Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2026 – 09:09 AM EDT

PDB ID	:	6UD5 / pdb_00006ud5
Title	:	Crystal structure of human tryptophan 2,3-dioxygenase in complex with carbon monoxide and tryptophan
Authors	:	Pham, K.N.; Lewis-Ballester, A.; Yeh, S.R.
Deposited on	:	2019-09-18
Resolution	:	2.05 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:

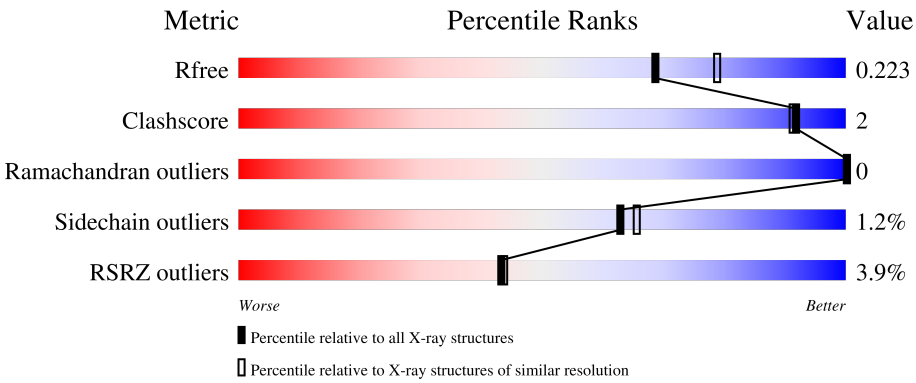
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	380	4% 88% • 8%
1	B	380	4% 86% 5% 9%
1	C	380	4% 86% • 10%
1	D	380	3% 90% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12705 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2946	1891	518	526	11	0	0	0
1	B	347	2898	1864	504	519	11	0	0	0
1	C	343	2825	1816	494	504	11	0	0	0
1	D	353	2963	1902	523	527	11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	UNP P48775
B	17	MET	-	initiating methionine	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	HIS	-	expression tag	UNP P48775
C	17	MET	-	initiating methionine	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775

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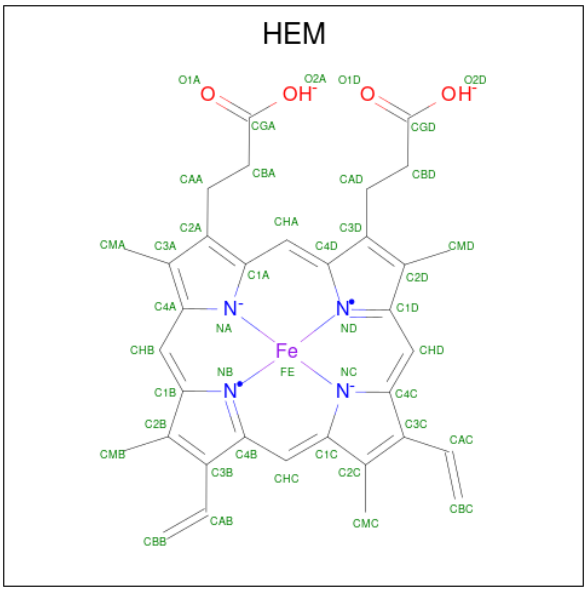
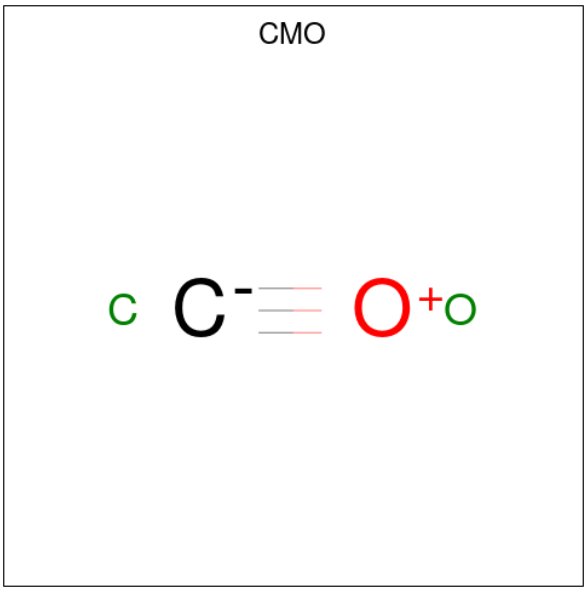
Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

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



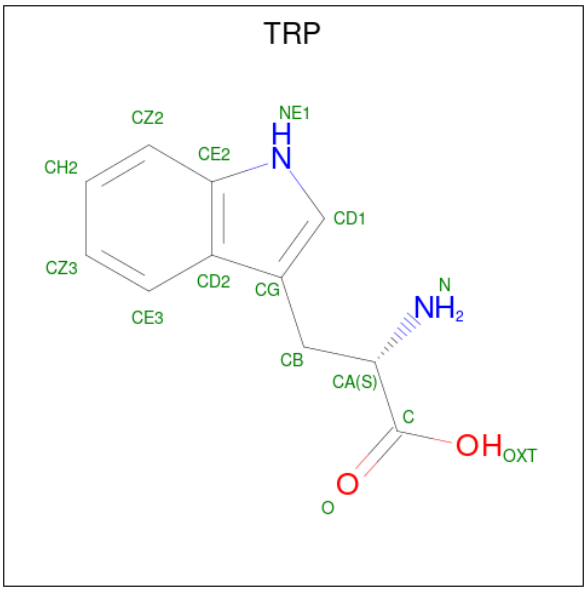
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	2	1	1	0	0
			Total	C	O		
3	B	1	2	1	1	0	0
			Total	C	O		
3	C	1	2	1	1	0	0
			Total	C	O		
3	D	1	2	1	1	0	0

- Molecule 4 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	15	11	2	2	0	0
			Total	C	N	O		
4	A	1	15	11	2	2	0	0
			Total	C	N	O		
4	B	1	15	11	2	2	0	0
			Total	C	N	O		
4	B	1	15	11	2	2	0	0
			Total	C	N	O		
4	C	1	15	11	2	2	0	0
			Total	C	N	O		
4	C	1	15	11	2	2	0	0
			Total	C	N	O		
4	D	1	15	11	2	2	0	0
			Total	C	N	O		
4	D	1	15	11	2	2	0	0

- Molecule 5 is water.

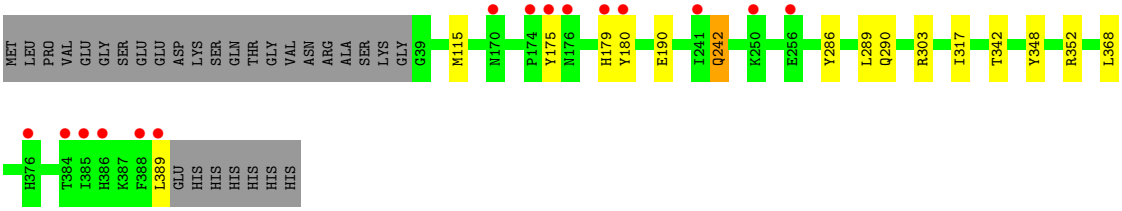
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	202	202	202	0	0
			Total	O		
5	B	214	214	214	0	0
			Total	O		
5	C	155	155	155	0	0
			Total	O		
5	D	202	202	202	0	0

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.

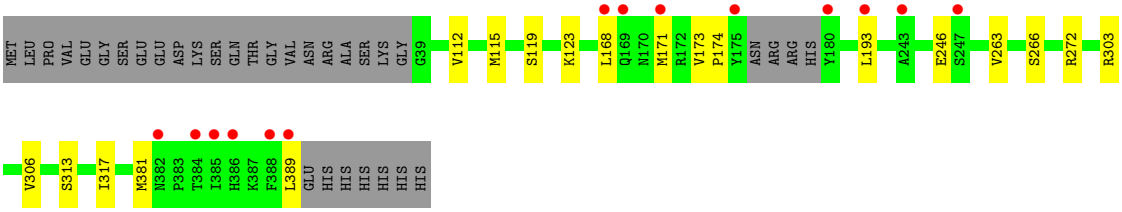
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain A:



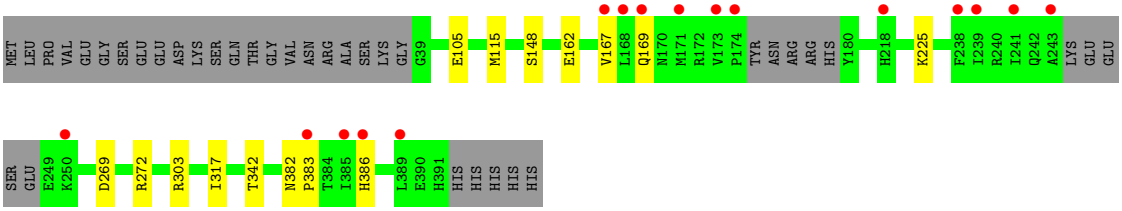
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain B:



• Molecule 1: Tryptophan 2,3-dioxygenase

Chain C:



• Molecule 1: Tryptophan 2,3-dioxygenase

Chain D:

MET
LEU
PRO
VAL
GLU
GLY
SER
GLU
GLU
ASP
LYS
SER
GLN
THR
GLY
VAL
ASN
ARG
ALA
SER
LYS
GLY
G39
M115
L168
M171
Y175
H179
D182
E190
E216
I241
E281
R303
I317
T342
P383
T384
I385
H386
K387
F388
L389
E390
H391
HIS

HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.72Å 154.49Å 88.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.05 19.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.97-2.05) 96.4 (19.97-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.183 , 0.217 0.190 , 0.223	Depositor DCC
R_{free} test set	6206 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 30.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12705	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, CMO

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	0.96	0/3015	1.42	0/4059
1	B	0.96	0/2965	1.41	0/3992
1	C	0.98	0/2891	1.43	0/3899
1	D	0.97	0/3033	1.40	0/4083
All	All	0.97	0/11904	1.42	0/16033

There are no bond length outliers.

There are no bond angle outliers.

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	2946	0	2924	8	0
1	B	2898	0	2872	8	0
1	C	2825	0	2753	7	0
1	D	2963	0	2945	5	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	30	0	18	1	0
4	B	30	0	18	0	0
4	C	30	0	18	1	0
4	D	30	0	18	1	0
5	A	202	0	0	0	0
5	B	214	0	0	0	0
5	C	155	0	0	1	0
5	D	202	0	0	0	0
All	All	12705	0	11686	37	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 2.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:HEM:HBC2	2:D:500:HEM:HHD	1.78	0.66
2:B:500:HEM:HBC2	2:B:500:HEM:HHD	1.84	0.59
2:A:500:HEM:HBC2	2:A:500:HEM:HHD	1.88	0.55
1:C:162:GLU:HB3	1:C:167:VAL:HG11	1.89	0.55
1:A:242:GLN:HA	1:A:242:GLN:HE21	1.73	0.53
1:D:342:THR:HG1	4:D:502:TRP:N	2.05	0.53
1:D:115:MET:HE3	1:D:317:ILE:CD1	2.39	0.53
1:C:105:GLU:OE1	1:C:303:ARG:HD2	2.10	0.52
1:A:342:THR:HG1	4:A:502:TRP:N	2.09	0.51
2:C:500:HEM:HBC2	2:C:500:HEM:HHD	1.93	0.50
1:B:112:VAL:HG21	1:B:306:VAL:CG1	2.41	0.50
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.42	0.50
2:A:500:HEM:HMB1	2:A:500:HEM:HBB2	1.95	0.48
1:D:303:ARG:HD3	1:D:389:LEU:HA	1.96	0.47
1:B:303:ARG:HD3	1:B:389:LEU:HA	1.98	0.46
1:C:382:ASN:HB2	1:C:383:PRO:HD2	1.98	0.46
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.46	0.46
1:B:112:VAL:HG21	1:B:306:VAL:HG13	1.98	0.45
1:C:342:THR:HG1	4:C:502:TRP:N	2.14	0.45
1:C:269:ASP:CG	1:C:272:ARG:HB2	2.41	0.45
1:C:148:SER:HB2	5:C:640:HOH:O	2.17	0.44
1:D:168:LEU:HB2	1:D:171:MET:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:VAL:O	1:B:266:SER:OG	2.28	0.44
2:B:500:HEM:HMB1	2:B:500:HEM:HBB2	1.99	0.44
2:A:500:HEM:HBB2	2:A:500:HEM:CMB	2.48	0.43
1:B:168:LEU:HD13	1:B:171:MET:HB2	2.01	0.43
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.49	0.43
1:A:289:LEU:HG	1:A:368:LEU:HD21	2.00	0.43
1:A:175:TYR:O	1:A:179:HIS:HB2	2.20	0.42
1:A:348:TYR:CZ	1:A:352:ARG:HD2	2.55	0.42
2:C:500:HEM:HMB1	2:C:500:HEM:HBB2	2.01	0.42
2:D:500:HEM:HBB2	2:D:500:HEM:HMB1	2.02	0.42
1:D:171:MET:HE3	1:D:171:MET:HA	2.02	0.42
1:B:173:VAL:HG13	1:B:174:PRO:HD2	2.03	0.41
1:A:303:ARG:HD3	1:A:389:LEU:HA	2.02	0.41
1:B:119:SER:O	1:B:123:LYS:HG2	2.21	0.40
1:A:286:TYR:O	1:A:290:GLN:HG3	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	349/380 (92%)	341 (98%)	8 (2%)	0	100	100
1	B	343/380 (90%)	337 (98%)	6 (2%)	0	100	100
1	C	337/380 (89%)	328 (97%)	9 (3%)	0	100	100
1	D	351/380 (92%)	346 (99%)	5 (1%)	0	100	100
All	All	1380/1520 (91%)	1352 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/348 (92%)	317 (99%)	3 (1%)	70	75
1	B	314/348 (90%)	309 (98%)	5 (2%)	55	56
1	C	300/348 (86%)	297 (99%)	3 (1%)	68	72
1	D	322/348 (92%)	318 (99%)	4 (1%)	63	65
All	All	1256/1392 (90%)	1241 (99%)	15 (1%)	63	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	TYR
1	A	190	GLU
1	A	242	GLN
1	B	193	LEU
1	B	246	GLU
1	B	272	ARG
1	B	313	SER
1	B	381	MET
1	C	169	GLN
1	C	225	LYS
1	C	386	HIS
1	D	182	ASP
1	D	190	GLU
1	D	216	GLU
1	D	281	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	64	ASN
1	A	242	GLN
1	A	253	GLN

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Mol	Chain	Res	Type
1	B	53	ASN
1	B	183	ASN
1	B	309	GLN
1	B	327	ASN
1	C	98	GLN
1	C	275	HIS
1	C	309	GLN
1	C	386	HIS
1	D	179	HIS
1	D	183	ASN
1	D	275	HIS
1	D	327	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)

16 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	CMO	A	501	-	0,1,1	-	-	-		
4	TRP	B	503	-	15,16,16	0.66	1 (6%)	18,22,22	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	B	500	1	50,50,50	1.55	9 (18%)	67,82,82	1.59	13 (19%)
4	TRP	A	502	-	15,16,16	0.65	1 (6%)	18,22,22	0.65	1 (5%)
4	TRP	B	502	-	15,16,16	0.71	1 (6%)	18,22,22	0.74	1 (5%)
2	HEM	D	500	1	50,50,50	1.57	7 (14%)	67,82,82	1.60	14 (20%)
4	TRP	D	503	-	15,16,16	0.65	1 (6%)	18,22,22	0.74	1 (5%)
4	TRP	D	502	-	15,16,16	0.60	0	18,22,22	0.55	0
4	TRP	C	502	-	15,16,16	0.67	1 (6%)	18,22,22	0.74	1 (5%)
3	CMO	D	501	-	0,1,1	-	-	-		
2	HEM	A	500	1	50,50,50	1.54	7 (14%)	67,82,82	1.59	14 (20%)
3	CMO	B	501	-	0,1,1	-	-	-		
4	TRP	C	503	-	15,16,16	0.71	1 (6%)	18,22,22	0.84	1 (5%)
3	CMO	C	501	-	0,1,1	-	-	-		
4	TRP	A	503	-	15,16,16	0.66	1 (6%)	18,22,22	0.75	1 (5%)
2	HEM	C	500	1	50,50,50	1.49	5 (10%)	67,82,82	1.67	15 (22%)

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
4	TRP	B	503	-	-	1/8/8/8	0/2/2/2
2	HEM	B	500	1	-	4/14/54/54	-
4	TRP	A	502	-	-	2/8/8/8	0/2/2/2
4	TRP	B	502	-	-	4/8/8/8	0/2/2/2
2	HEM	D	500	1	-	3/14/54/54	-
4	TRP	D	503	-	-	1/8/8/8	0/2/2/2
4	TRP	D	502	-	-	2/8/8/8	0/2/2/2
4	TRP	C	502	-	-	4/8/8/8	0/2/2/2
2	HEM	A	500	1	-	2/14/54/54	-
4	TRP	C	503	-	-	1/8/8/8	0/2/2/2
4	TRP	A	503	-	-	1/8/8/8	0/2/2/2
2	HEM	C	500	1	-	2/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	FE-NB	5.52	2.11	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	FE-NB	5.16	2.10	1.94
2	A	500	HEM	FE-NB	5.16	2.10	1.94
2	C	500	HEM	FE-NB	5.12	2.10	1.94
2	A	500	HEM	FE-NC	4.11	2.08	1.95
2	C	500	HEM	FE-NC	4.07	2.08	1.95
2	B	500	HEM	FE-NC	3.94	2.08	1.95
2	D	500	HEM	FE-NC	3.67	2.07	1.95
2	D	500	HEM	C1B-NB	-3.44	1.34	1.40
2	B	500	HEM	C1B-NB	-3.32	1.34	1.40
2	A	500	HEM	C1B-NB	-3.16	1.34	1.40
2	C	500	HEM	C1B-NB	-3.04	1.35	1.40
2	B	500	HEM	C4D-ND	-2.86	1.35	1.40
2	A	500	HEM	C4D-ND	-2.58	1.35	1.40
2	D	500	HEM	C4D-ND	-2.57	1.35	1.40
2	C	500	HEM	C4D-ND	-2.55	1.35	1.40
2	D	500	HEM	C1C-C2C	-2.47	1.40	1.45
2	A	500	HEM	C3B-C4B	2.42	1.49	1.44
4	B	502	TRP	OXT-C	-2.39	1.23	1.30
2	A	500	HEM	C1C-C2C	-2.36	1.40	1.45
2	C	500	HEM	C3B-C4B	2.35	1.49	1.44
4	C	503	TRP	OXT-C	-2.35	1.23	1.30
2	B	500	HEM	C1D-ND	-2.34	1.34	1.38
2	B	500	HEM	C1C-C2C	-2.33	1.40	1.45
2	D	500	HEM	C1D-ND	-2.31	1.34	1.38
2	D	500	HEM	C4B-NB	-2.30	1.34	1.38
4	B	503	TRP	OXT-C	-2.18	1.23	1.30
4	C	502	TRP	OXT-C	-2.18	1.23	1.30
4	A	503	TRP	OXT-C	-2.15	1.23	1.30
4	D	503	TRP	OXT-C	-2.14	1.23	1.30
4	A	502	TRP	OXT-C	-2.14	1.23	1.30
2	A	500	HEM	C1D-ND	-2.13	1.34	1.38
2	B	500	HEM	O2D-CGD	-2.11	1.23	1.30
2	B	500	HEM	FE-ND	-2.09	1.88	1.94
2	B	500	HEM	C4B-NB	-2.04	1.34	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	CHC-C4B-NB	4.56	129.32	124.42
2	D	500	HEM	CHC-C4B-NB	4.35	129.10	124.42
2	A	500	HEM	CHC-C4B-NB	4.32	129.07	124.42
2	C	500	HEM	CHC-C4B-NB	4.17	128.91	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	HEM	C1B-NB-C4B	4.01	109.96	105.21
2	B	500	HEM	CHD-C1D-ND	3.97	128.70	124.42
2	D	500	HEM	CBD-CAD-C3D	-3.87	101.82	112.53
2	A	500	HEM	CBD-CAD-C3D	-3.82	101.97	112.53
2	C	500	HEM	CBD-CAD-C3D	-3.74	102.19	112.53
2	C	500	HEM	CHA-C4D-ND	3.69	128.93	124.37
2	D	500	HEM	CHA-C4D-ND	3.67	128.90	124.37
2	B	500	HEM	CBD-CAD-C3D	-3.54	102.74	112.53
2	B	500	HEM	C1B-NB-C4B	3.52	109.38	105.21
2	A	500	HEM	C1B-NB-C4B	3.52	109.38	105.21
2	D	500	HEM	C1B-NB-C4B	3.44	109.28	105.21
2	A	500	HEM	CHD-C1D-ND	3.40	128.08	124.42
2	C	500	HEM	CHD-C1D-ND	3.38	128.06	124.42
2	B	500	HEM	CHA-C4D-ND	3.37	128.54	124.37
2	A	500	HEM	CHA-C4D-ND	3.22	128.35	124.37
2	C	500	HEM	CHB-C1B-NB	3.07	128.16	124.37
2	D	500	HEM	CHD-C1D-ND	3.02	127.67	124.42
4	C	503	TRP	OXT-C-O	-2.99	117.30	124.08
2	B	500	HEM	CHD-C1D-C2D	-2.91	120.44	125.03
2	B	500	HEM	CHB-C1B-NB	2.73	127.74	124.37
2	C	500	HEM	C3B-C4B-NB	-2.73	107.51	109.47
2	C	500	HEM	CHD-C1D-C2D	-2.72	120.74	125.03
4	B	503	TRP	OXT-C-O	-2.62	118.13	124.08
2	A	500	HEM	CHD-C1D-C2D	-2.62	120.89	125.03
2	A	500	HEM	C3B-C4B-NB	-2.58	107.62	109.47
2	D	500	HEM	CHA-C4D-C3D	-2.56	120.51	125.23
2	A	500	HEM	CHA-C4D-C3D	-2.54	120.54	125.23
2	D	500	HEM	C1A-CHA-C4D	-2.54	120.27	126.25
2	A	500	HEM	CAC-C3C-C4C	2.53	130.86	124.82
2	D	500	HEM	O2D-CGD-CBD	2.52	121.95	114.00
4	C	502	TRP	OXT-C-O	-2.51	118.39	124.08
4	B	502	TRP	OXT-C-O	-2.49	118.42	124.08
2	C	500	HEM	C1A-CHA-C4D	-2.47	120.45	126.25
2	D	500	HEM	O2D-CGD-O1D	-2.43	117.07	123.33
4	A	503	TRP	OXT-C-O	-2.43	118.58	124.08
2	D	500	HEM	CMD-C2D-C1D	2.42	128.82	125.03
2	C	500	HEM	CAC-C3C-C4C	2.42	130.60	124.82
2	D	500	HEM	CHB-C1B-NB	2.42	127.36	124.37
2	C	500	HEM	O2D-CGD-CBD	2.41	121.60	114.00
2	C	500	HEM	CMD-C2D-C1D	2.38	128.76	125.03
2	A	500	HEM	CHB-C1B-NB	2.38	127.31	124.37
2	C	500	HEM	CHA-C4D-C3D	-2.35	120.89	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	503	TRP	OXT-C-O	-2.31	118.85	124.08
2	B	500	HEM	CHA-C4D-C3D	-2.30	120.98	125.23
2	B	500	HEM	O2D-CGD-CBD	2.29	121.25	114.00
2	D	500	HEM	CHD-C1D-C2D	-2.29	121.41	125.03
2	A	500	HEM	CMD-C2D-C1D	2.28	128.60	125.03
4	A	502	TRP	OXT-C-O	-2.15	119.21	124.08
2	B	500	HEM	CAC-C3C-C4C	2.14	129.92	124.82
2	A	500	HEM	CHD-C4C-NC	2.13	126.77	124.45
2	A	500	HEM	C1A-CHA-C4D	-2.10	121.31	126.25
2	B	500	HEM	C4B-C3B-C2B	-2.09	105.36	107.28
2	C	500	HEM	O2A-CGA-CBA	2.08	120.57	114.00
2	D	500	HEM	C4C-NC-C1C	2.08	109.21	105.82
2	A	500	HEM	C4C-NC-C1C	2.04	109.15	105.82
2	B	500	HEM	O2D-CGD-O1D	-2.03	118.10	123.33
2	C	500	HEM	CHD-C4C-NC	2.02	126.65	124.45
2	B	500	HEM	CHD-C4C-NC	2.02	126.65	124.45
2	D	500	HEM	C3B-C4B-NB	-2.00	108.03	109.47

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C4C-C3C-CAC-CBC
4	B	502	TRP	CA-CB-CG-CD1
4	A	502	TRP	CA-CB-CG-CD1
4	A	502	TRP	CA-CB-CG-CD2
4	C	502	TRP	CA-CB-CG-CD1
4	D	502	TRP	CA-CB-CG-CD1
4	B	502	TRP	CA-CB-CG-CD2
4	C	502	TRP	CA-CB-CG-CD2
4	D	502	TRP	CA-CB-CG-CD2
4	B	502	TRP	O-C-CA-CB
4	B	502	TRP	OXT-C-CA-CB
2	C	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O2A
2	D	500	HEM	CAA-CBA-CGA-O1A
4	D	503	TRP	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
4	C	502	TRP	OXT-C-CA-CB
4	C	502	TRP	O-C-CA-CB
4	A	503	TRP	CA-CB-CG-CD2
2	B	500	HEM	CAD-CBD-CGD-O2D
4	B	503	TRP	CA-CB-CG-CD2
4	C	503	TRP	CA-CB-CG-CD2
2	B	500	HEM	CAD-CBD-CGD-O1D

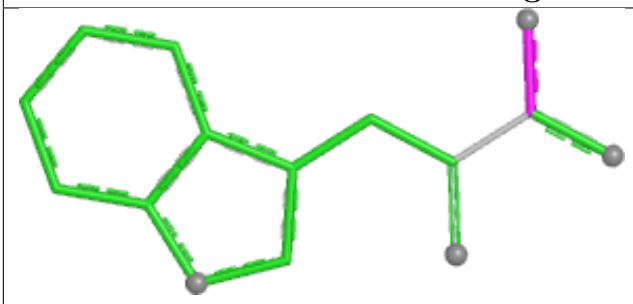
There are no ring outliers.

7 monomers are involved in 12 short contacts:

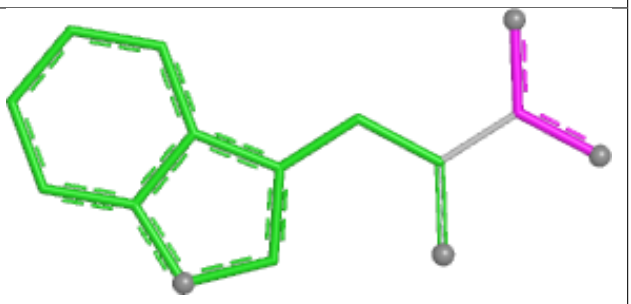
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	2	0
4	A	502	TRP	1	0
2	D	500	HEM	2	0
4	D	502	TRP	1	0
4	C	502	TRP	1	0
2	A	500	HEM	3	0
2	C	500	HEM	2	0

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.

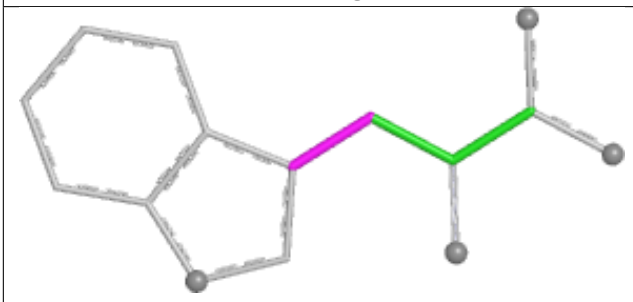
Ligand TRP B 503



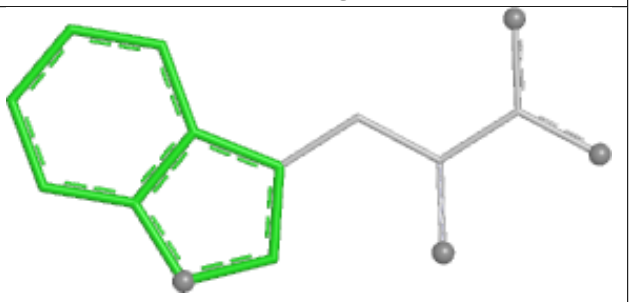
Bond lengths



Bond angles

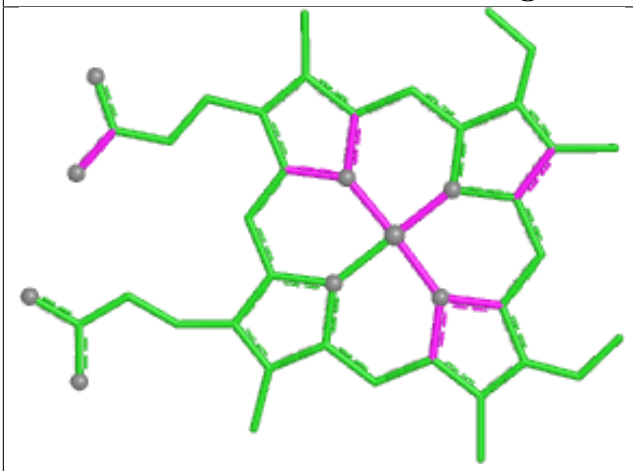


Torsions



Rings

Ligand HEM B 500



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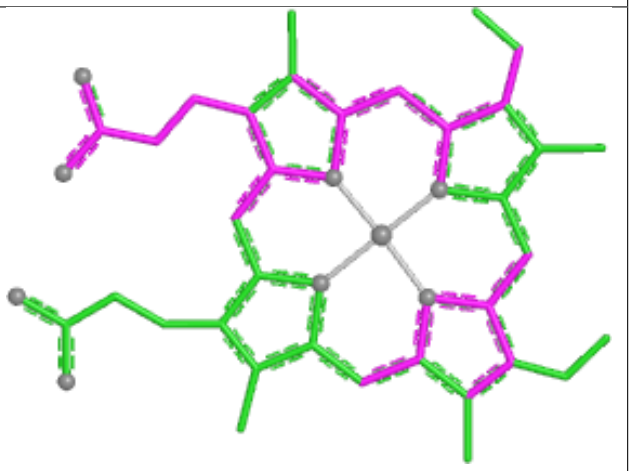

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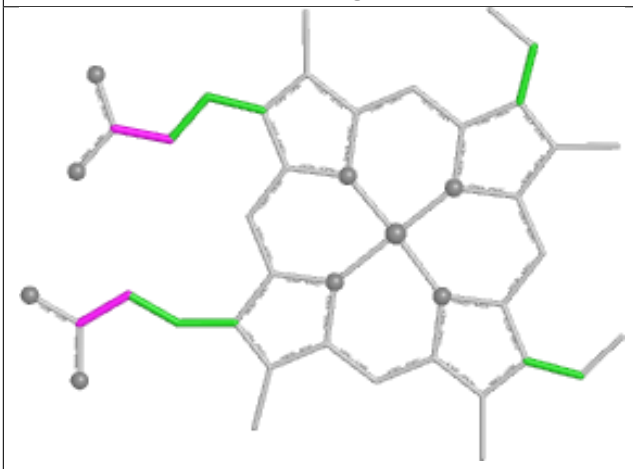

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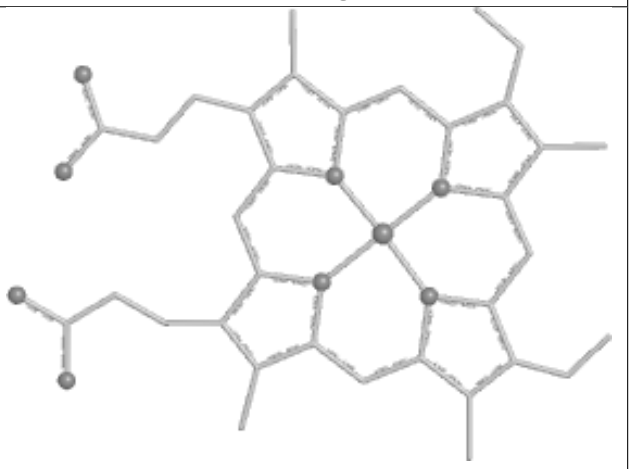
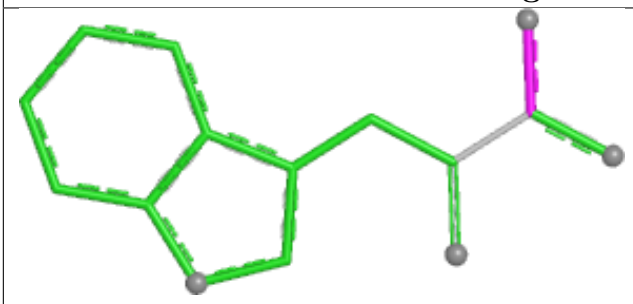


Rings

Ligand TRP A 502



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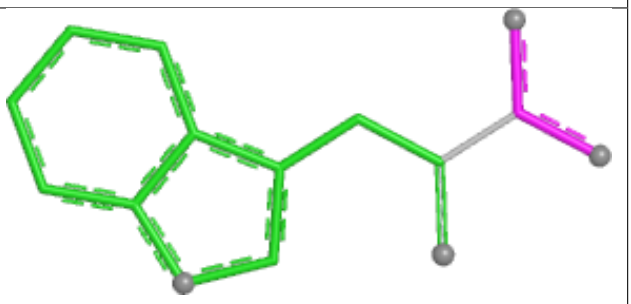
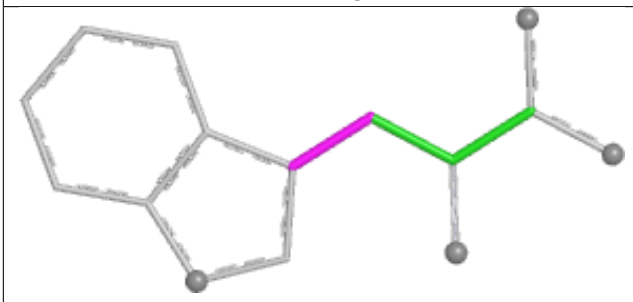


Bond angles



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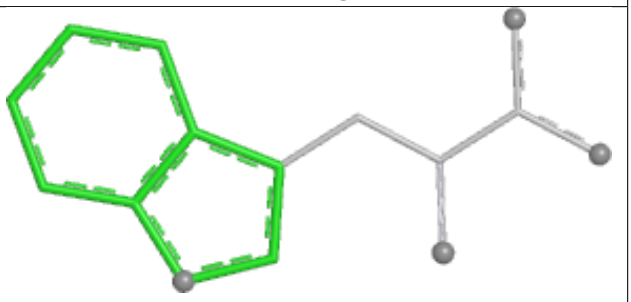
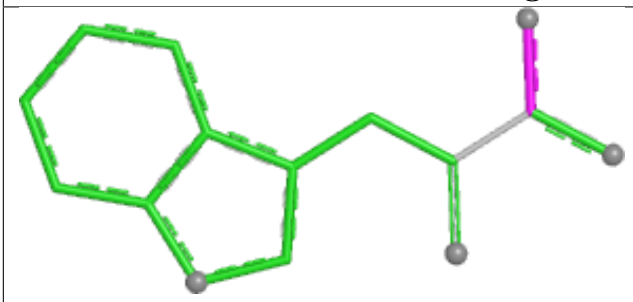


Rings

Ligand TRP B 502



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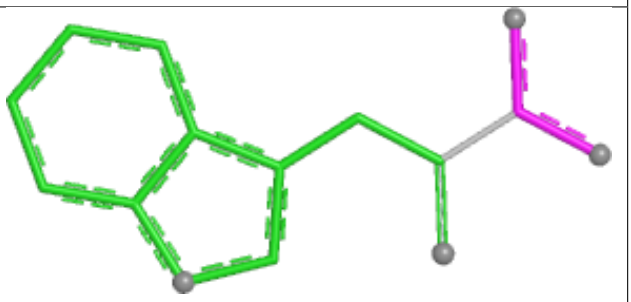

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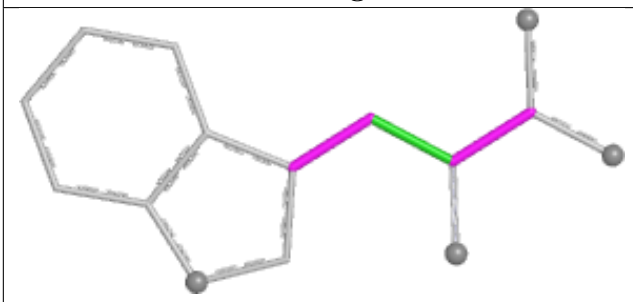

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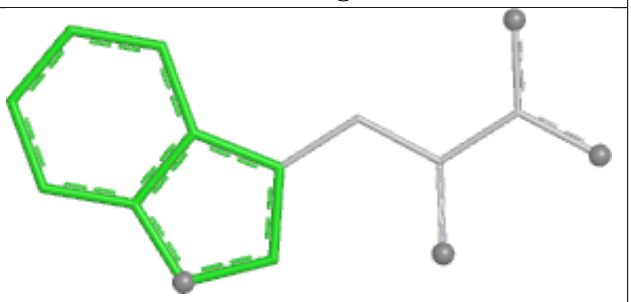
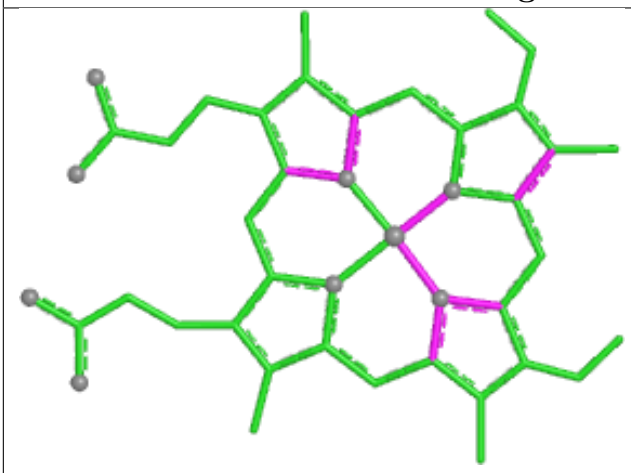


Rings

Ligand HEM D 500



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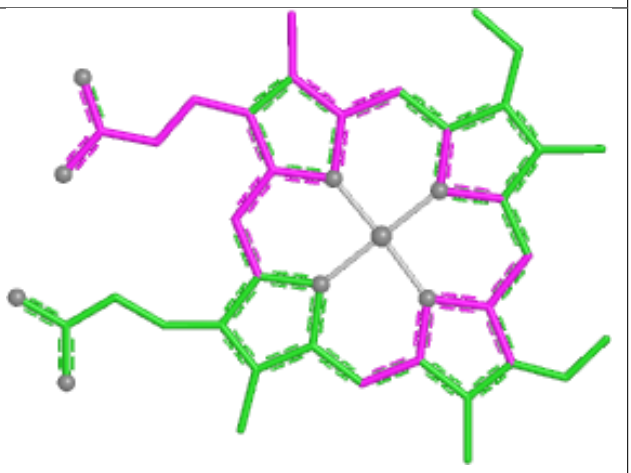

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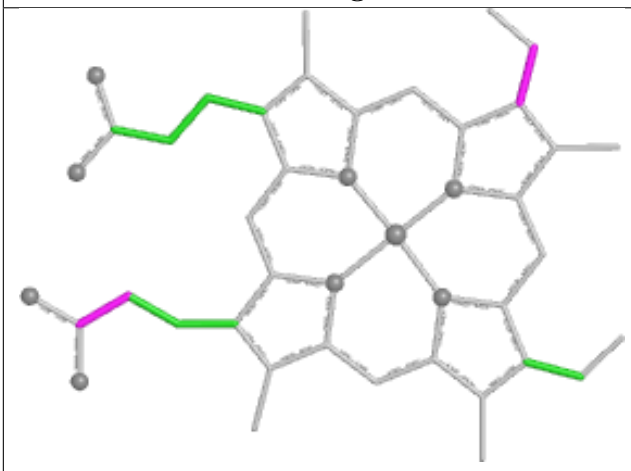

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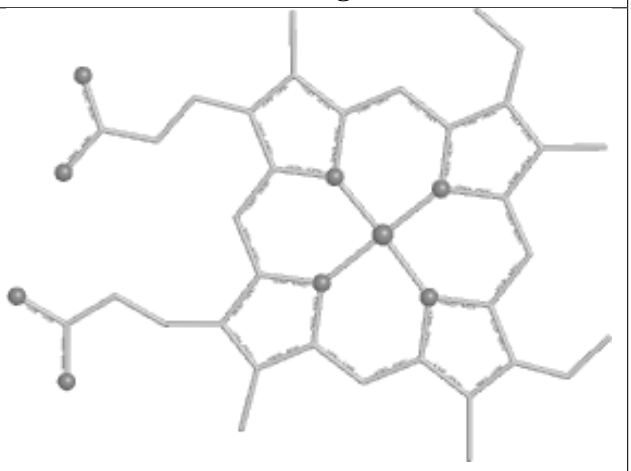
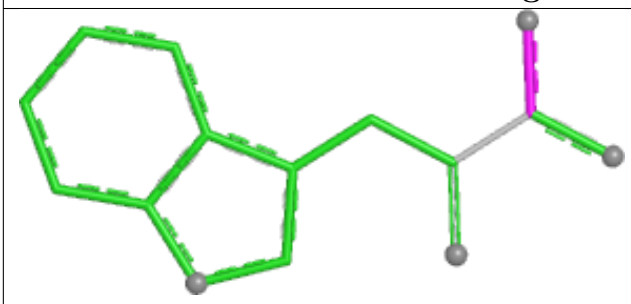
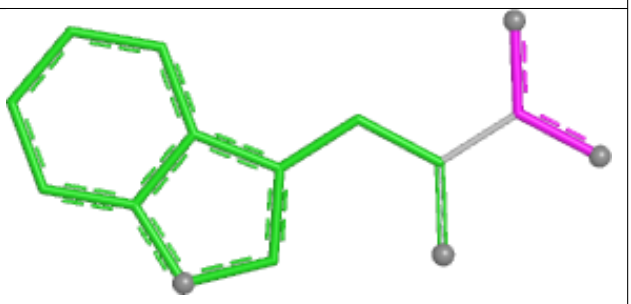


Rings

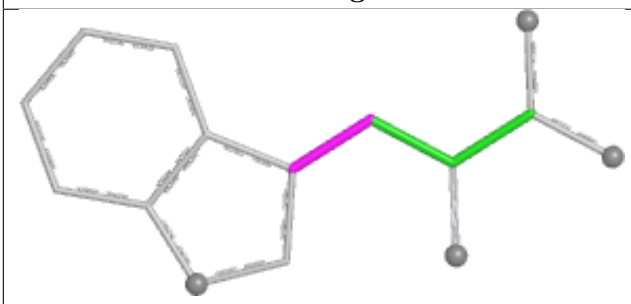
Ligand TRP D 503



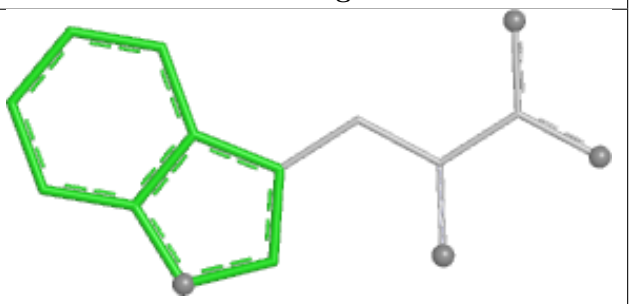
Bond lengths



Bond angles

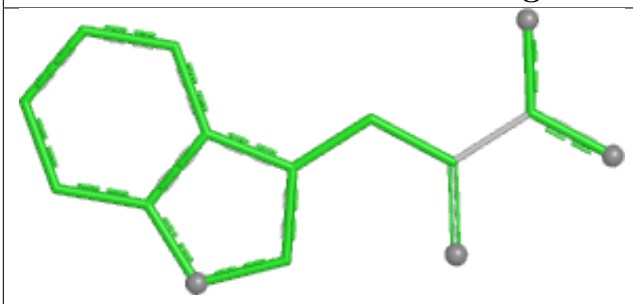


Torsions



Rings

Ligand TRP D 502



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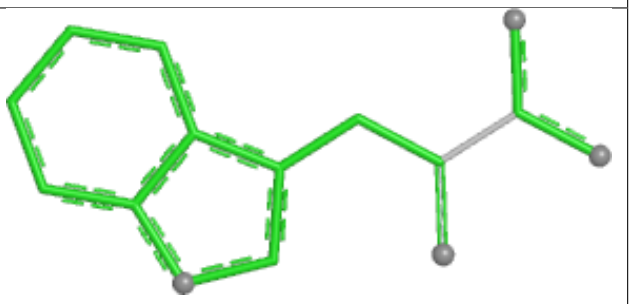

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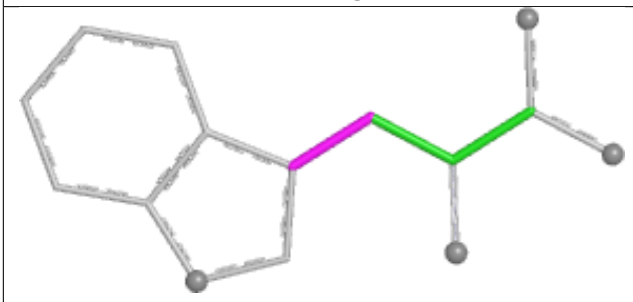

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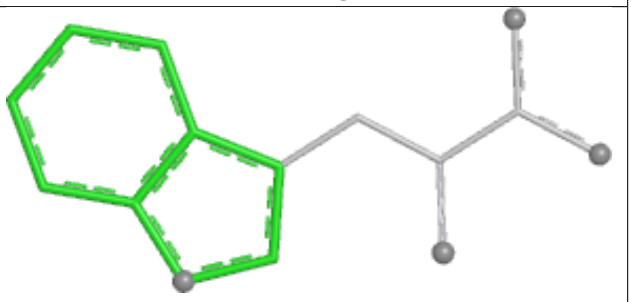
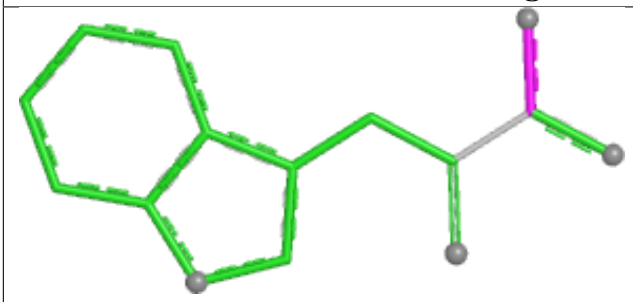


Rings

Ligand TRP C 502



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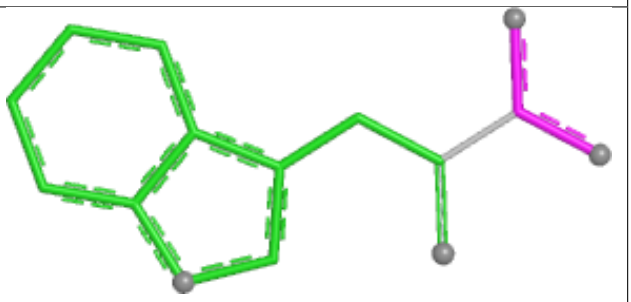
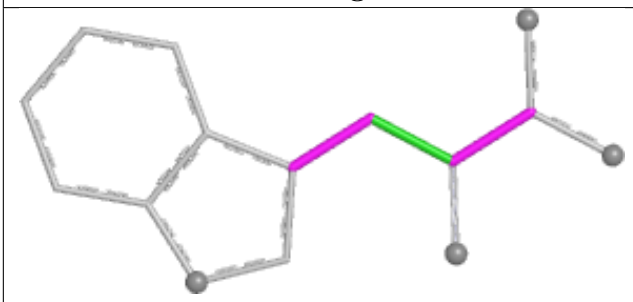


Bond angles



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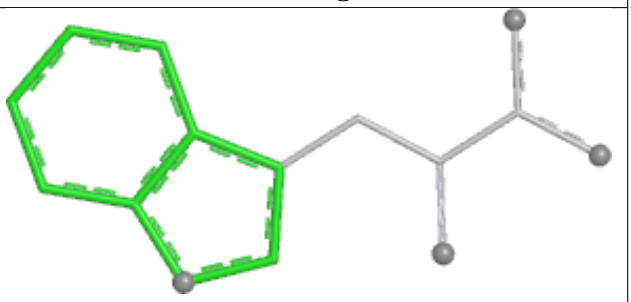
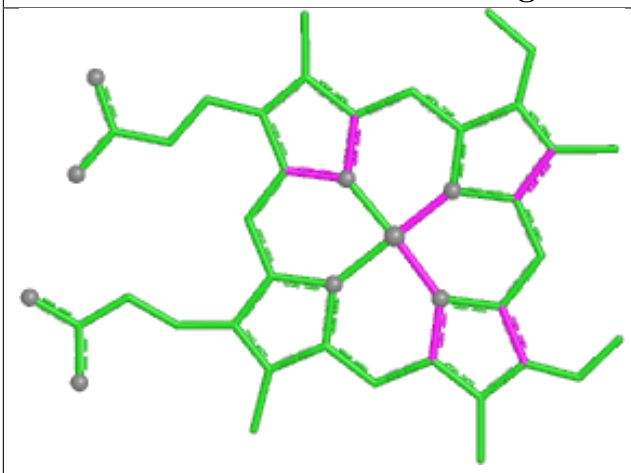


Rings

Ligand HEM A 500



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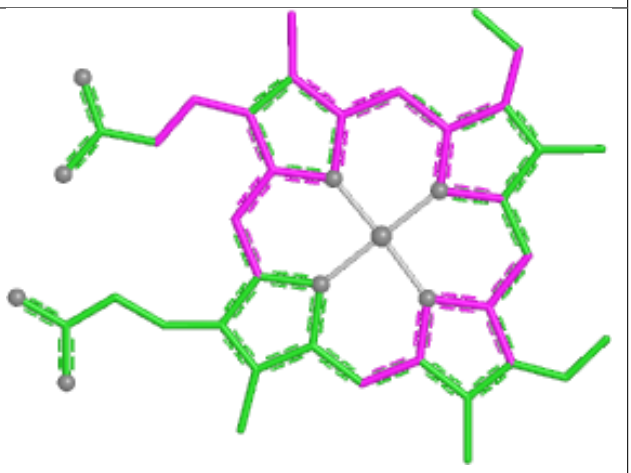
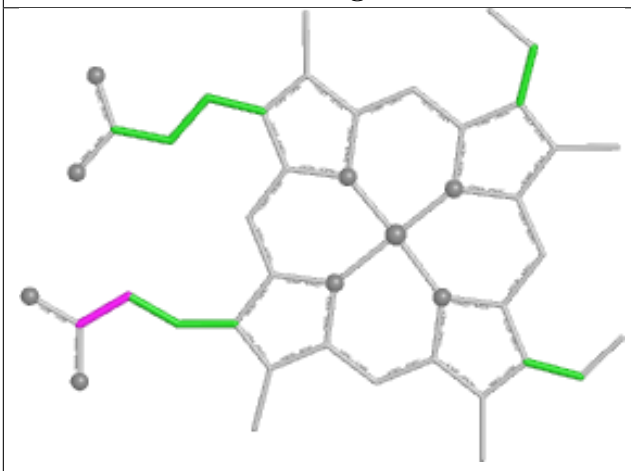


Bond angles



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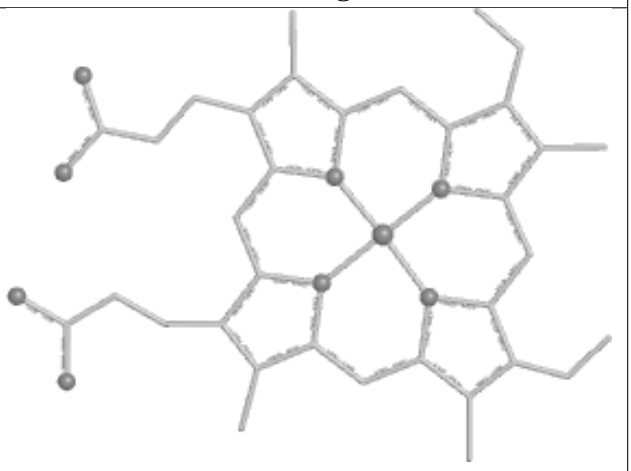
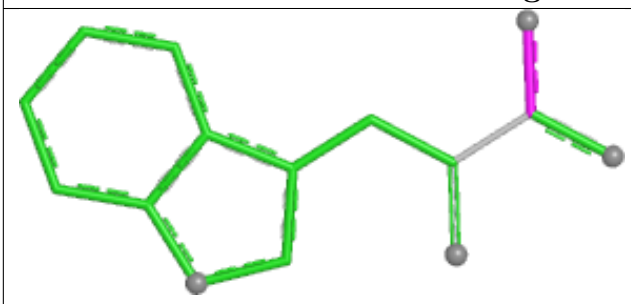


Rings

Ligand TRP C 503



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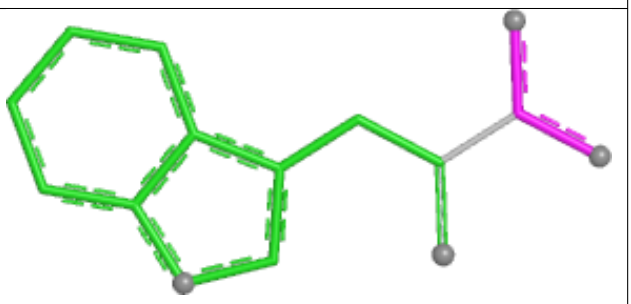
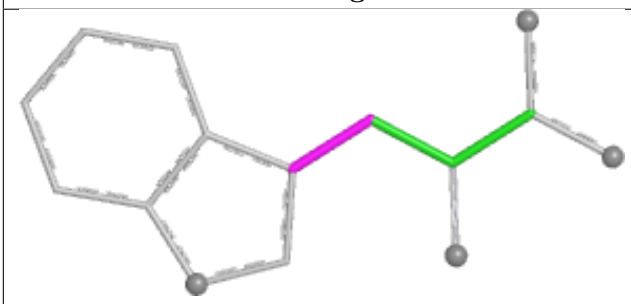


Bond angles



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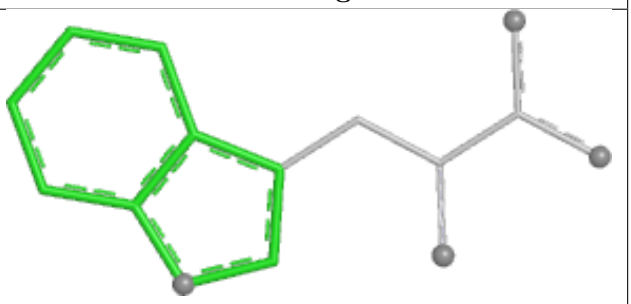
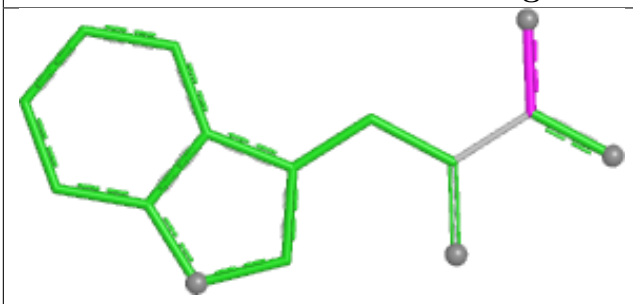
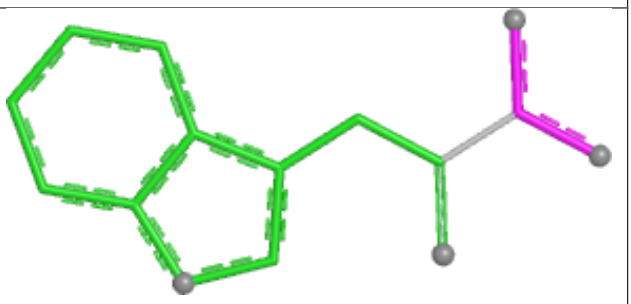


Rings

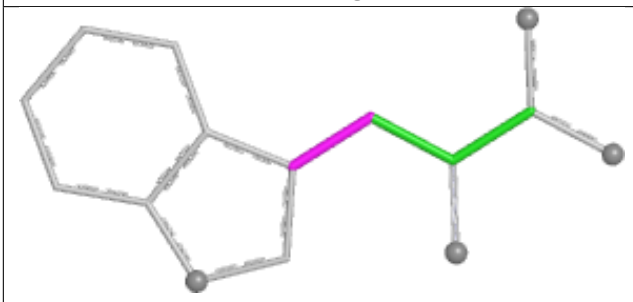
Ligand TRP A 503



Bond lengths



Bond angles



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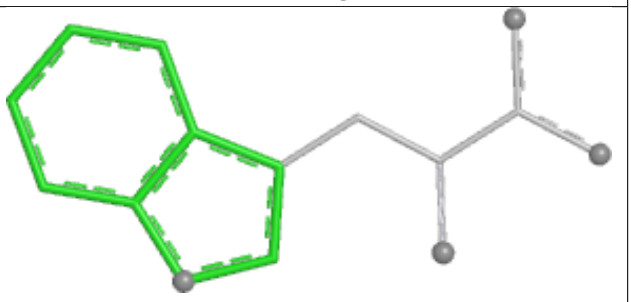
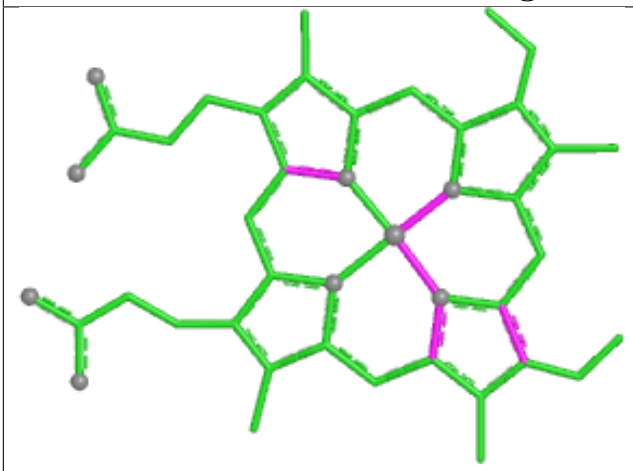


Rings

Ligand HEM C 500



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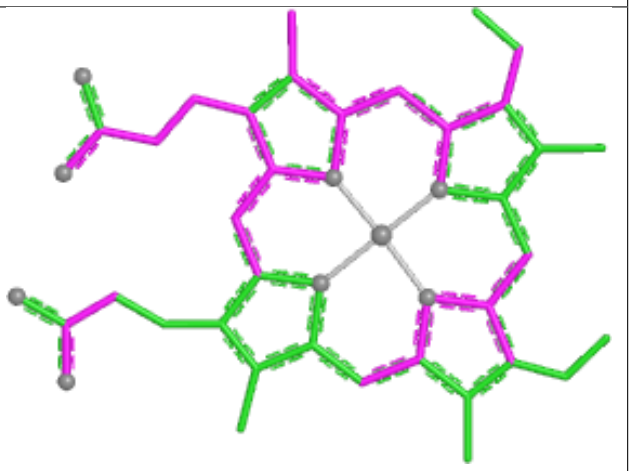
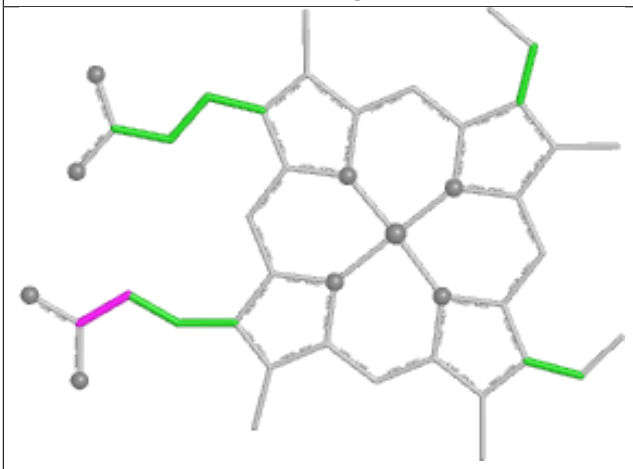


Bond angles



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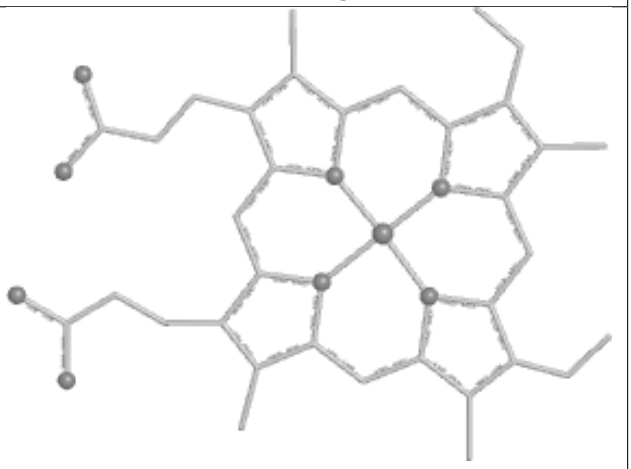

Rings

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	351/380 (92%)	-0.04	15 (4%)	40	40	23, 34, 77, 117	0
1	B	347/380 (91%)	-0.09	14 (4%)	42	42	23, 34, 70, 91	0
1	C	343/380 (90%)	0.15	16 (4%)	36	36	24, 38, 85, 107	0
1	D	353/380 (92%)	-0.07	10 (2%)	55	57	22, 34, 77, 100	0
All	All	1394/1520 (91%)	-0.01	55 (3%)	43	44	22, 35, 78, 117	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	385	ILE	3.9
1	A	176	ASN	3.9
1	C	389	LEU	3.8
1	B	169	GLN	3.7
1	A	385	ILE	3.7
1	A	389	LEU	3.6
1	B	389	LEU	3.4
1	A	384	THR	3.3
1	D	389	LEU	3.1
1	B	386	HIS	3.1
1	C	174	PRO	3.1
1	B	175	TYR	2.9
1	C	173	VAL	2.8
1	D	388	PHE	2.8
1	A	175	TYR	2.8
1	C	243	ALA	2.8
1	A	250	LYS	2.8
1	A	170	ASN	2.8
1	C	386	HIS	2.7
1	C	168	LEU	2.7
1	D	385	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	382	ASN	2.6
1	B	384	THR	2.6
1	B	193	LEU	2.6
1	C	385	ILE	2.6
1	C	241	ILE	2.5
1	D	384	THR	2.4
1	D	179	HIS	2.4
1	A	180	TYR	2.4
1	D	383	PRO	2.4
1	B	168	LEU	2.4
1	C	250	LYS	2.4
1	B	243	ALA	2.3
1	D	175	TYR	2.3
1	C	167	VAL	2.3
1	A	179	HIS	2.2
1	A	256	GLU	2.2
1	B	171	MET	2.2
1	C	171	MET	2.2
1	A	386	HIS	2.2
1	B	388	PHE	2.2
1	C	169	GLN	2.2
1	B	247	SER	2.2
1	C	218	HIS	2.1
1	D	168	LEU	2.1
1	C	238	PHE	2.1
1	A	241	ILE	2.1
1	A	376	HIS	2.1
1	C	239	ILE	2.1
1	D	241	ILE	2.1
1	A	388	PHE	2.1
1	A	174	PRO	2.0
1	B	180	TYR	2.0
1	D	386	HIS	2.0
1	C	383	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

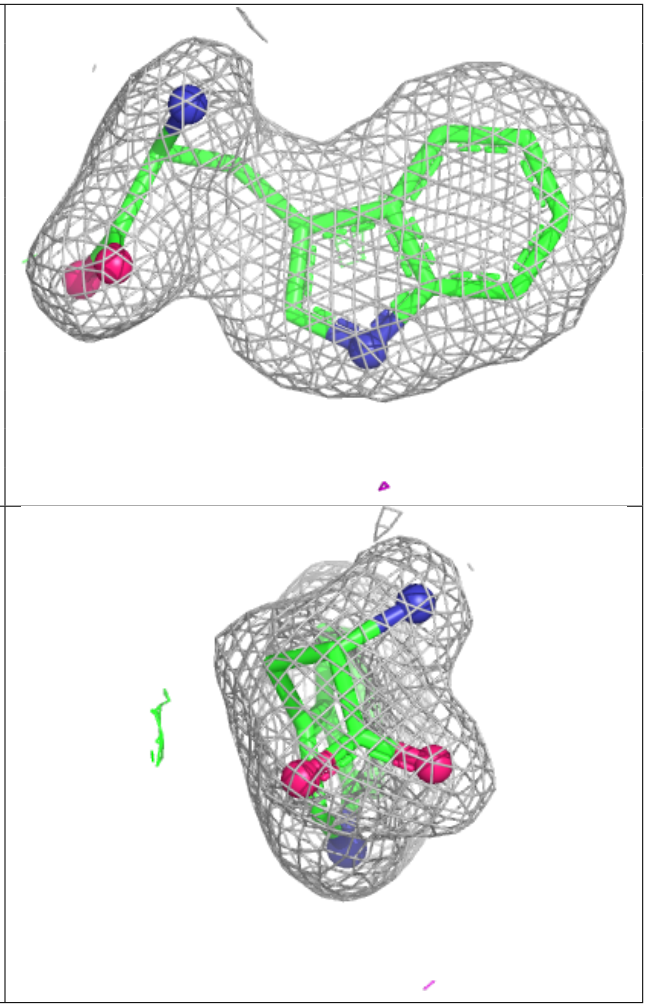
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

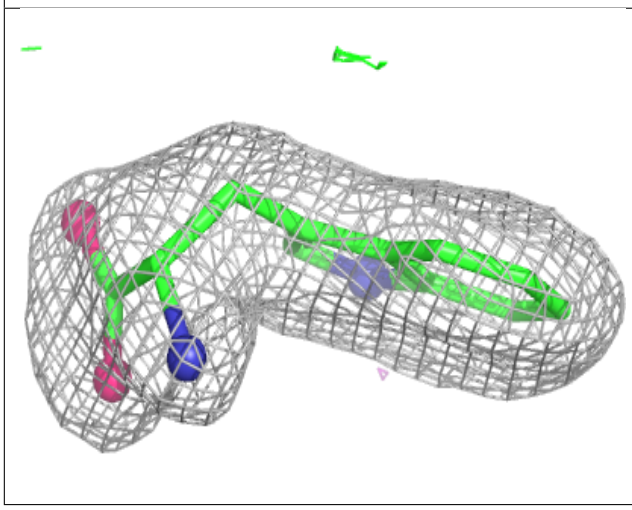
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CMO	A	501	2/2	0.94	0.10	34,34,34,41	0
4	TRP	C	503	15/15	0.94	0.07	33,36,44,50	0
4	TRP	D	503	15/15	0.94	0.07	30,32,41,43	0
4	TRP	C	502	15/15	0.95	0.06	34,35,36,36	0
4	TRP	A	503	15/15	0.95	0.06	28,31,35,37	0
4	TRP	B	503	15/15	0.95	0.06	29,31,36,37	0
3	CMO	B	501	2/2	0.96	0.07	33,33,33,35	0
4	TRP	B	502	15/15	0.96	0.06	28,29,35,37	0
4	TRP	A	502	15/15	0.96	0.06	33,34,38,38	0
3	CMO	D	501	2/2	0.97	0.06	34,34,34,34	0
4	TRP	D	502	15/15	0.97	0.05	29,30,32,32	0
3	CMO	C	501	2/2	0.97	0.07	31,31,31,35	0
2	HEM	A	500	43/43	0.98	0.06	29,33,36,37	0
2	HEM	B	500	43/43	0.98	0.05	25,28,31,37	0
2	HEM	C	500	43/43	0.98	0.06	28,30,33,35	0
2	HEM	D	500	43/43	0.98	0.05	26,28,30,31	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 TRP C 503:

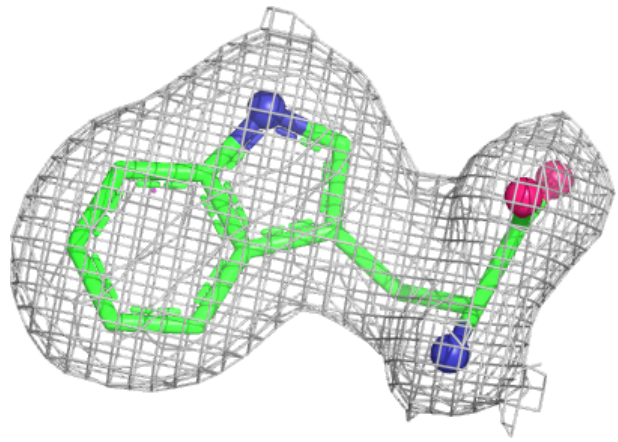
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

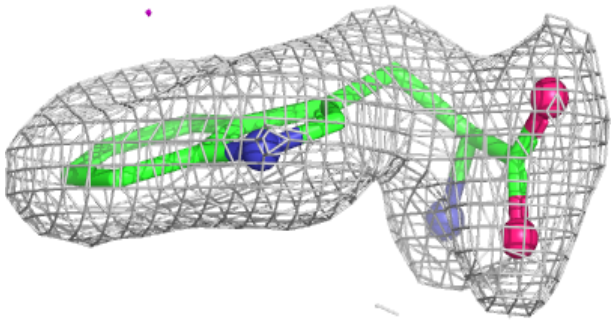


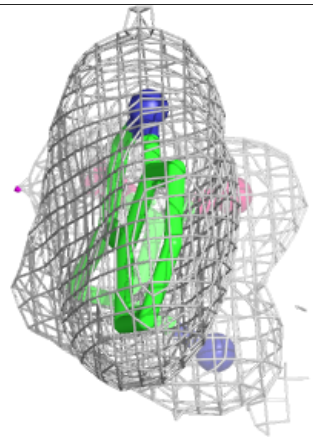


Electron density around TRP D 503:

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

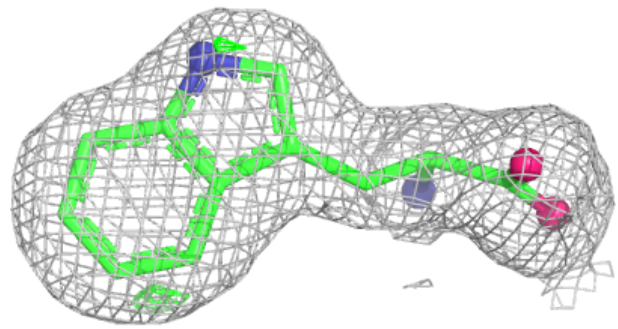


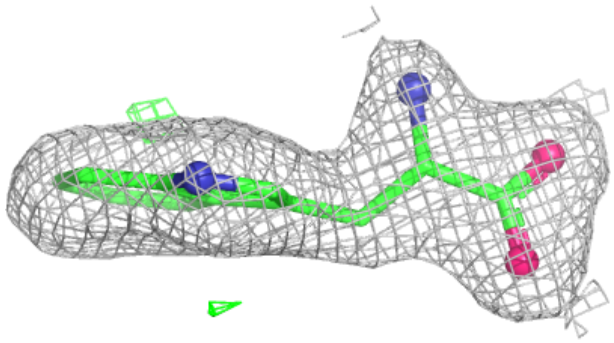


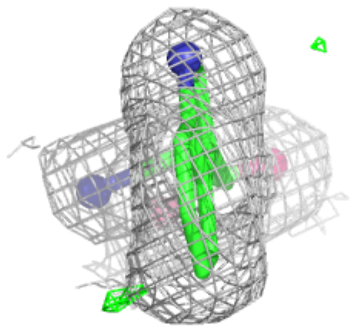


Electron density around TRP C 502:

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

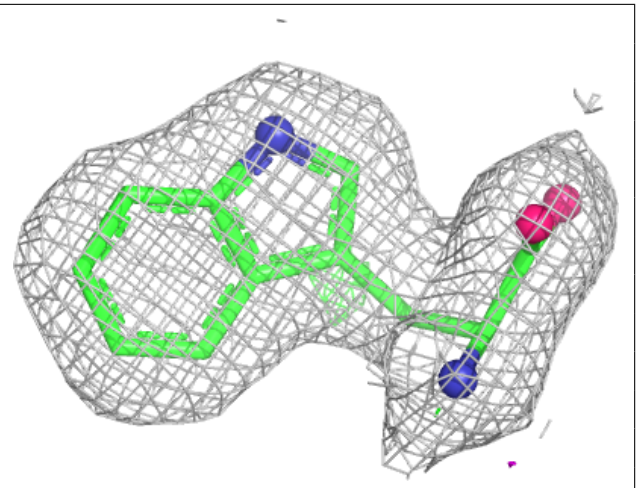


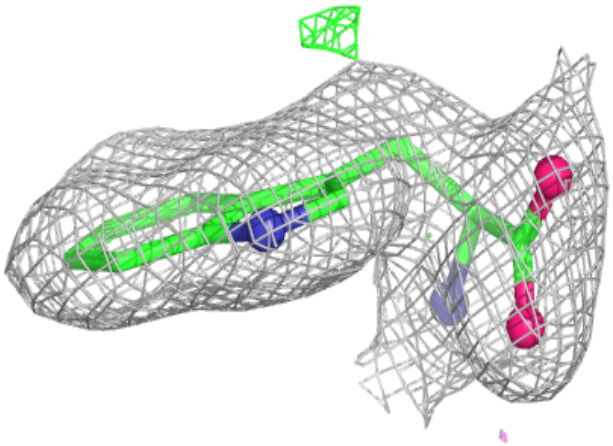


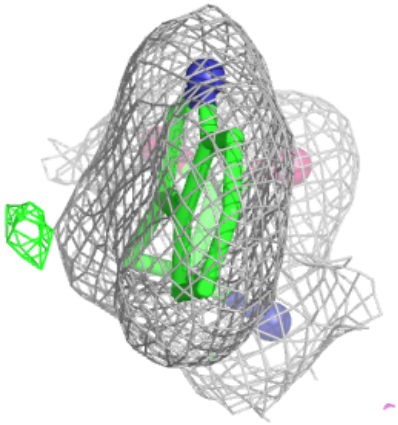


Electron density around TRP A 503:

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

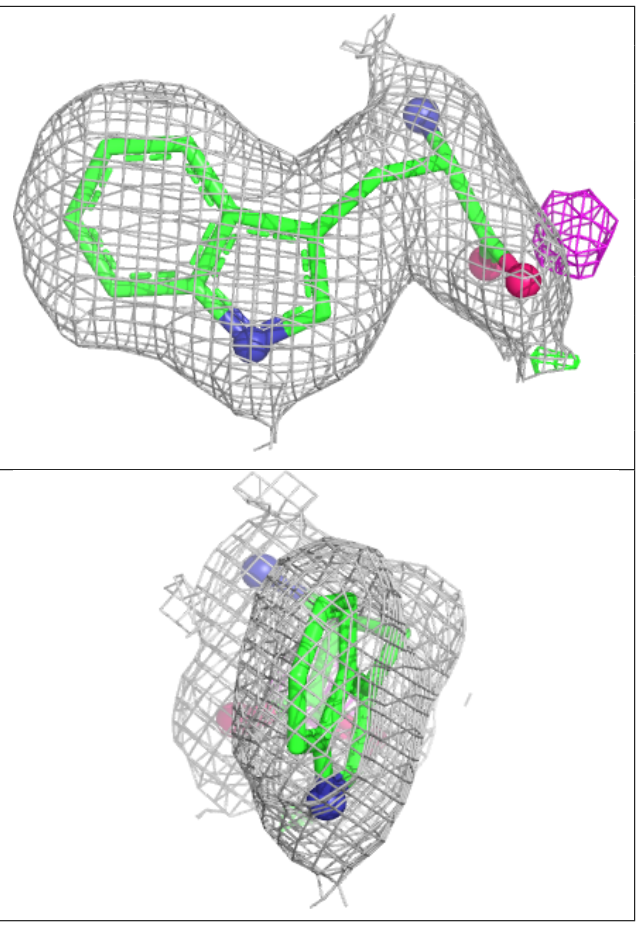






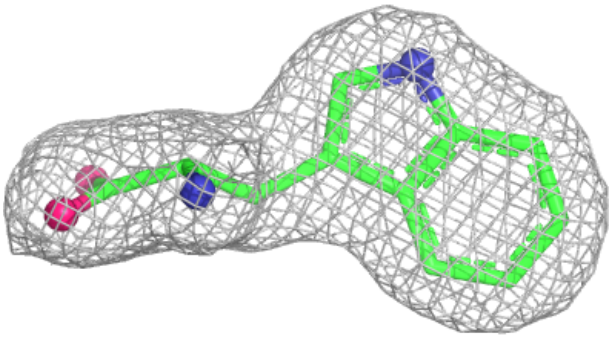
Electron density around TRP B 503:

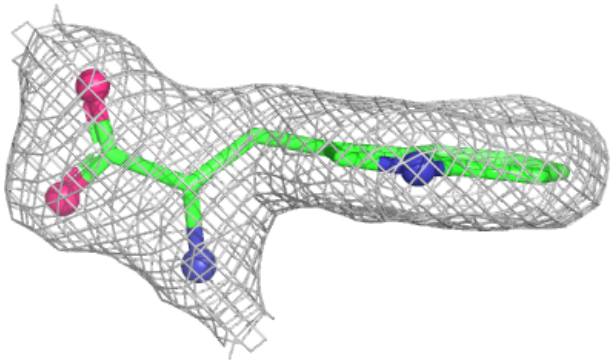
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

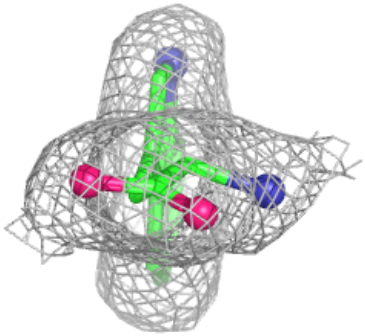


Electron density around TRP B 502:

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

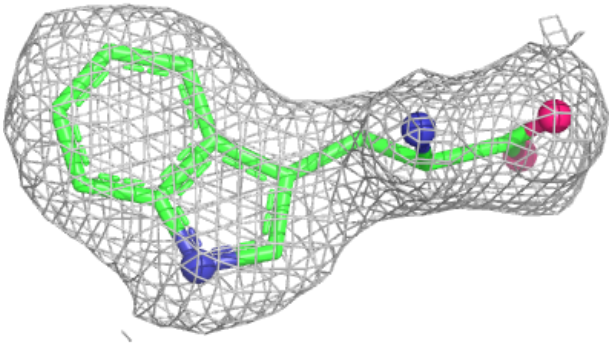


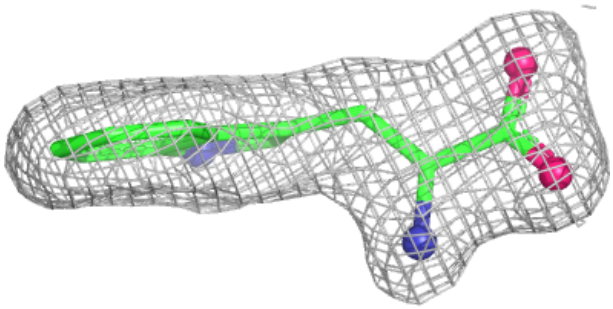


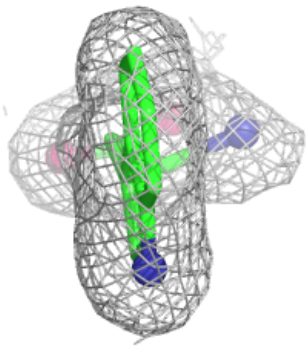


Electron density around TRP A 502:

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

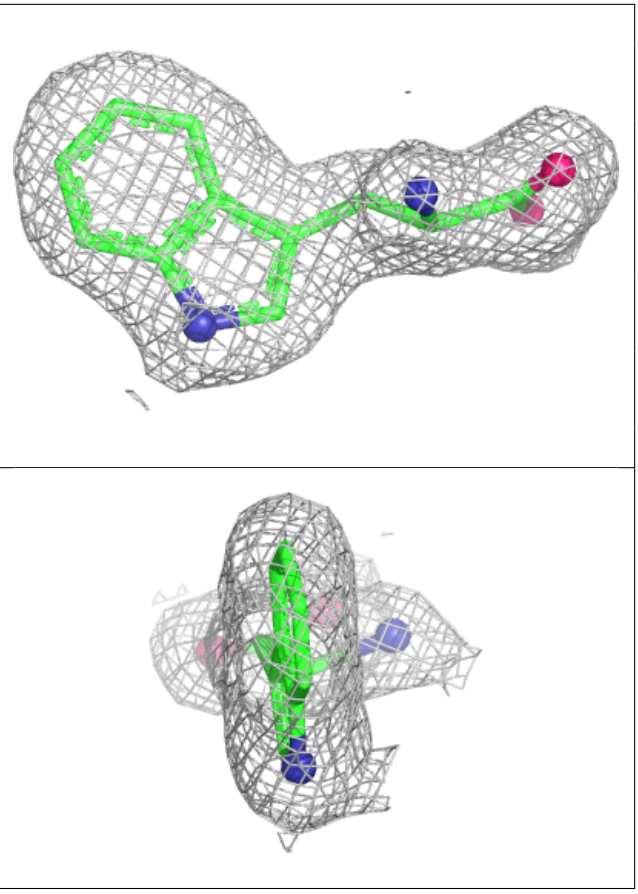






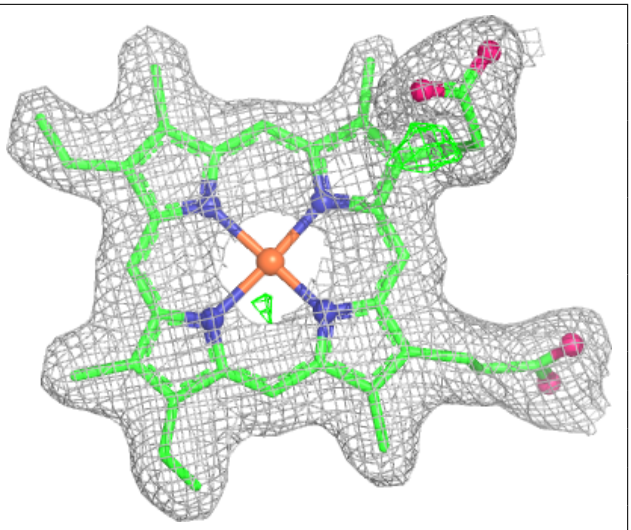
Electron density around TRP D 502:

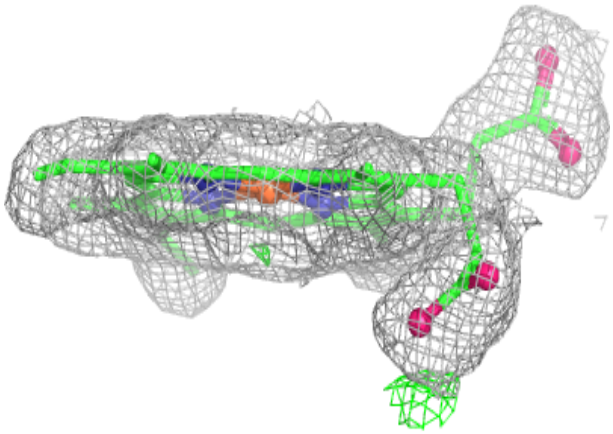
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

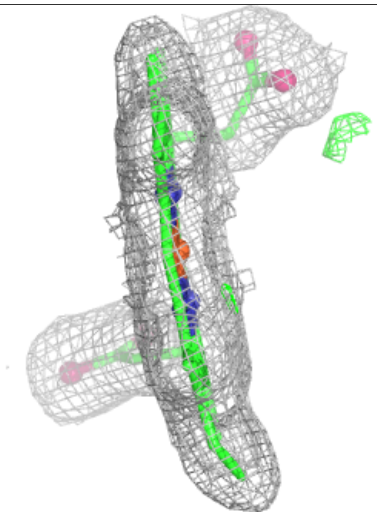


Electron density around HEM A 500:

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

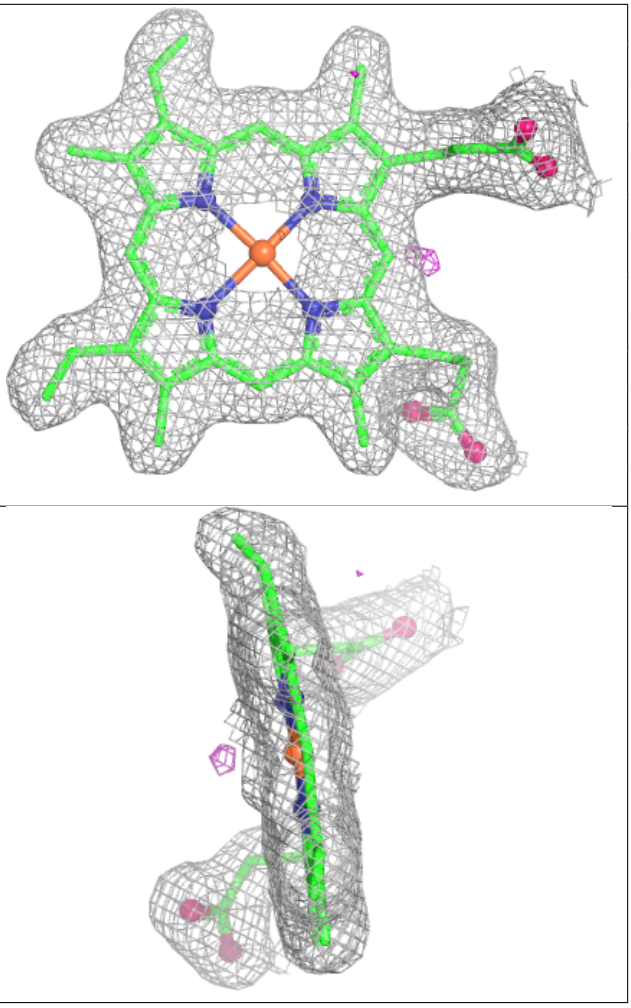






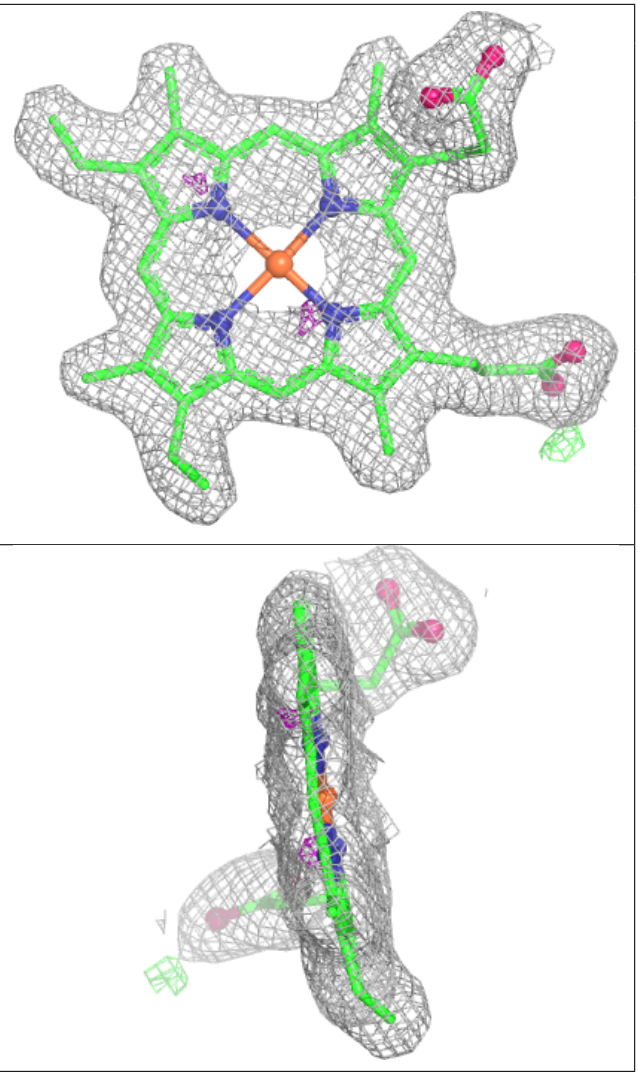
Electron density around HEM B 500:

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



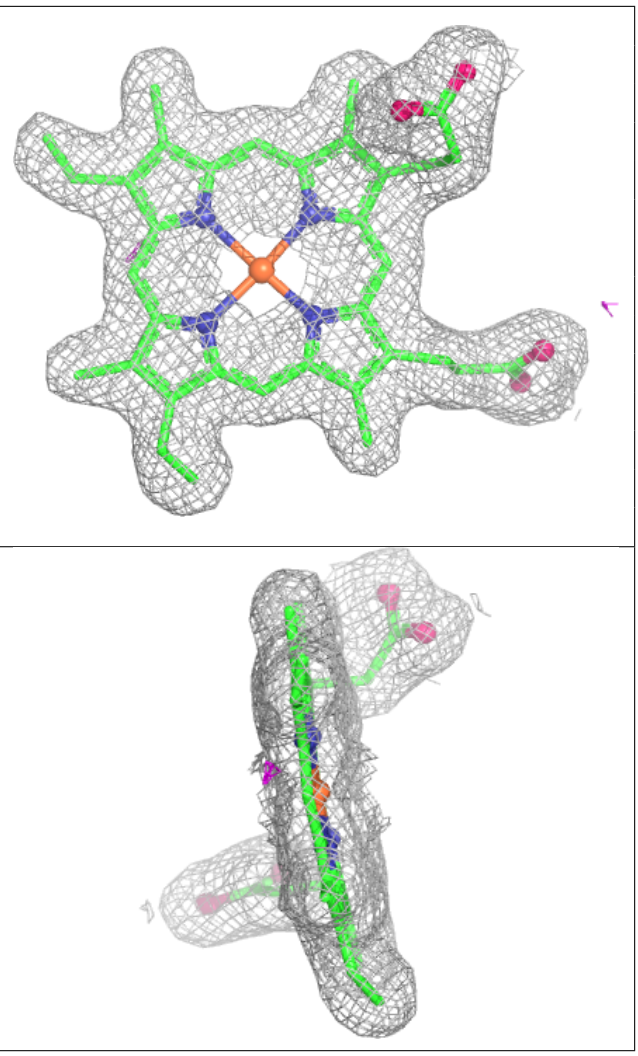
Electron density around HEM C 500:

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



Electron density around HEM D 500:

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.