



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2021 – 12:09 PM EST

PDB ID : 6UD5
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

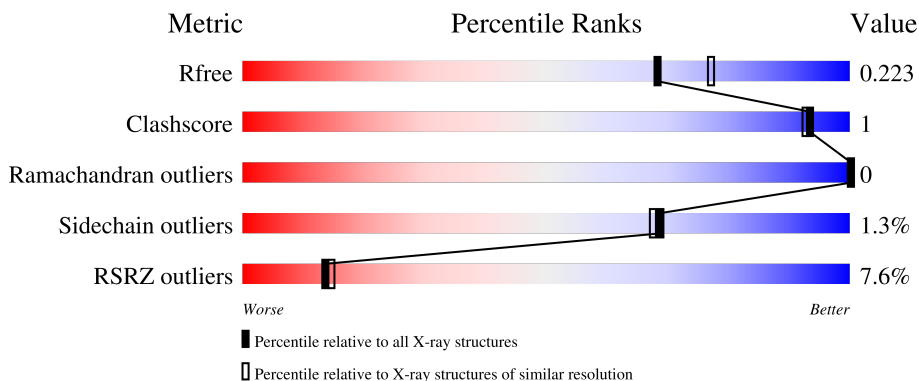
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


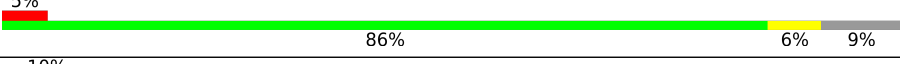

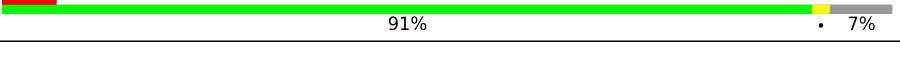
The reported resolution of this entry is 2.05 Å.

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	380	
1	B	380	
1	C	380	
1	D	380	

2 Entry composition

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

There are 32 discrepancies between the modelled and reference sequences:

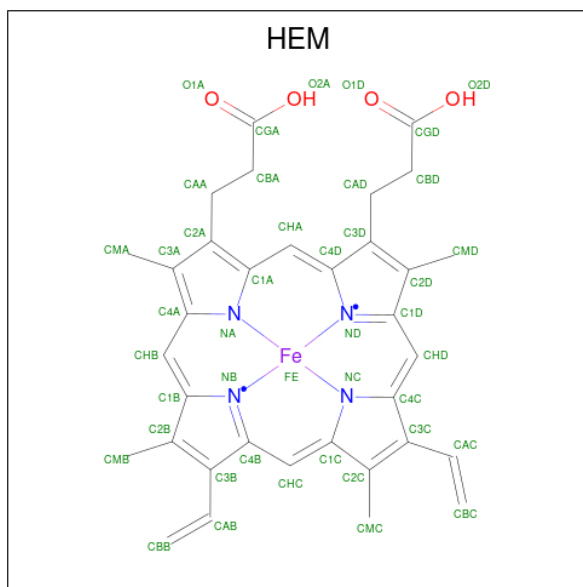
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression 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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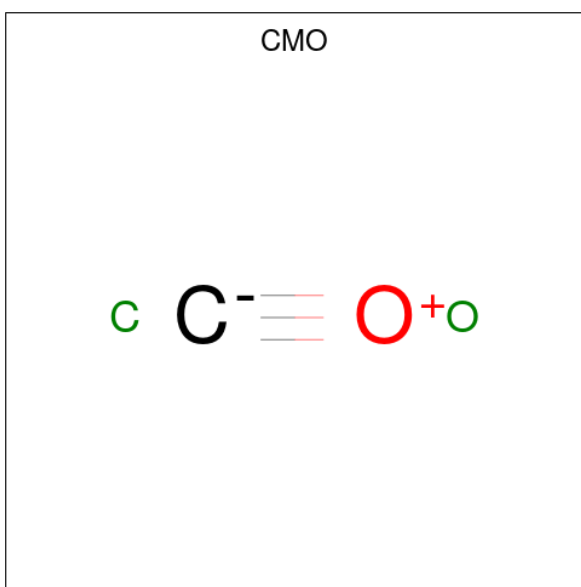
Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression 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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



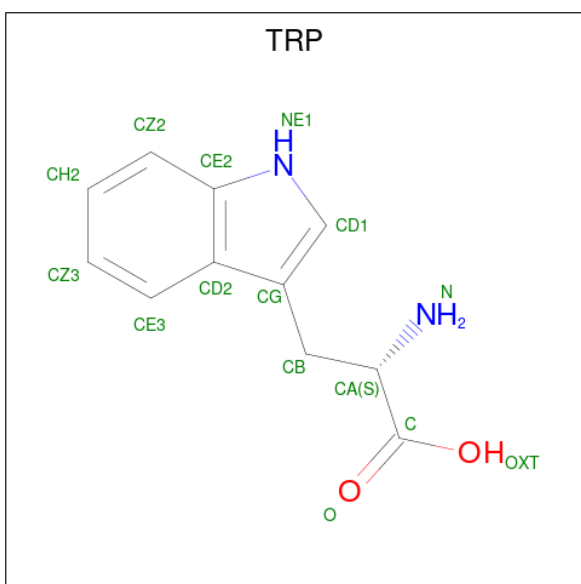
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

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



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

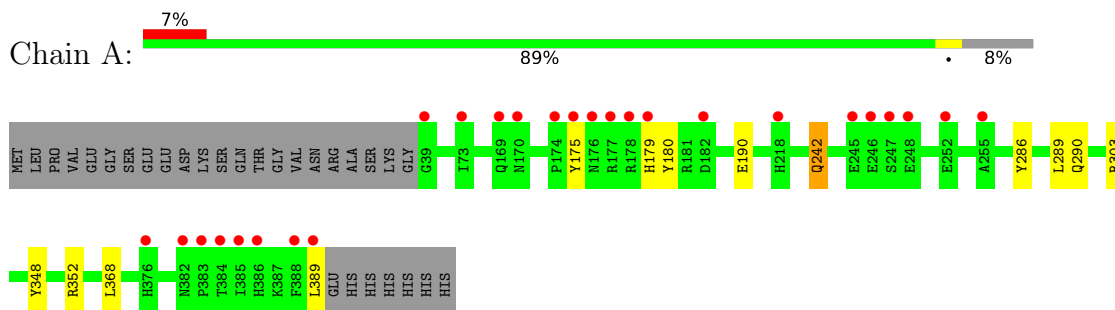
- Molecule 5 is water.

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

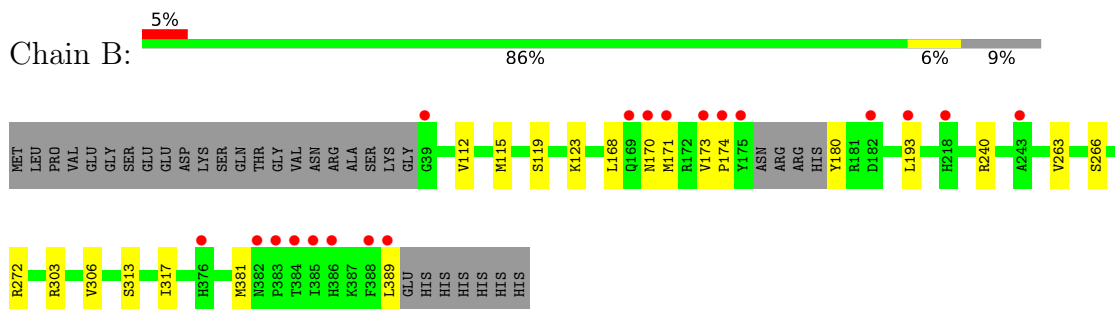
3 Residue-property plots [i](#)

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.

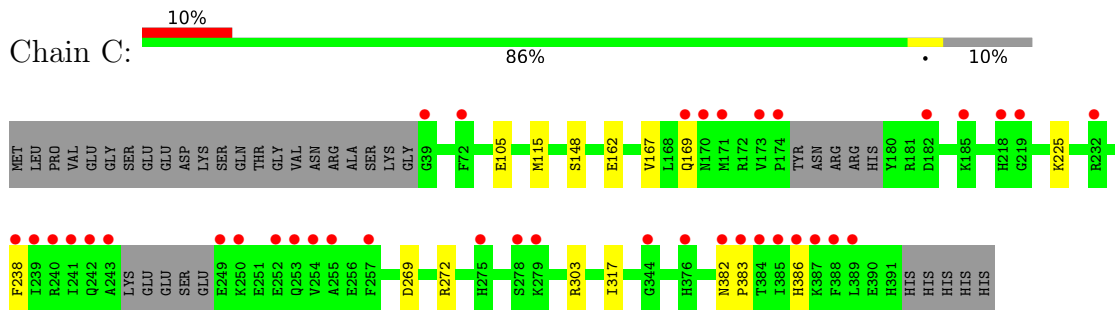
- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase

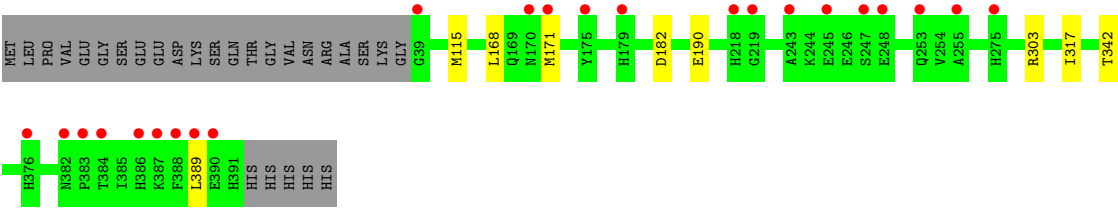


- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase





4 Data and refinement statistics

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) 96.5 (19.97-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.17%)	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)	0.35 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	0/3015	0.69	0/4059
1	B	0.64	0/2965	0.69	0/3992
1	C	0.65	0/2891	0.69	0/3899
1	D	0.64	0/3033	0.68	0/4083
All	All	0.64	0/11904	0.69	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	6	0
1	B	2898	0	2872	8	0
1	C	2825	0	2753	6	0
1	D	2963	0	2945	4	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	0	0
4	B	30	0	18	0	0
4	C	30	0	18	0	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	33	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 1.

All (33) 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:HHH	2:D:500:HEM:HBC2	1.78	0.66
2:B:500:HEM:HHH	2:B:500:HEM:HBC2	1.84	0.59
1:D:342:THR:HG1	4:D:502:TRP:N	2.03	0.56
2:A:500:HEM:HBC2	2:A:500:HEM:HHH	1.88	0.55
1:C:162:GLU:HB3	1:C:167:VAL:HG11	1.89	0.55
1:A:242:GLN:HE21	1:A:242:GLN:HA	1.73	0.53
1:C:105:GLU:OE1	1:C:303:ARG:HD2	2.10	0.52
2:C:500:HEM:HBC2	2:C:500:HEM:HHH	1.93	0.50
1:B:112:VAL:HG21	1:B:306:VAL:CG1	2.41	0.50
2:A:500:HEM:HBB2	2:A:500:HEM:HMB1	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:B:112:VAL:HG21	1:B:306:VAL:HG13	1.98	0.45
1:D:115:MET:HE3	1:D:317:ILE:CD1	2.46	0.45
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.46	0.44
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HBB2	2:C:500:HEM:HMB1	2.01	0.42
2:D:500:HEM:HMB1	2:D:500:HEM:HBB2	2.02	0.42
1:B:173:VAL:HG13	1:B:174:PRO:HD2	2.03	0.41
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.50	0.41
1:A:303:ARG:HD3	1:A:389:LEU:HA	2.02	0.41
1:C:269:ASP:CG	1:C:272:ARG:HB2	2.41	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%)	78	79
1	B	314/348 (90%)	307 (98%)	7 (2%)	52	46
1	C	300/348 (86%)	296 (99%)	4 (1%)	69	67
1	D	322/348 (92%)	320 (99%)	2 (1%)	86	87
All	All	1256/1392 (90%)	1240 (99%)	16 (1%)	69	67

All (16) 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	170	ASN
1	B	180	TYR
1	B	193	LEU
1	B	240	ARG
1	B	272	ARG
1	B	313	SER
1	B	381	MET
1	C	169	GLN
1	C	225	LYS
1	C	238	PHE
1	C	386	HIS
1	D	182	ASP
1	D	190	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	242	GLN
1	A	253	GLN
1	A	327	ASN
1	C	98	GLN
1	C	242	GLN
1	C	386	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2	0,1,1	0.00	-	-		
3	CMO	C	501	2	0,1,1	0.00	-	-		
2	HEM	D	500	1,3	27,50,50	0.85	1 (3%)	17,82,82	1.86	2 (11%)
4	TRP	B	503	-	12,16,16	0.68	0	12,22,22	0.84	0
2	HEM	B	500	1,3	27,50,50	0.87	1 (3%)	17,82,82	1.73	2 (11%)
2	HEM	A	500	1,3	27,50,50	0.84	2 (7%)	17,82,82	1.82	3 (17%)
4	TRP	A	502	-	12,16,16	0.67	0	12,22,22	0.89	0
3	CMO	D	501	2	0,1,1	0.00	-	-		
4	TRP	C	503	-	12,16,16	0.72	0	12,22,22	0.86	0
4	TRP	D	503	-	12,16,16	0.72	0	12,22,22	0.79	0
4	TRP	A	503	-	12,16,16	0.68	0	12,22,22	0.86	1 (8%)
3	CMO	B	501	2	0,1,1	0.00	-	-		
4	TRP	D	502	-	12,16,16	0.73	0	12,22,22	0.81	0
4	TRP	B	502	-	12,16,16	0.70	0	12,22,22	0.94	1 (8%)
4	TRP	C	502	-	12,16,16	0.70	0	12,22,22	0.91	0
2	HEM	C	500	1,3	27,50,50	0.83	0	17,82,82	1.81	3 (17%)

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	D	503	-	-	0/3/8/8	0/2/2/2
4	TRP	B	503	-	-	0/3/8/8	0/2/2/2
2	HEM	D	500	1,3	-	0/6/54/54	-
2	HEM	B	500	1,3	-	0/6/54/54	-
2	HEM	A	500	1,3	-	0/6/54/54	-
4	TRP	A	502	-	-	1/3/8/8	0/2/2/2
4	TRP	C	503	-	-	0/3/8/8	0/2/2/2
4	TRP	A	503	-	-	0/3/8/8	0/2/2/2
4	TRP	D	502	-	-	1/3/8/8	0/2/2/2
4	TRP	B	502	-	-	1/3/8/8	0/2/2/2
4	TRP	C	502	-	-	1/3/8/8	0/2/2/2
2	HEM	C	500	1,3	-	0/6/54/54	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C4D-C3D	2.11	1.47	1.42
2	D	500	HEM	C4D-C3D	2.10	1.47	1.42
2	A	500	HEM	C3B-C2B	-2.06	1.37	1.40
2	B	500	HEM	C3B-C2B	-2.03	1.37	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	HEM	CBD-CAD-C3D	-5.78	101.82	112.48
2	A	500	HEM	CBD-CAD-C3D	-5.71	101.97	112.48
2	C	500	HEM	CBD-CAD-C3D	-5.58	102.19	112.48
2	B	500	HEM	CBD-CAD-C3D	-5.28	102.74	112.48
2	B	500	HEM	CAD-CBD-CGD	3.30	118.21	112.67
2	D	500	HEM	CAD-CBD-CGD	3.13	117.93	112.67
2	A	500	HEM	CAD-CBD-CGD	2.63	117.08	112.67
2	C	500	HEM	CBA-CAA-C2A	-2.54	107.80	112.49
2	C	500	HEM	C1D-C2D-C3D	-2.20	105.47	107.00
2	A	500	HEM	CBA-CAA-C2A	-2.12	108.58	112.49
4	B	502	TRP	CH2-CZ2-CE2	-2.05	117.13	120.08
4	A	503	TRP	CH2-CZ2-CE2	-2.01	117.19	120.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

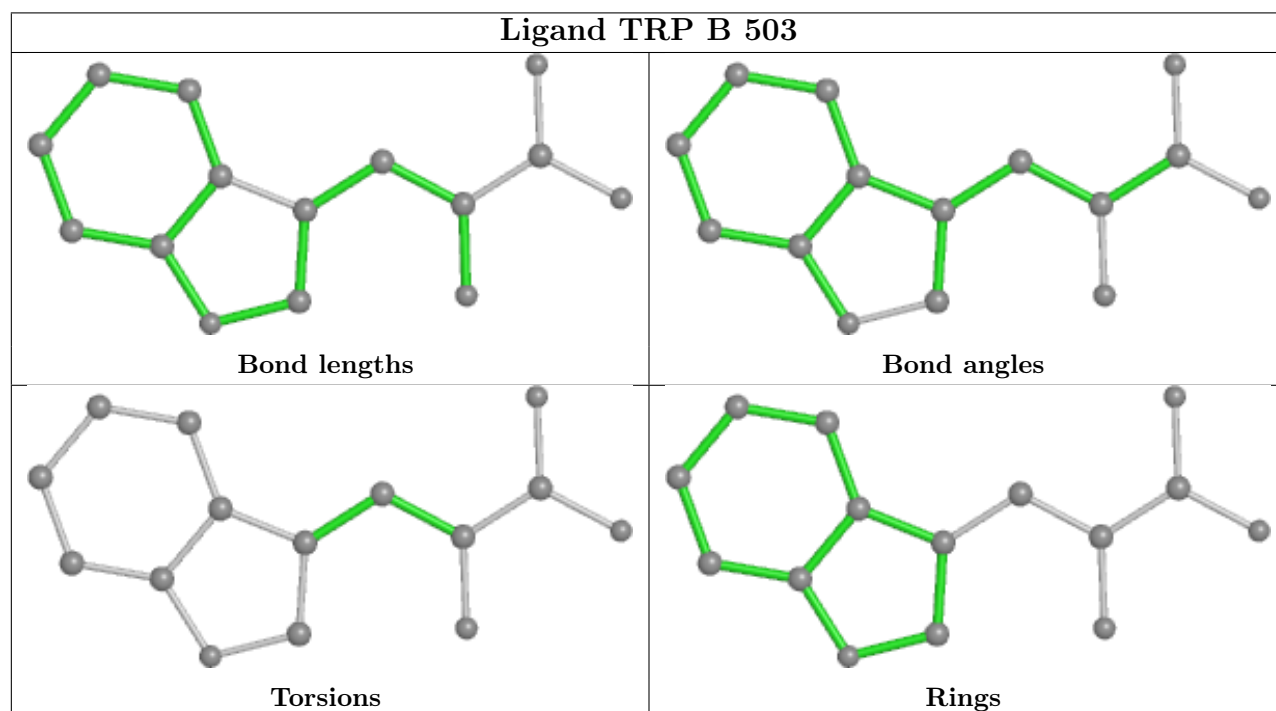
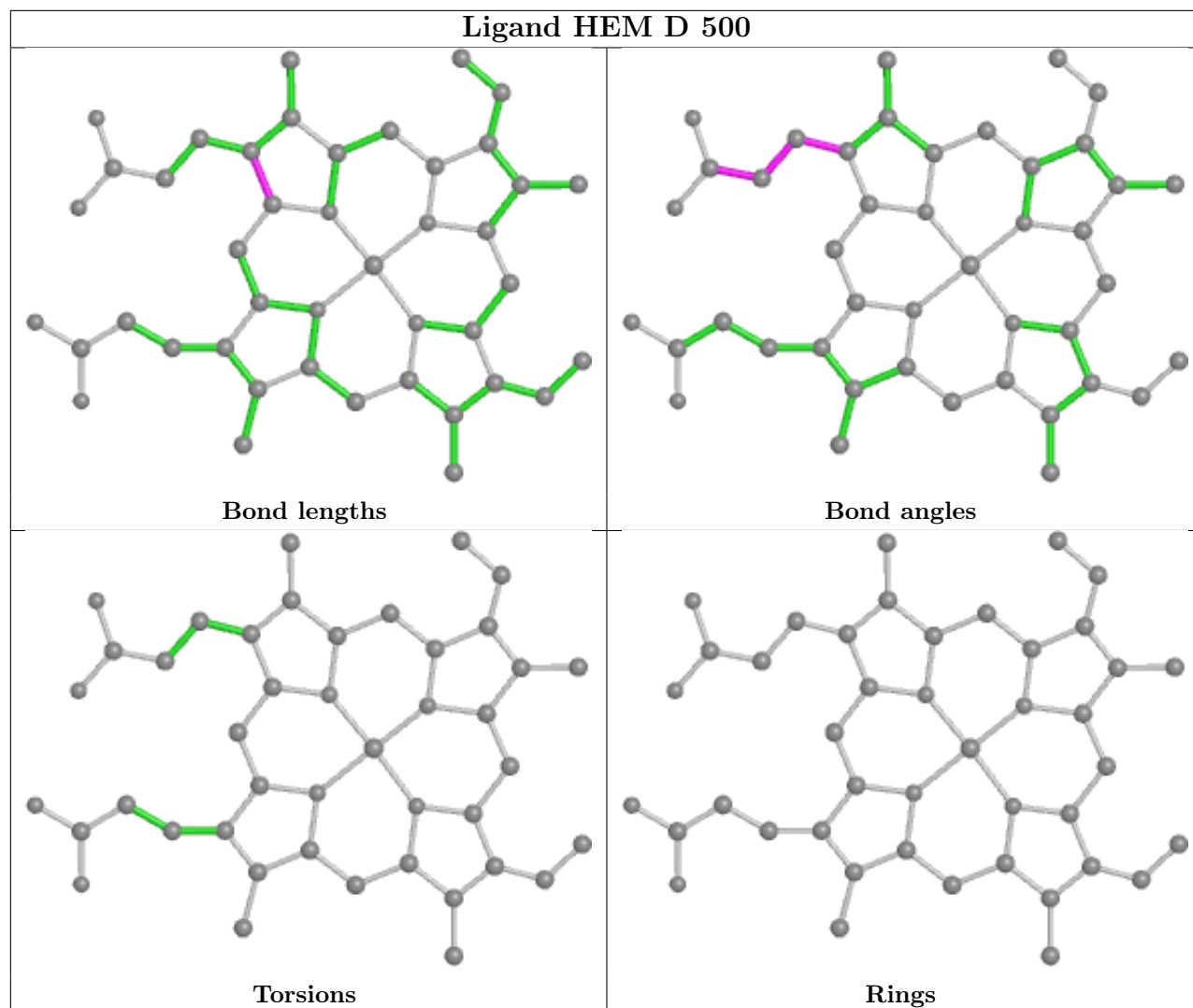
Mol	Chain	Res	Type	Atoms
4	A	502	TRP	CA-CB-CG-CD1
4	D	502	TRP	CA-CB-CG-CD1
4	B	502	TRP	CA-CB-CG-CD1
4	C	502	TRP	CA-CB-CG-CD1

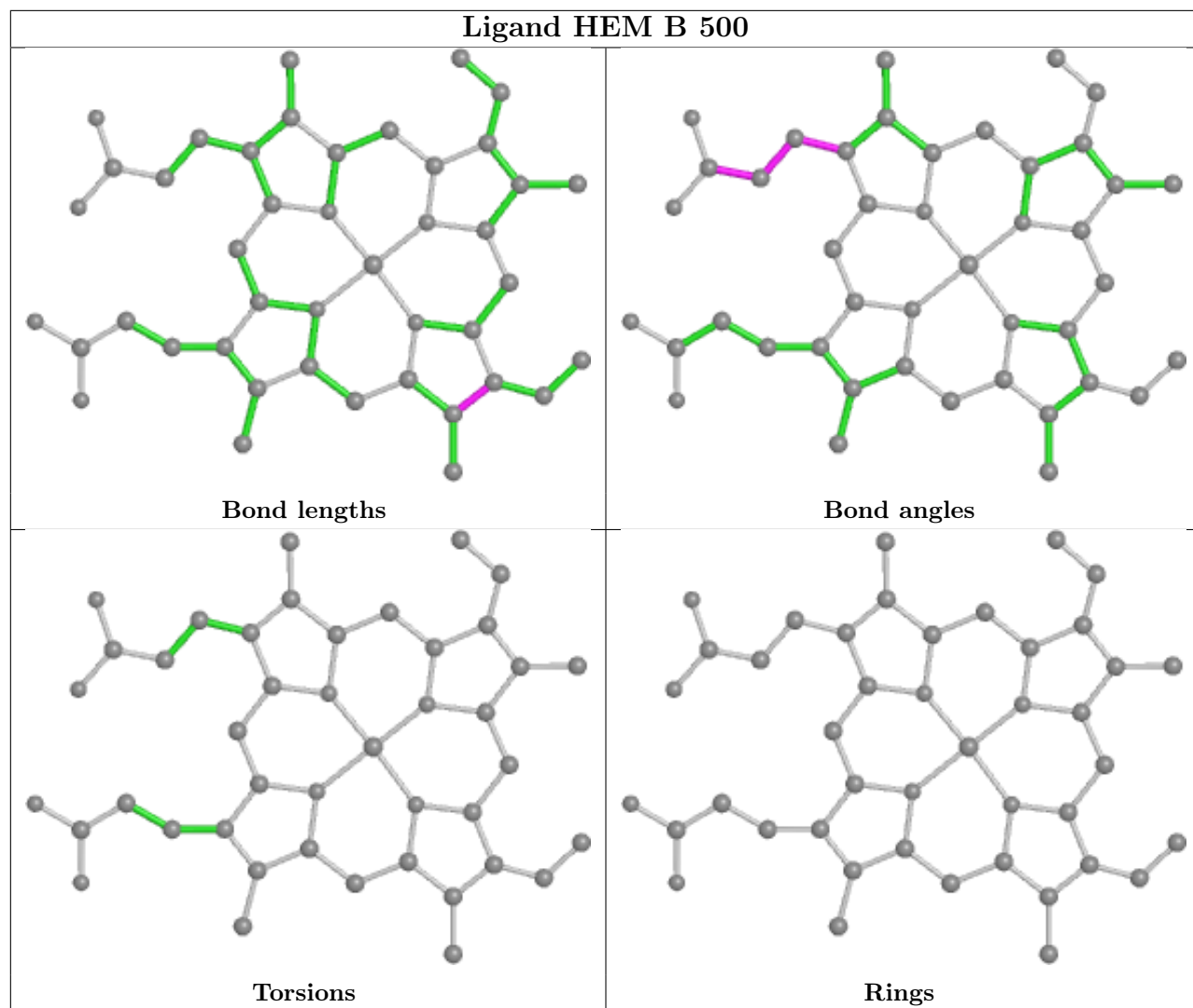
There are no ring outliers.

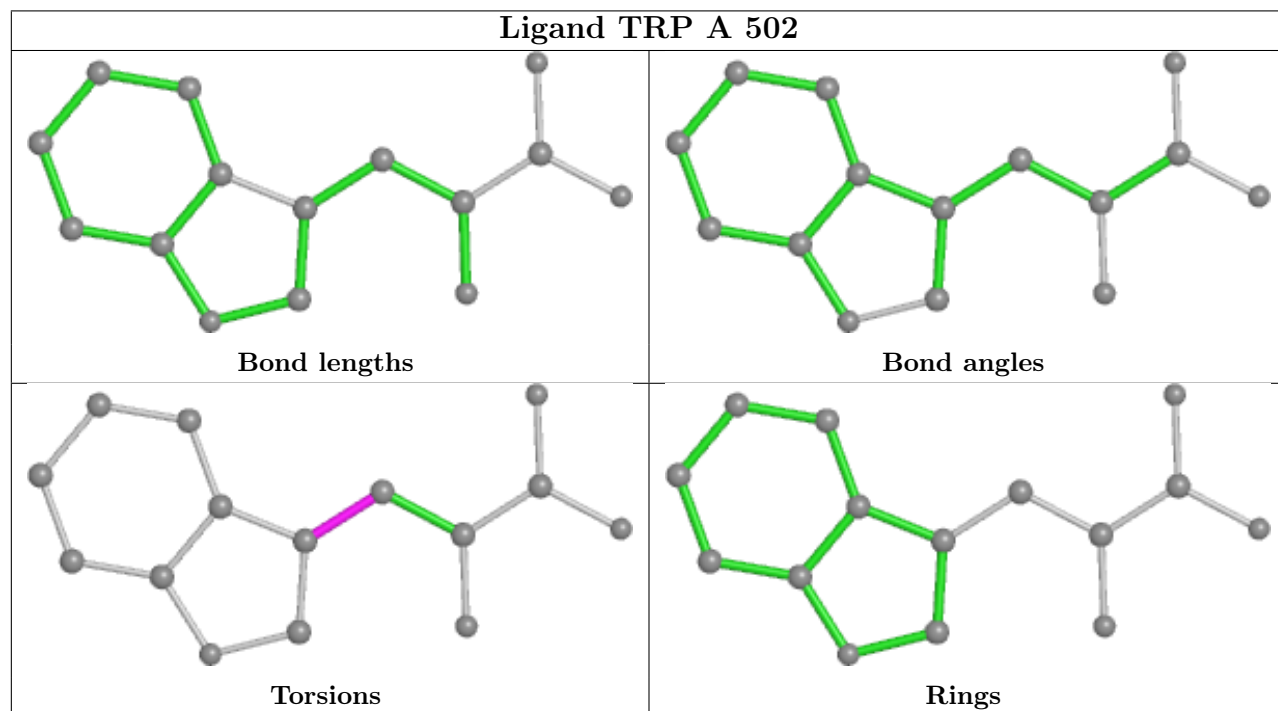
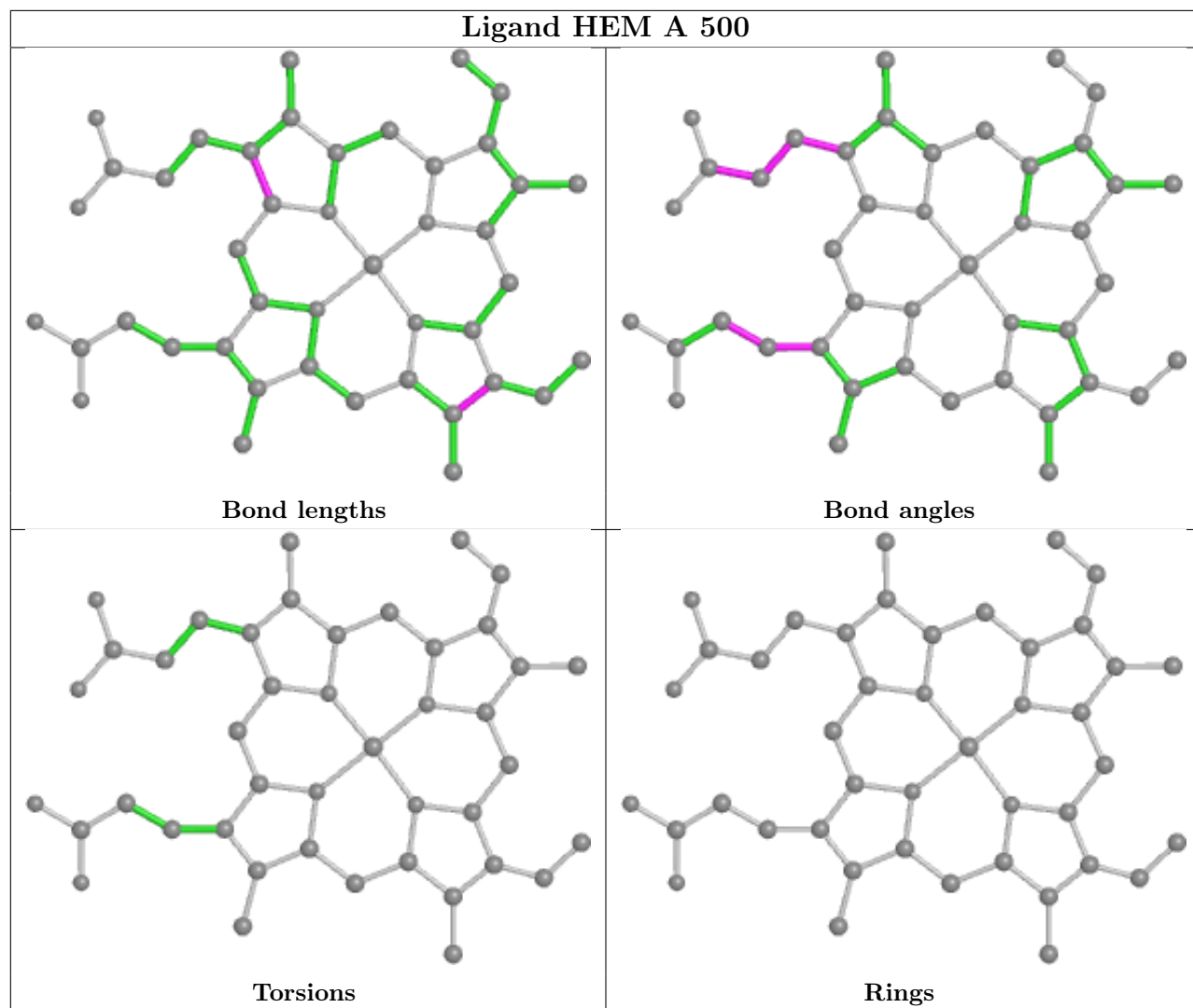
5 monomers are involved in 10 short contacts:

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

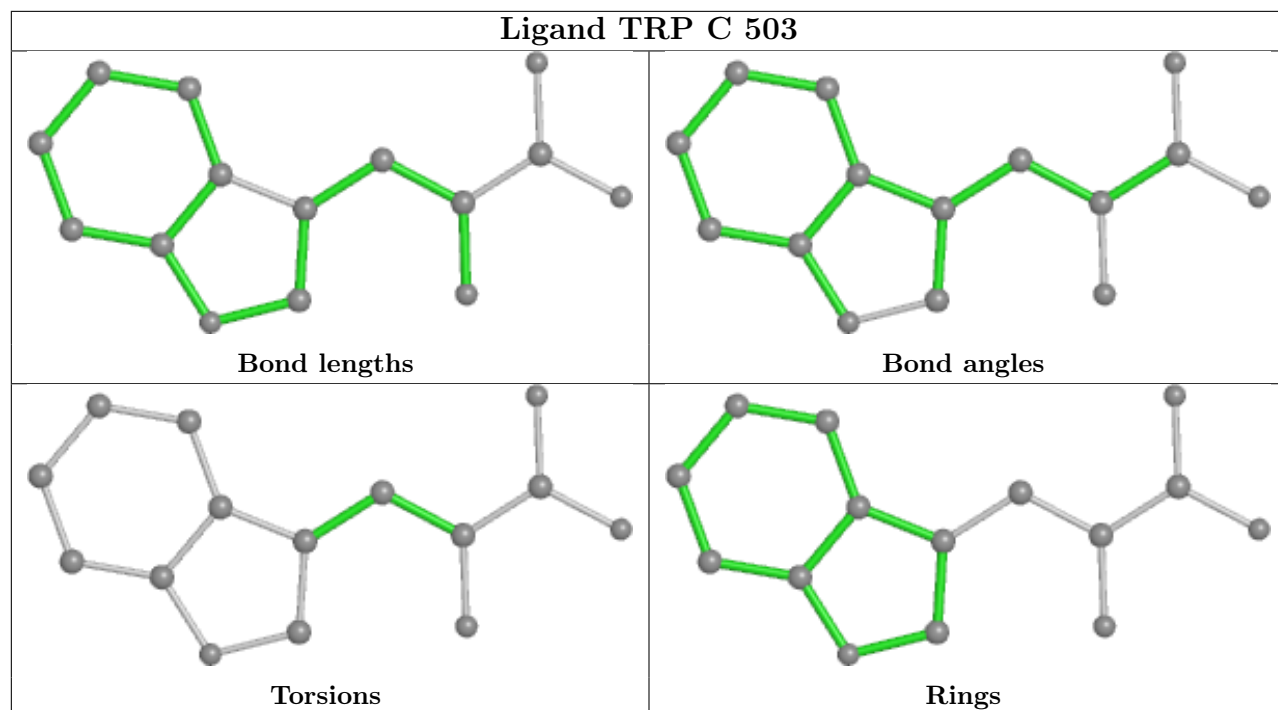
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



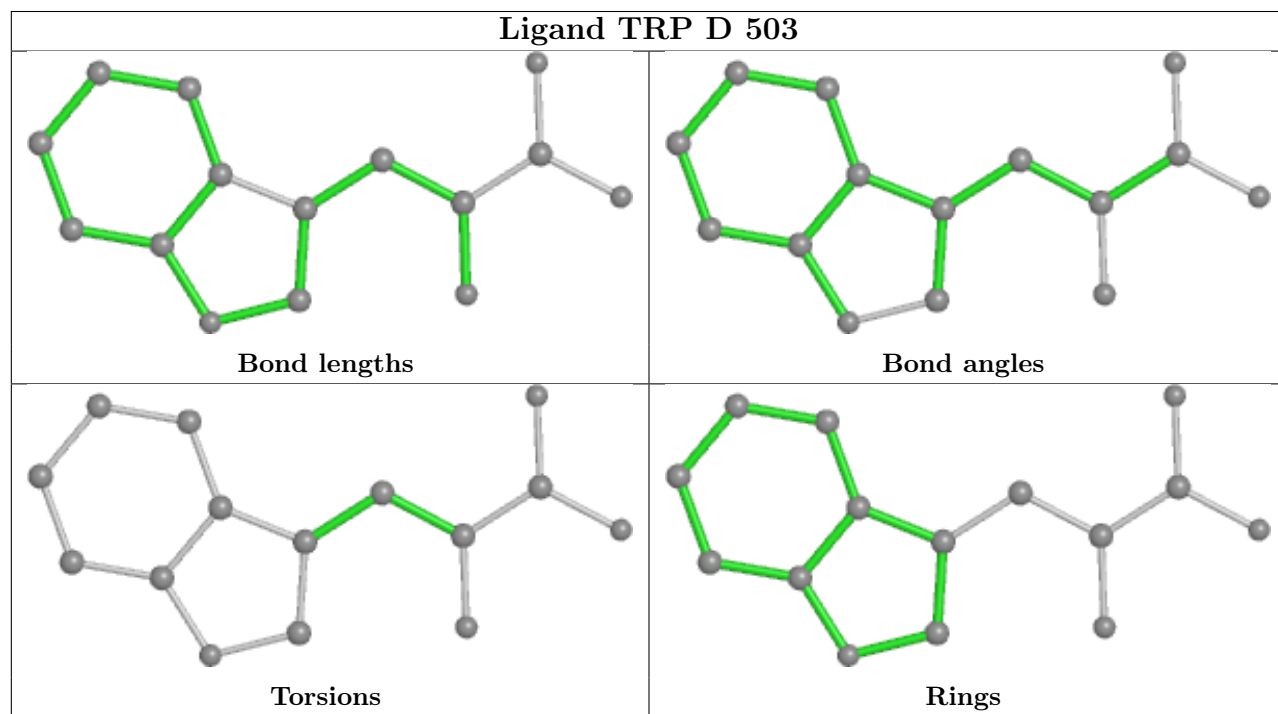




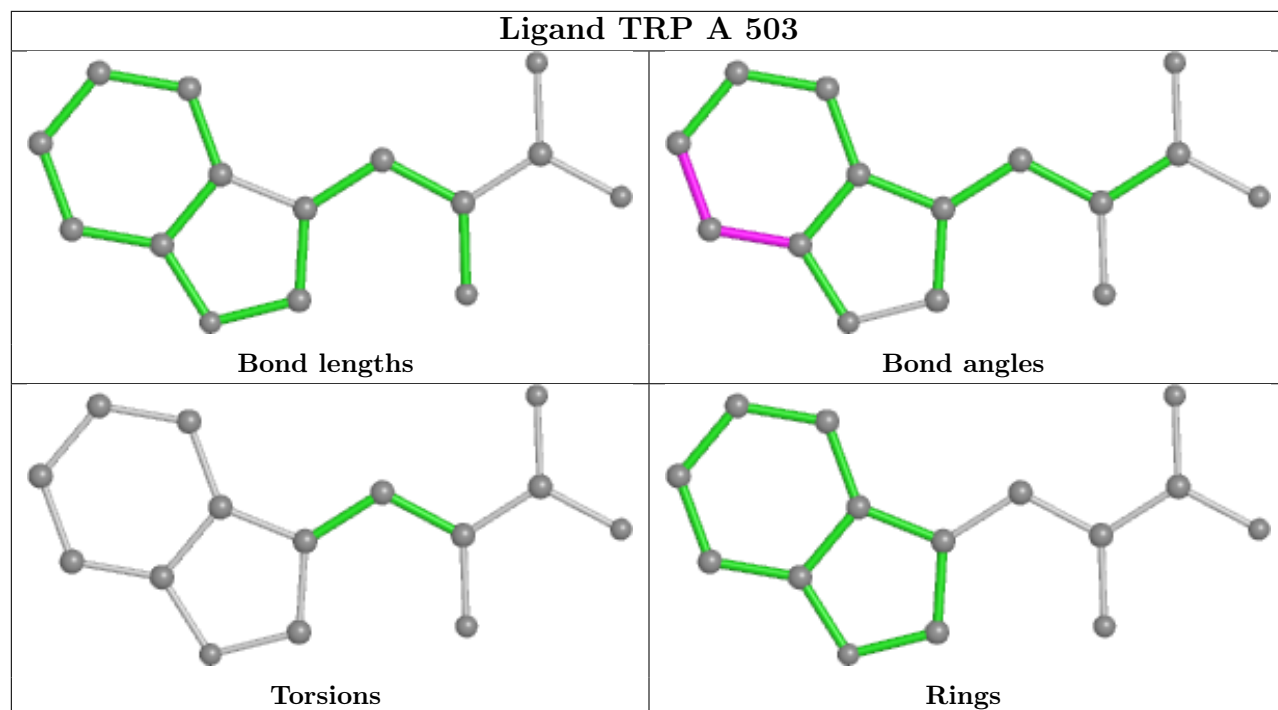
Ligand TRP C 503



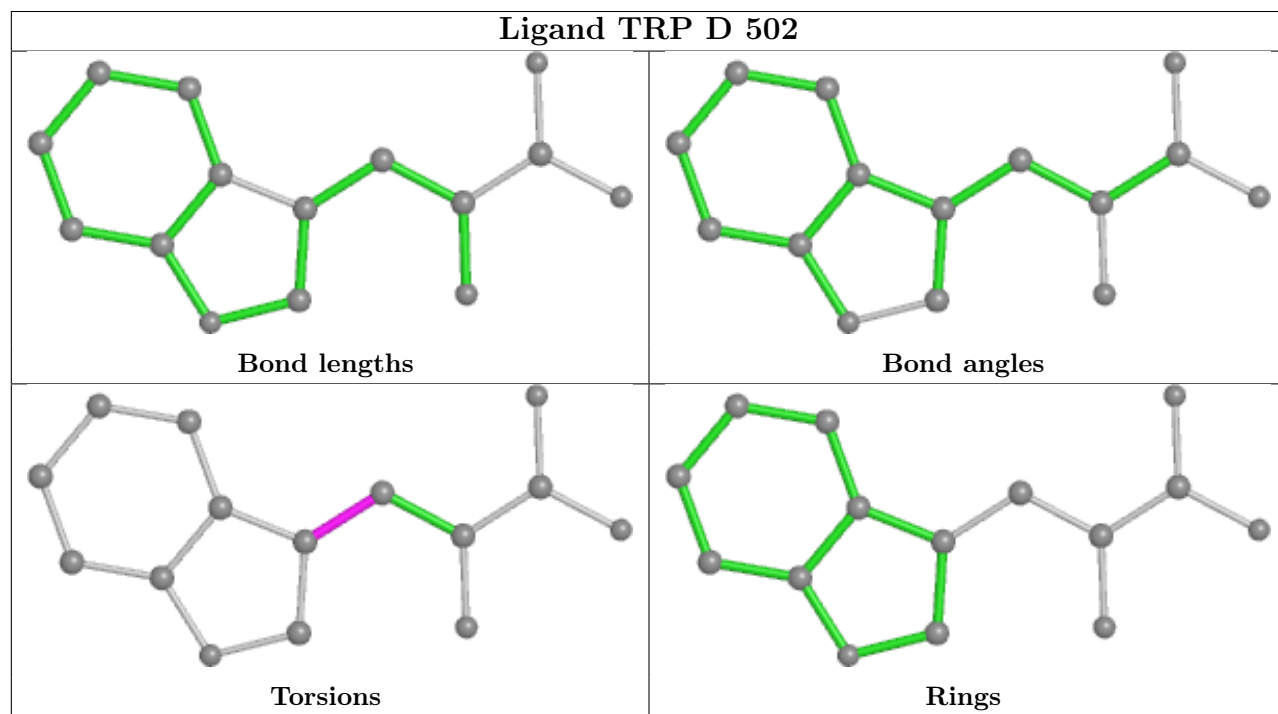
Ligand TRP D 503



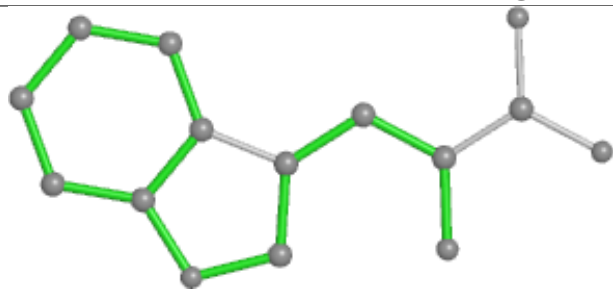
Ligand TRP A 503



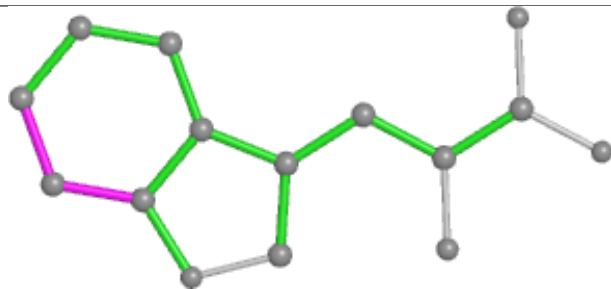
Ligand TRP D 502



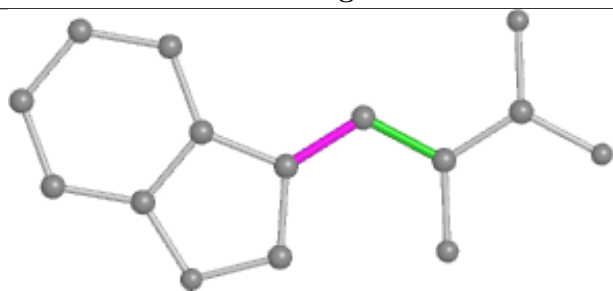
Ligand TRP B 502



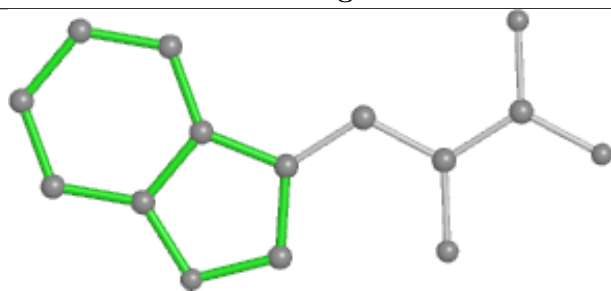
Bond lengths



Bond angles

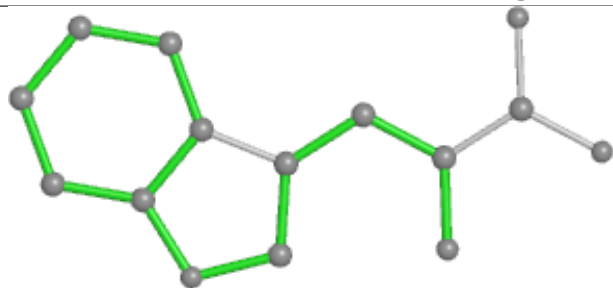


Torsions

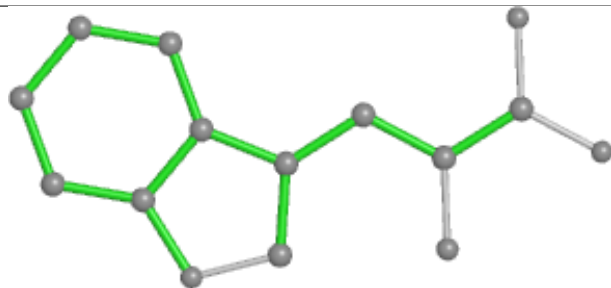


Rings

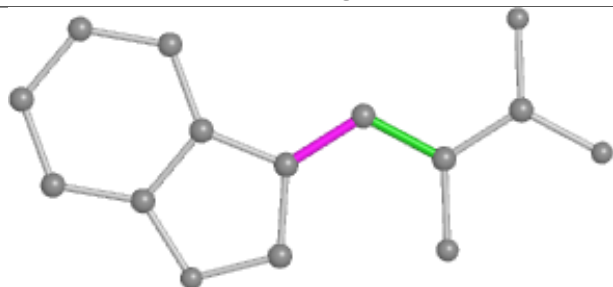
Ligand TRP C 502



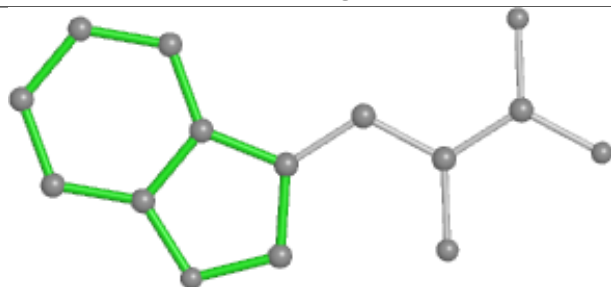
Bond lengths



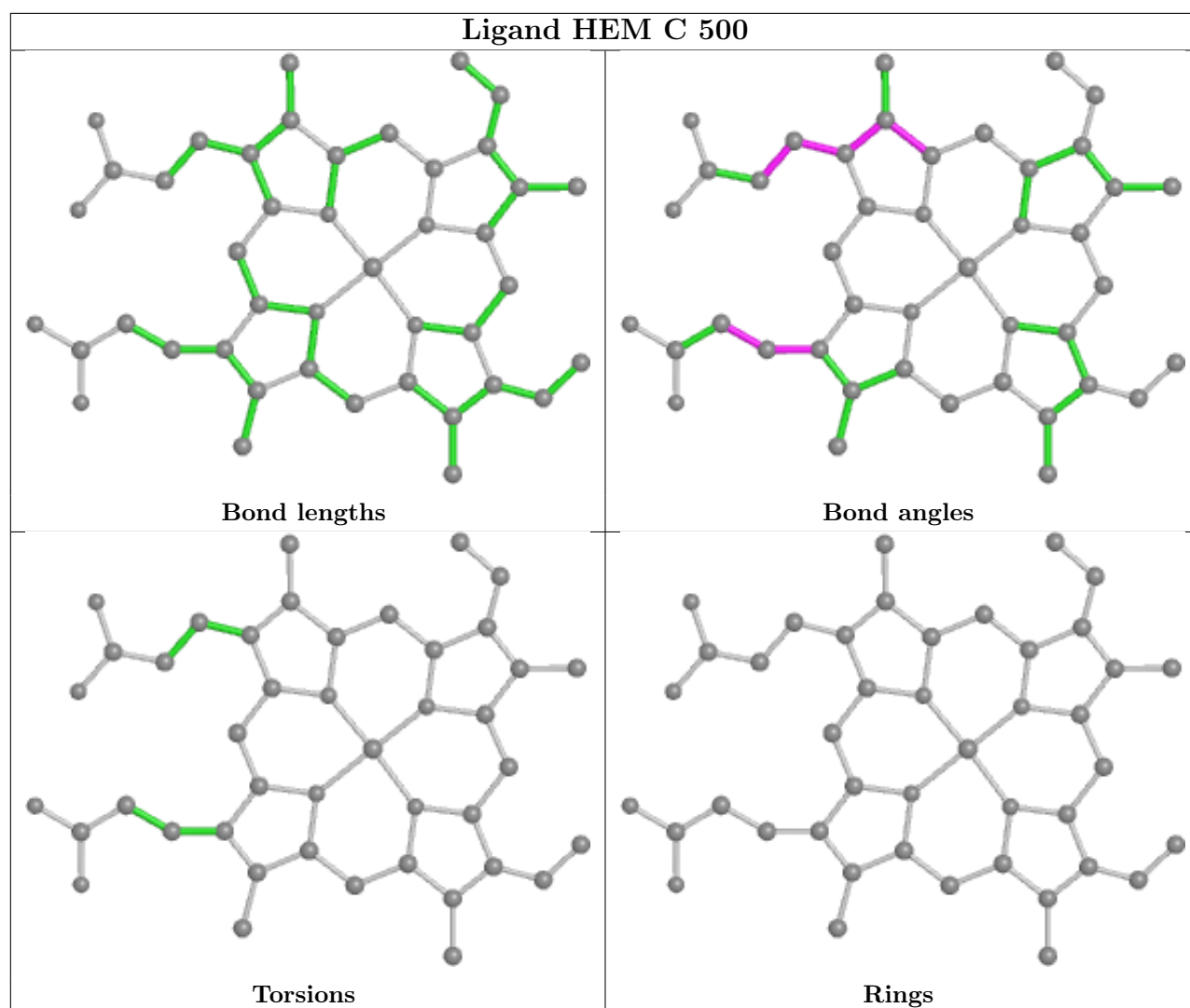
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.14	26 (7%) 14 16	23, 34, 77, 117	0
1	B	347/380 (91%)	0.00	19 (5%) 25 27	23, 34, 70, 91	0
1	C	343/380 (90%)	0.34	38 (11%) 5 5	24, 38, 85, 107	0
1	D	353/380 (92%)	0.11	23 (6%) 18 20	22, 34, 77, 100	0
All	All	1394/1520 (91%)	0.15	106 (7%) 13 14	22, 35, 78, 117	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ARG	7.1
1	A	384	THR	6.5
1	C	383	PRO	6.5
1	A	174	PRO	6.3
1	D	383	PRO	5.8
1	C	218	HIS	5.6
1	C	239	ILE	5.6
1	B	174	PRO	5.5
1	A	383	PRO	5.1
1	C	384	THR	5.1
1	D	388	PHE	5.0
1	C	386	HIS	4.7
1	D	248	GLU	4.7
1	A	179	HIS	4.6
1	B	175	TYR	4.6
1	B	386	HIS	4.5
1	C	254	VAL	4.5
1	B	384	THR	4.4
1	A	388	PHE	4.4
1	B	383	PRO	4.3
1	A	386	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	384	THR	4.2
1	C	238	PHE	4.2
1	C	169	GLN	4.2
1	C	219	GLY	4.2
1	C	388	PHE	4.1
1	A	176	ASN	4.1
1	C	243	ALA	4.0
1	D	218	HIS	4.0
1	C	255	ALA	3.9
1	B	171	MET	3.8
1	A	385	ILE	3.8
1	B	382	ASN	3.8
1	C	382	ASN	3.8
1	C	249	GLU	3.7
1	C	173	VAL	3.6
1	C	171	MET	3.6
1	C	182	ASP	3.6
1	C	241	ILE	3.6
1	A	248	GLU	3.5
1	C	389	LEU	3.5
1	A	389	LEU	3.5
1	B	169	GLN	3.5
1	B	388	PHE	3.4
1	A	170	ASN	3.4
1	B	182	ASP	3.4
1	A	245	GLU	3.4
1	B	385	ILE	3.4
1	D	387	LYS	3.4
1	B	39	GLY	3.4
1	A	382	ASN	3.3
1	D	243	ALA	3.3
1	A	175	TYR	3.2
1	D	382	ASN	3.1
1	C	376	HIS	3.1
1	A	246	GLU	3.1
1	C	242	GLN	3.0
1	C	385	ILE	3.0
1	D	386	HIS	3.0
1	C	170	ASN	3.0
1	A	177	ARG	3.0
1	D	39	GLY	3.0
1	A	255	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	245	GLU	2.9
1	C	174	PRO	2.9
1	D	376	HIS	2.9
1	B	170	ASN	2.8
1	C	232	ARG	2.8
1	C	250	LYS	2.8
1	A	247	SER	2.8
1	C	275	HIS	2.7
1	C	252	GLU	2.7
1	D	219	GLY	2.7
1	D	247	SER	2.6
1	B	218	HIS	2.6
1	B	173	VAL	2.6
1	C	387	LYS	2.5
1	D	389	LEU	2.5
1	C	240	ARG	2.5
1	B	193	LEU	2.5
1	D	255	ALA	2.5
1	C	257	PHE	2.4
1	C	344	GLY	2.4
1	D	175	TYR	2.4
1	A	169	GLN	2.4
1	A	73	ILE	2.3
1	D	170	ASN	2.3
1	C	253	GLN	2.3
1	A	39	GLY	2.3
1	D	253	GLN	2.3
1	A	182	ASP	2.3
1	D	179	HIS	2.3
1	A	218	HIS	2.2
1	C	185	LYS	2.2
1	D	171	MET	2.2
1	D	275	HIS	2.2
1	B	389	LEU	2.2
1	B	376	HIS	2.2
1	D	390	GLU	2.1
1	A	252	GLU	2.1
1	C	279	LYS	2.1
1	C	39	GLY	2.1
1	A	376	HIS	2.0
1	C	72	PHE	2.0
1	B	243	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	278	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

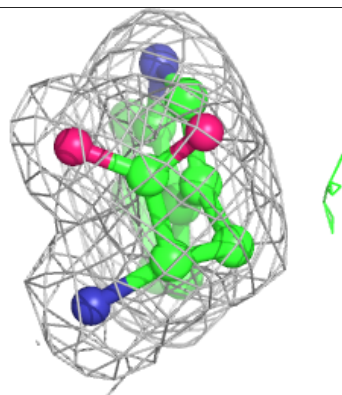
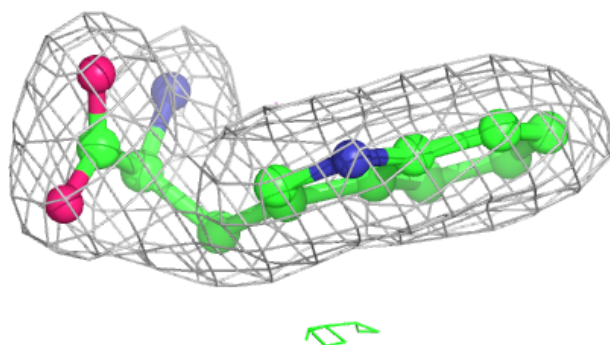
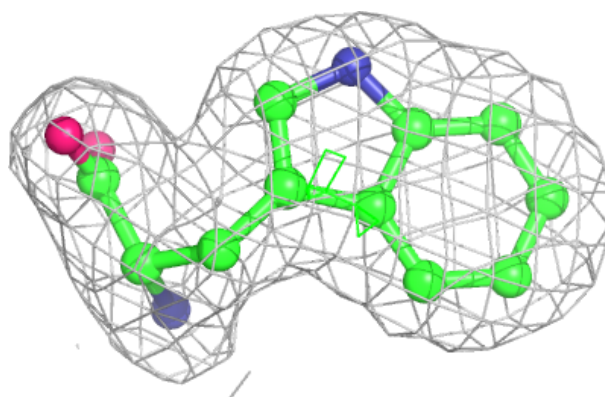
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TRP	C	503	15/15	0.93	0.11	33,36,44,50	0
4	TRP	D	503	15/15	0.94	0.11	30,32,41,43	0
4	TRP	B	503	15/15	0.95	0.09	29,31,36,37	0
4	TRP	C	502	15/15	0.95	0.11	34,35,36,36	0
4	TRP	A	502	15/15	0.96	0.11	33,34,38,38	0
4	TRP	D	502	15/15	0.97	0.09	29,30,32,32	0
4	TRP	B	502	15/15	0.97	0.12	28,29,35,37	0
4	TRP	A	503	15/15	0.97	0.08	28,31,35,37	0
2	HEM	C	500	43/43	0.97	0.10	28,30,33,35	0
2	HEM	B	500	43/43	0.98	0.13	25,28,31,37	0
3	CMO	B	501	2/2	0.98	0.12	33,33,33,35	0
2	HEM	A	500	43/43	0.98	0.12	29,33,36,37	0
3	CMO	C	501	2/2	0.98	0.11	31,31,31,35	0
2	HEM	D	500	43/43	0.98	0.10	26,28,30,31	0
3	CMO	A	501	2/2	0.98	0.14	34,34,34,41	0
3	CMO	D	501	2/2	0.99	0.15	34,34,34,34	0

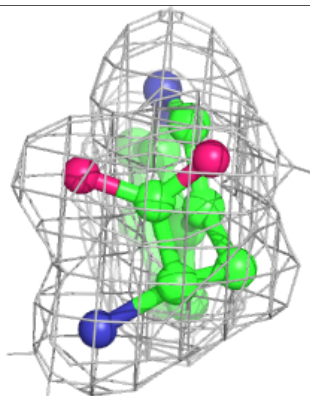
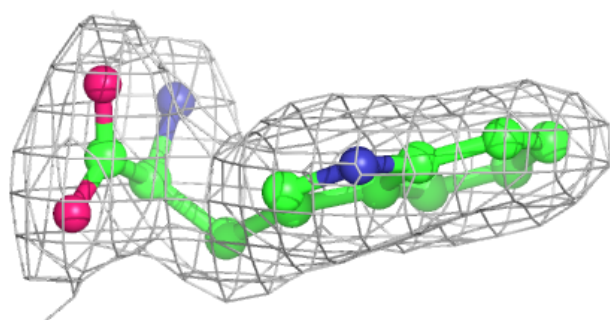
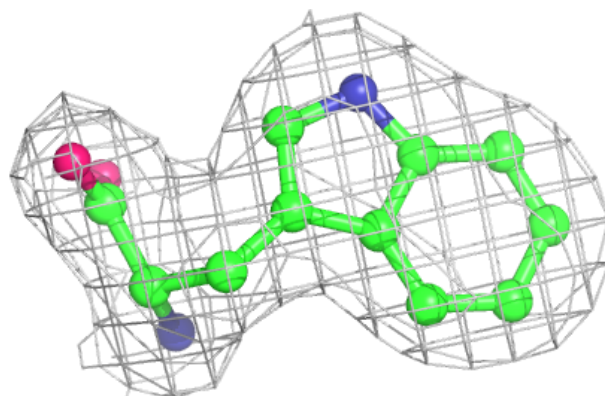
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

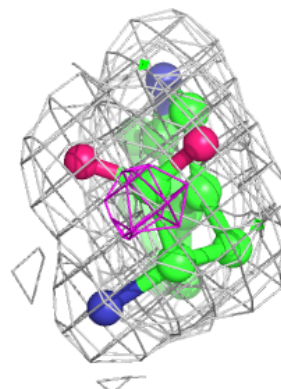
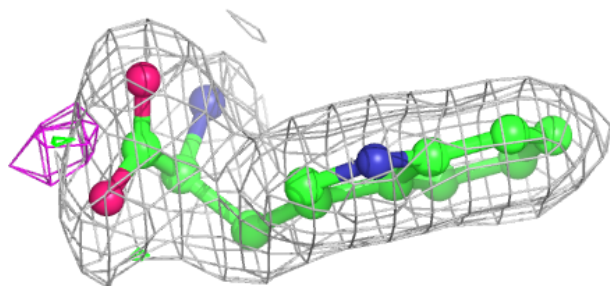
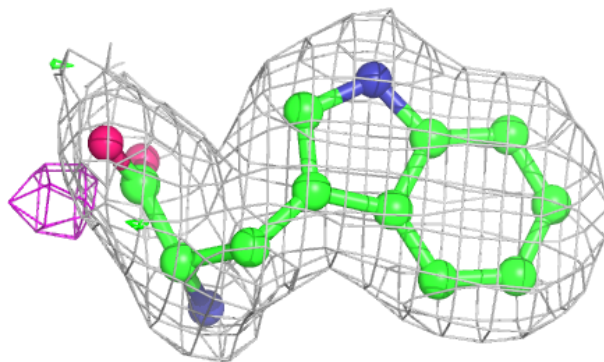
**Electron density around TRP D 503:**

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

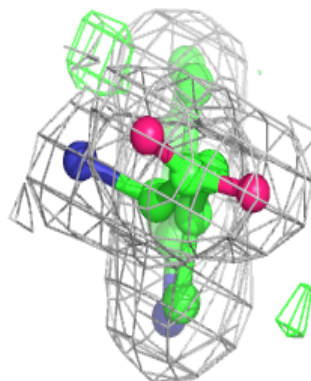
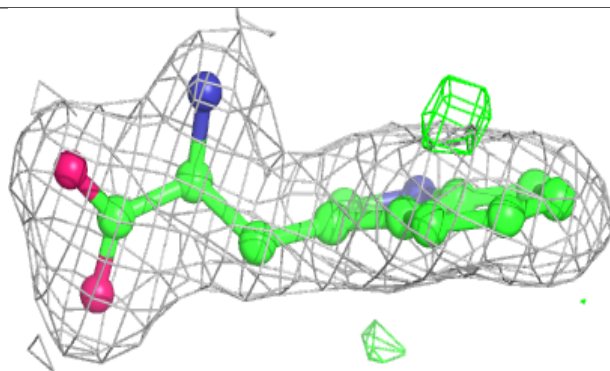
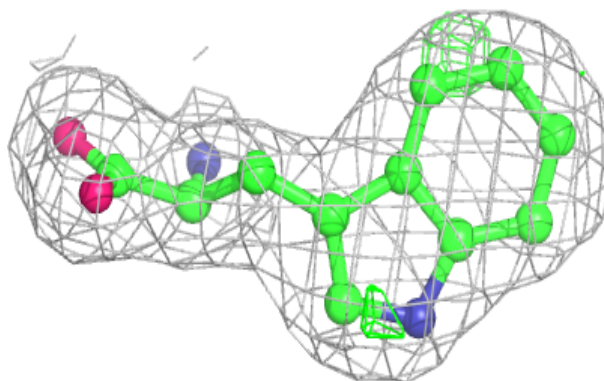


Electron density around TRP B 503:

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

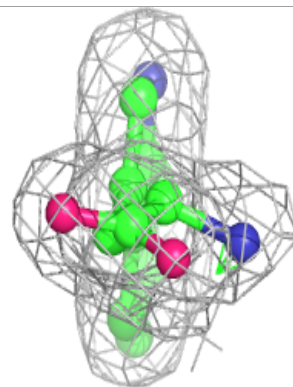
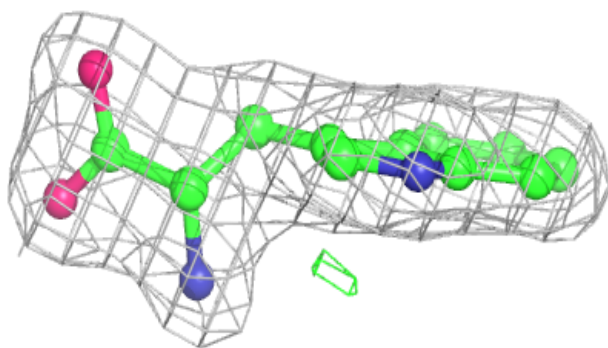
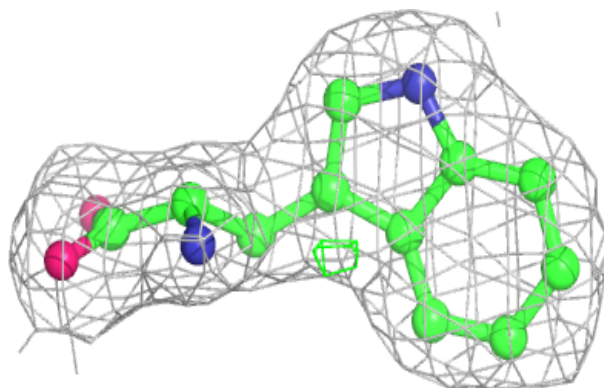
**Electron density around TRP C 502:**

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

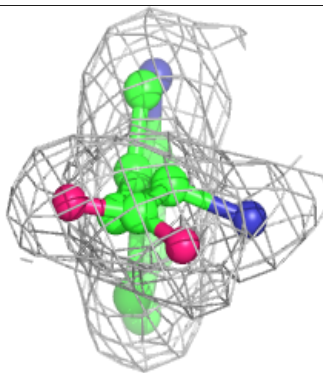
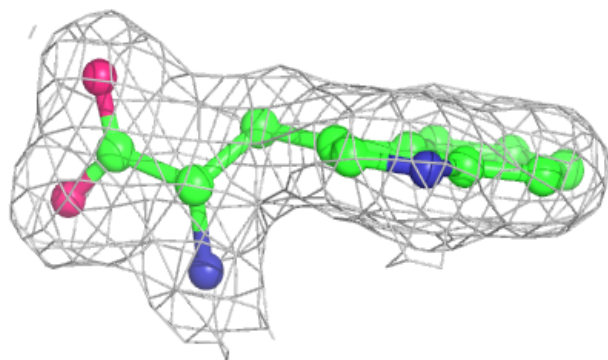
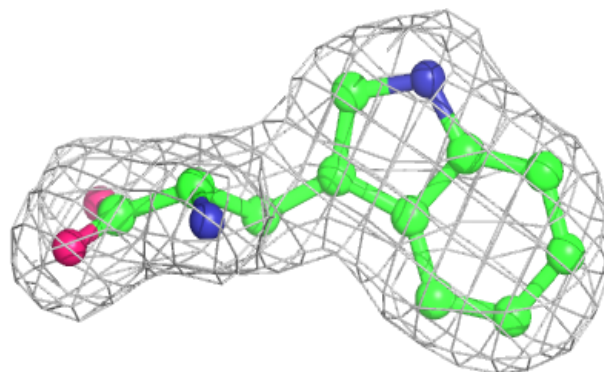


Electron density around TRP A 502:

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

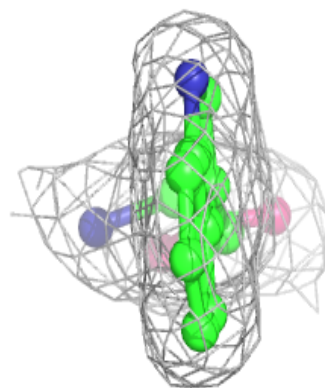
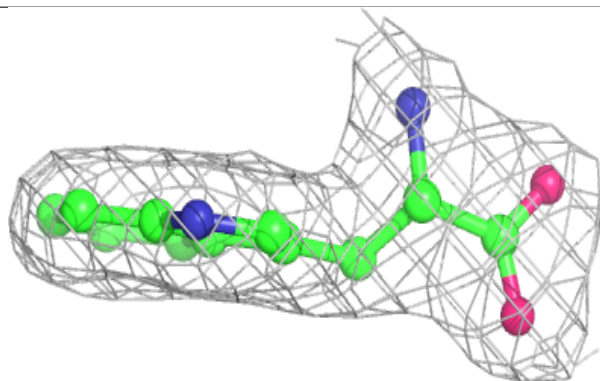
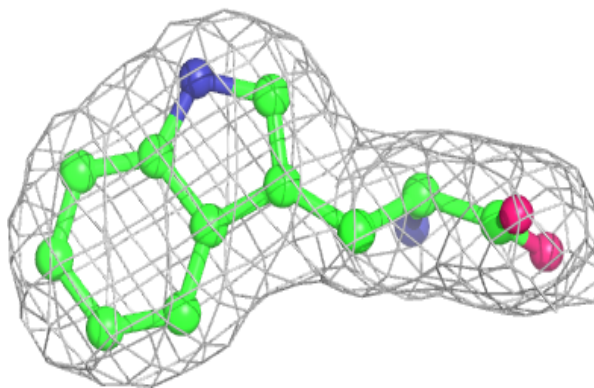
**Electron density around TRP D 502:**

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

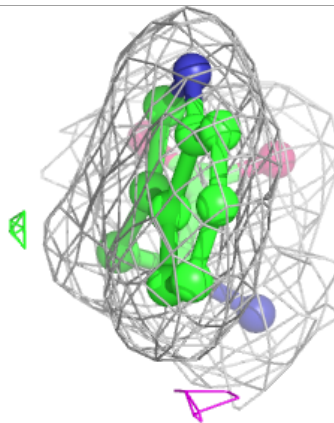
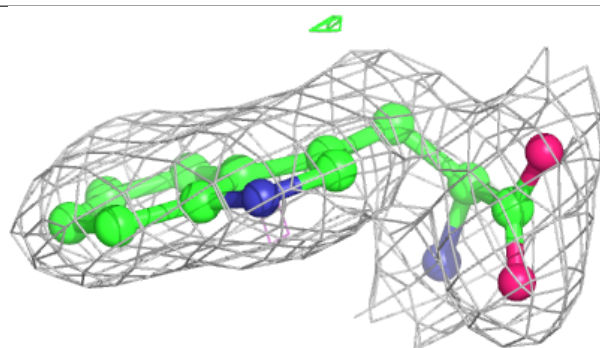
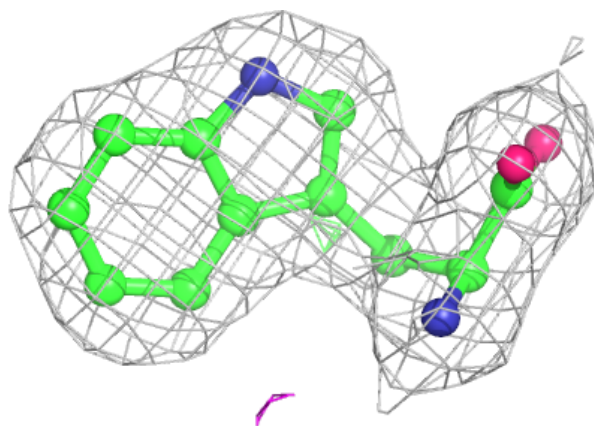


Electron density around TRP B 502:

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

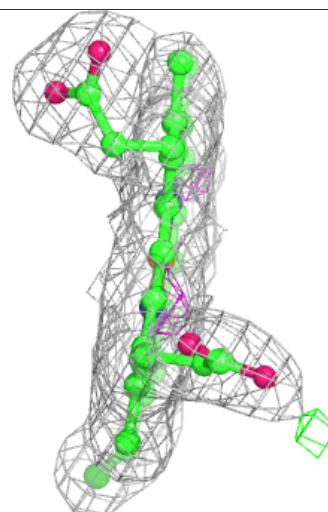
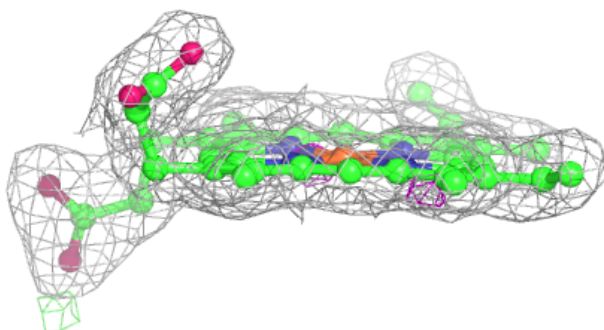
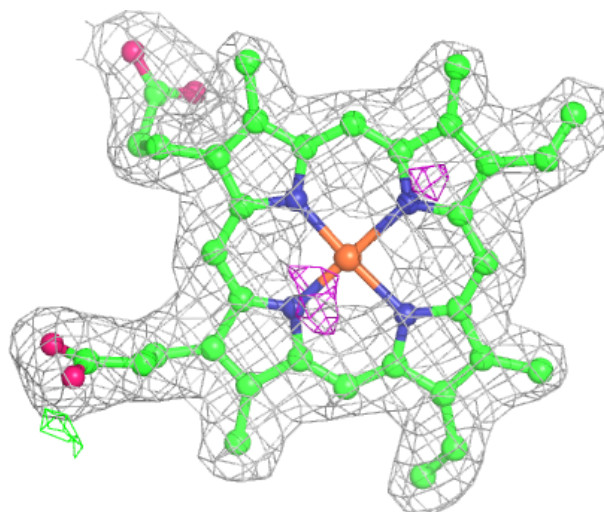
**Electron density around TRP A 503:**

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



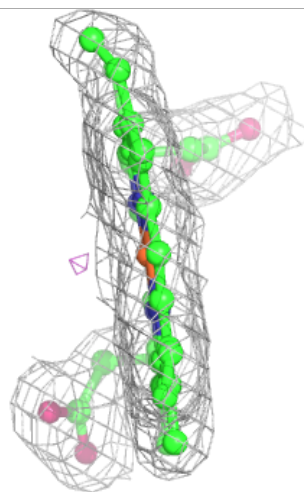
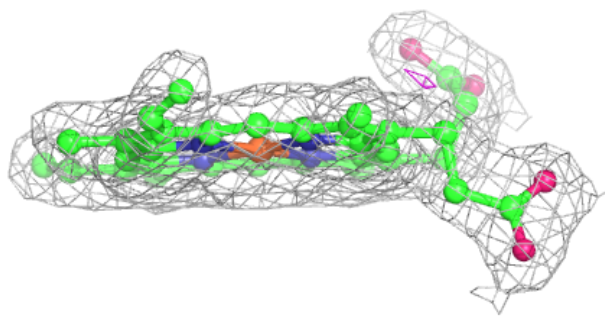
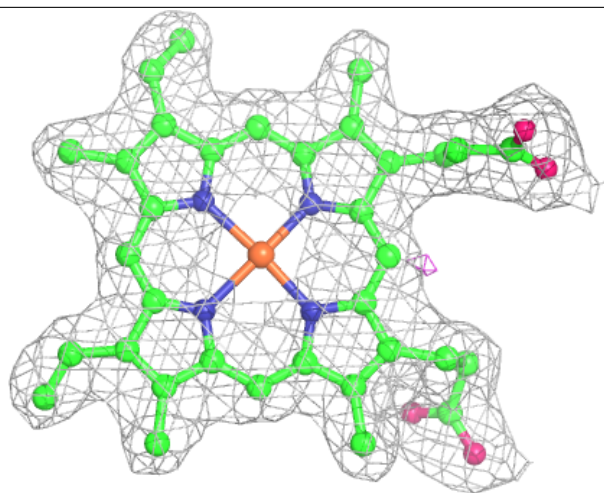
Electron density around HEM C 500:

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



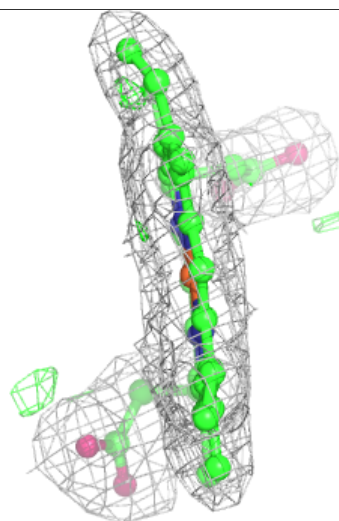
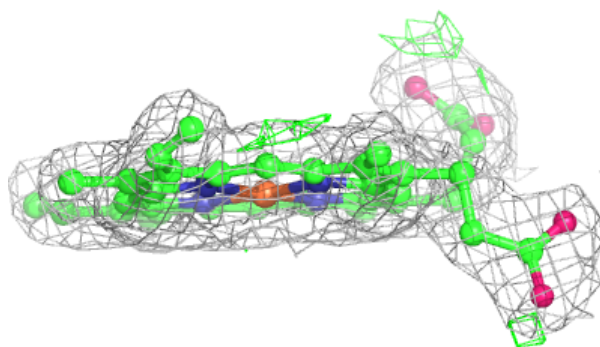
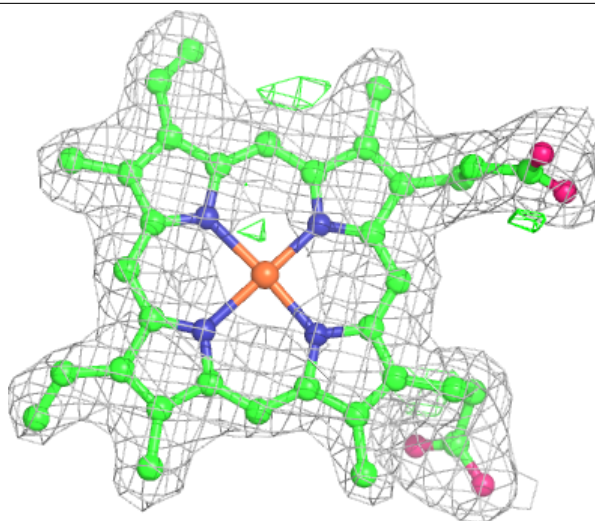
Electron density around HEM B 500:

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



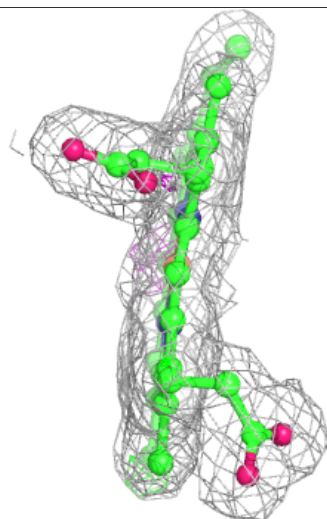
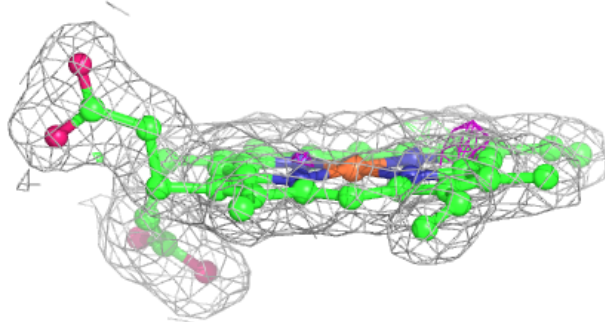
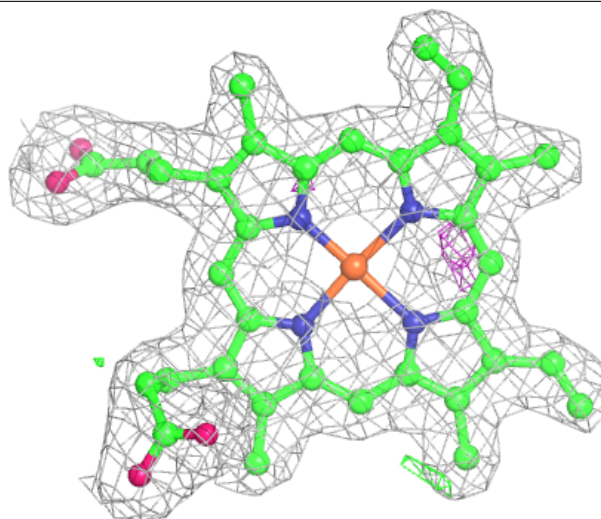
Electron density around HEM A 500:

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



Electron density around HEM 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.