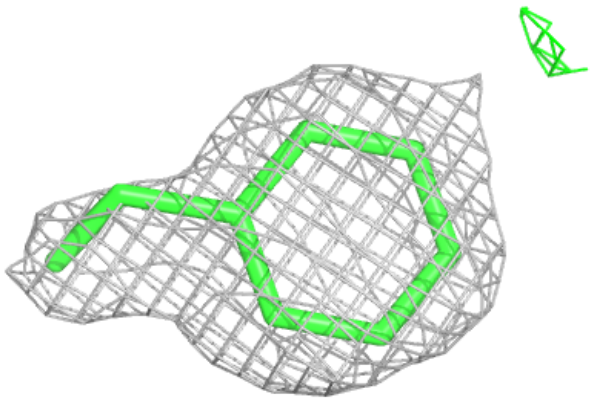
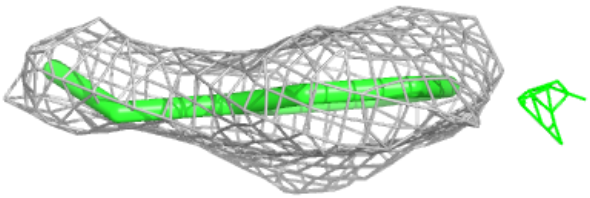
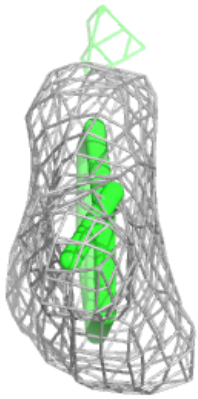
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

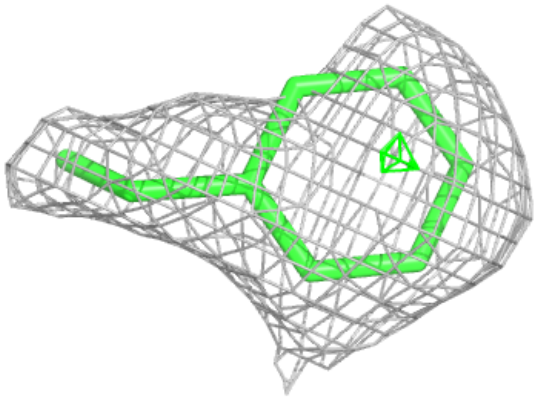


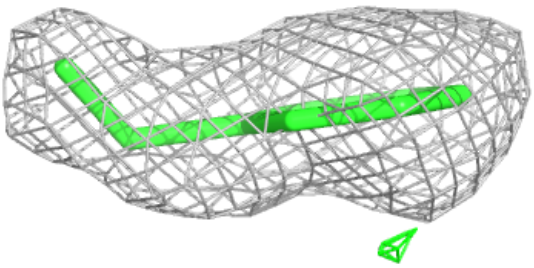


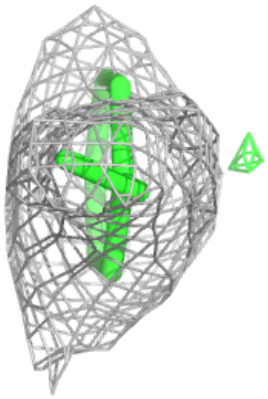


Electron density around SYN A 506:

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







Electron density around IC6 B 504 (B):

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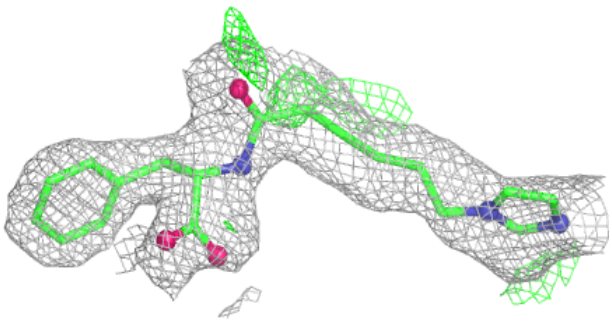
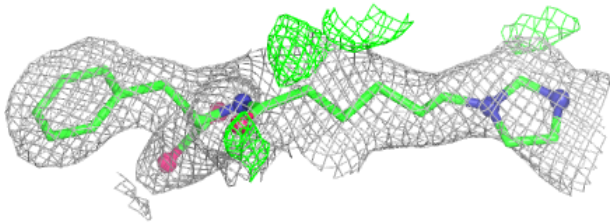
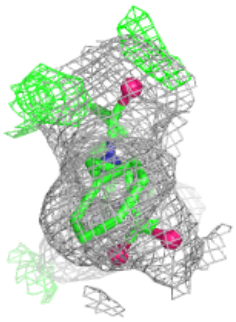
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around IC6 A 504 (B):

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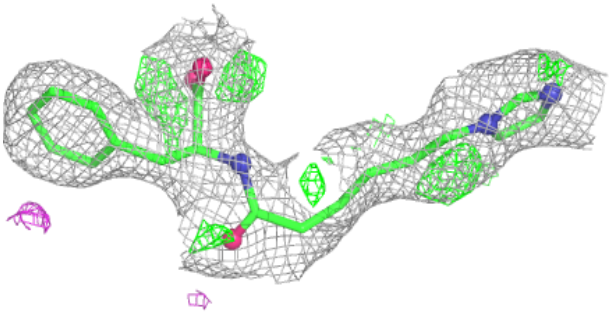
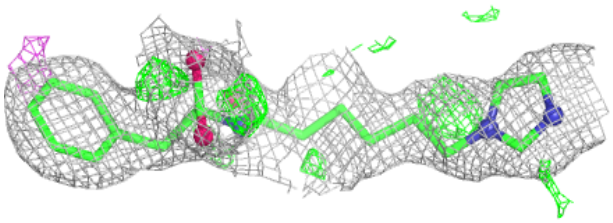
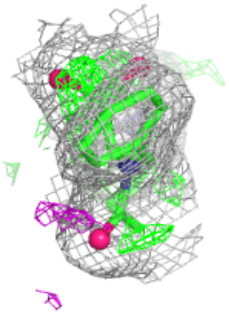
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around IC6 B 502 (A):

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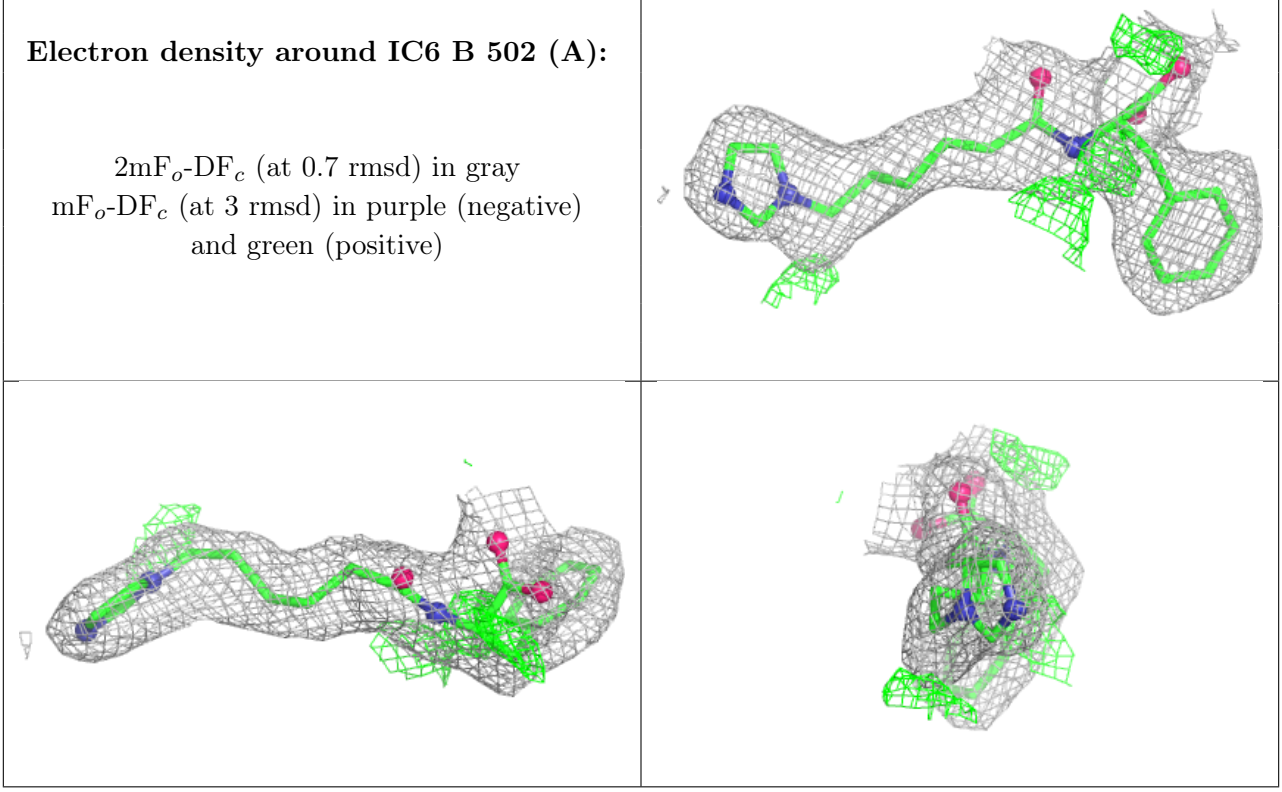
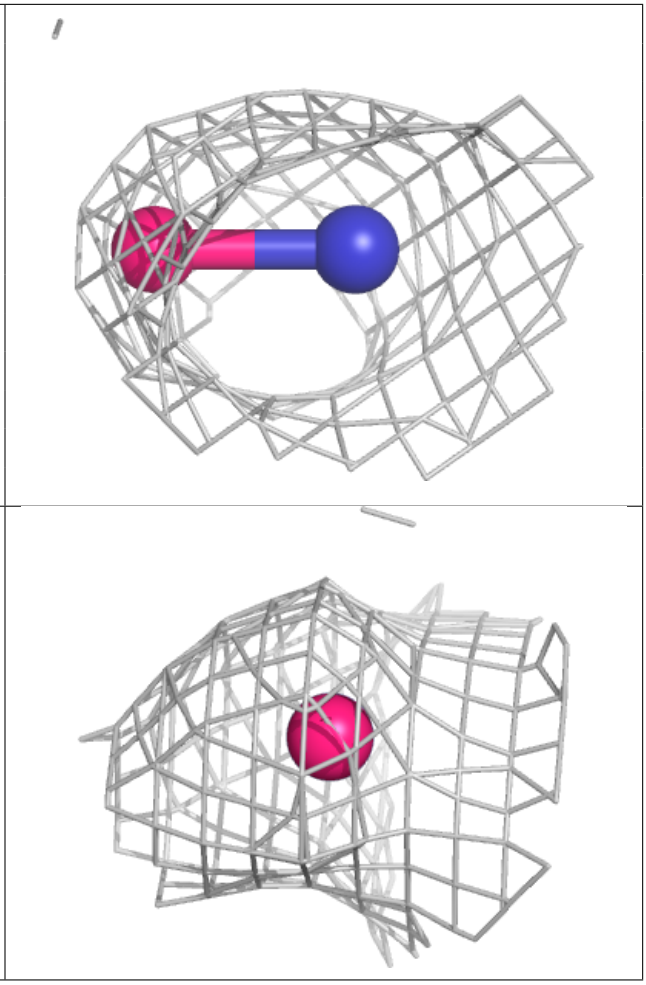
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



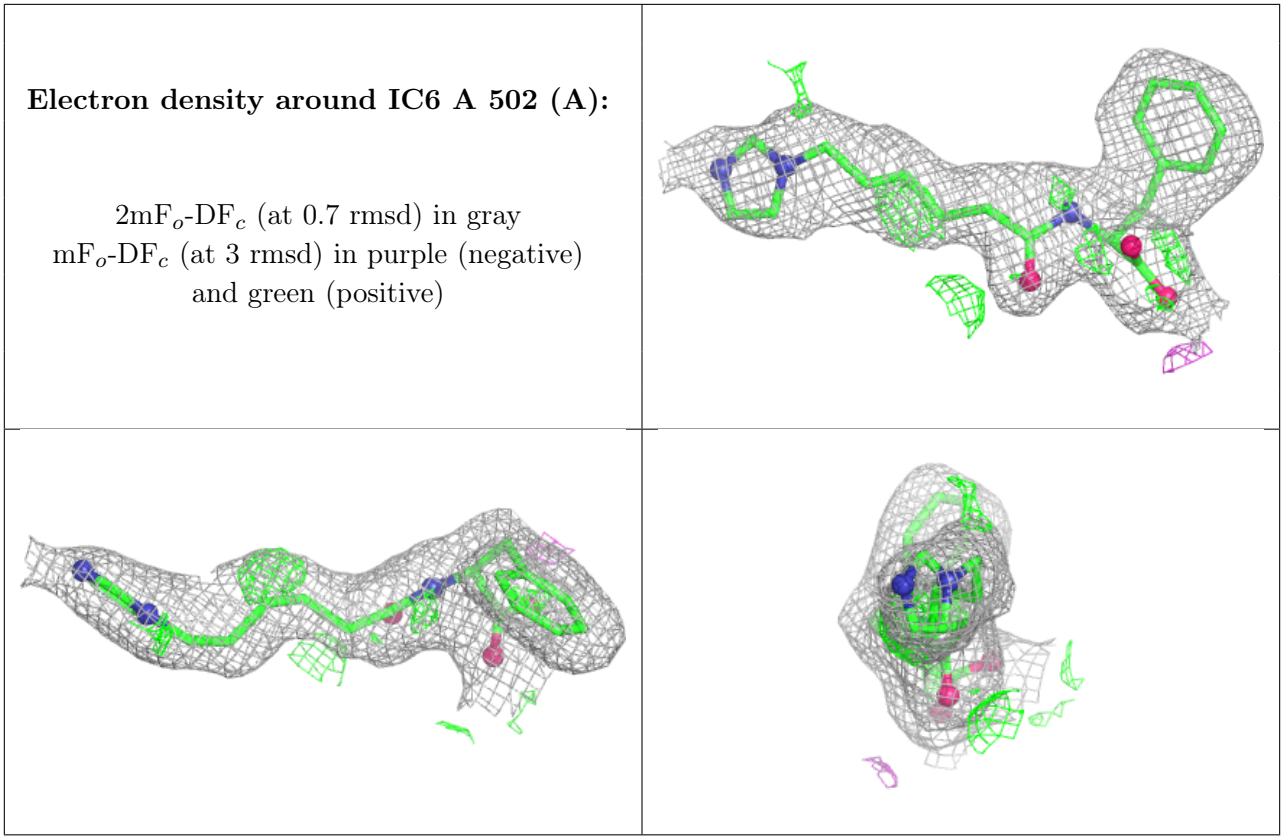
Electron density around HOA A 503:

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



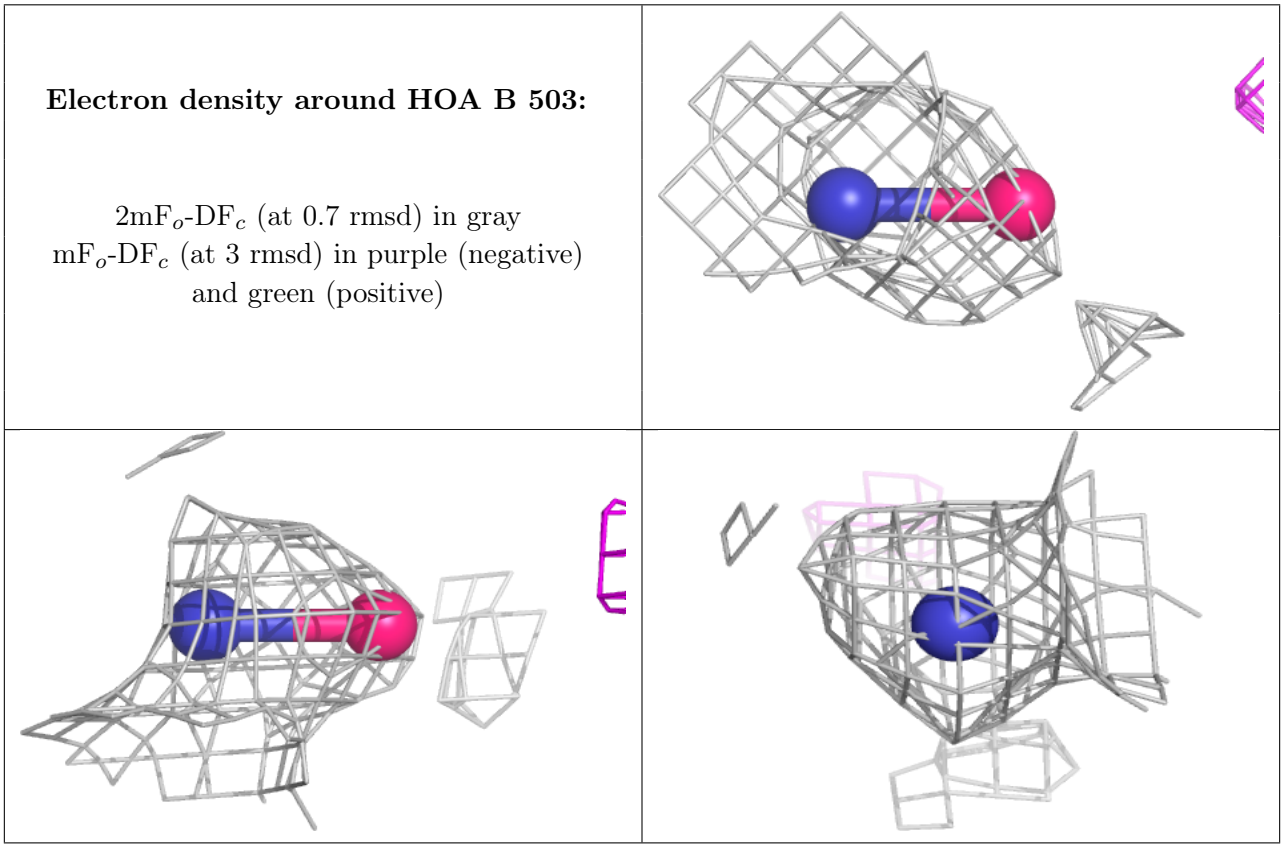
Electron density around IC6 A 502 (A):

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



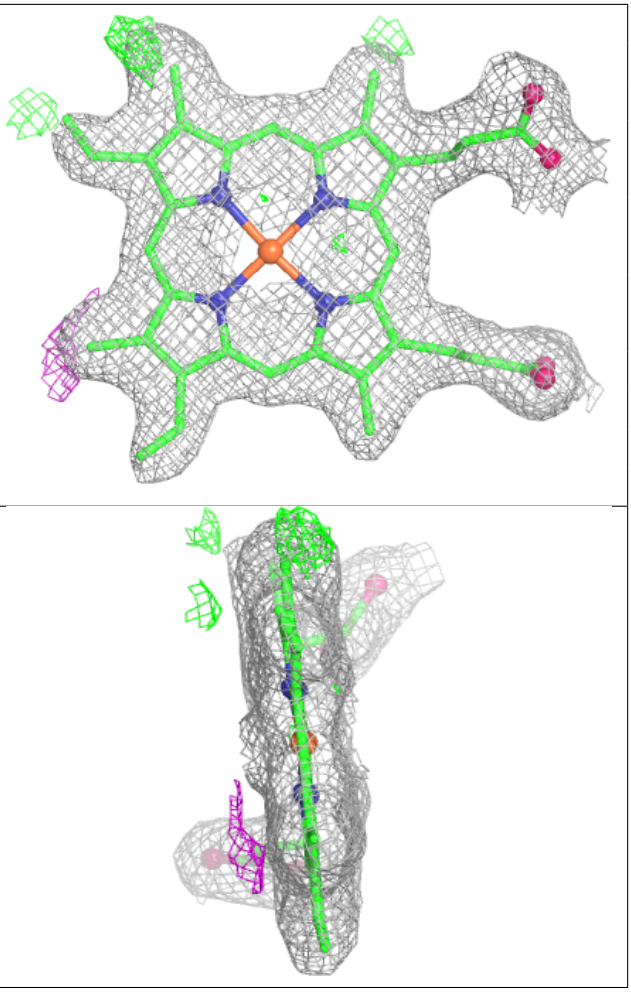
Electron density around HOA B 503:

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



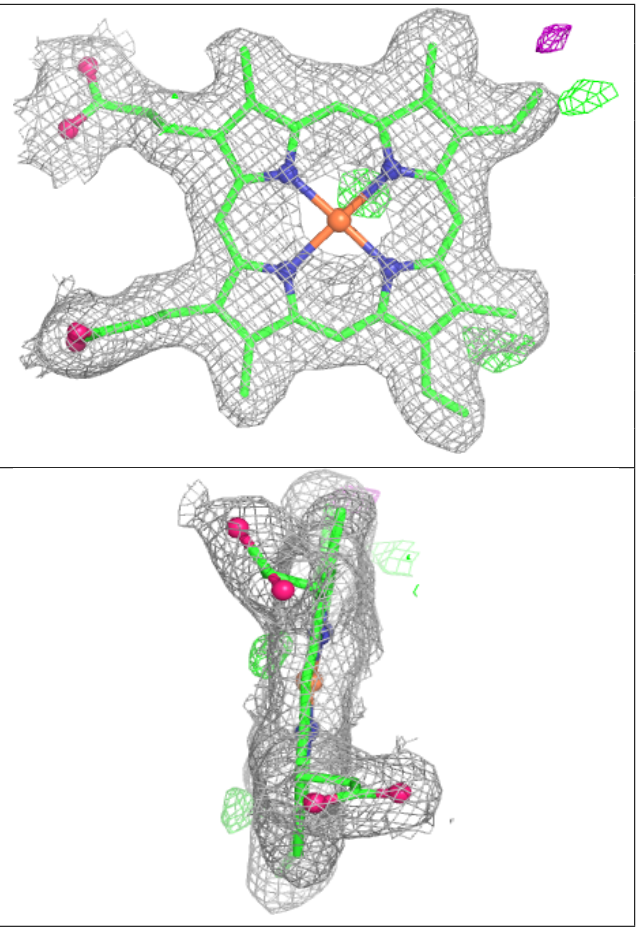
Electron density around HEM B 501:

$2mF_o$-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.