



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2021 – 12:04 PM EST

PDB ID : 6UBP
Title : Crystal structure of a photochemical intermediate of human indoleamine 2,3-dioxygenase 1 in complex with carbon monoxide and tryptophan
Authors : Pham, K.N.; Yeh, S.R.
Deposited on : 2019-09-12
Resolution : 2.95 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

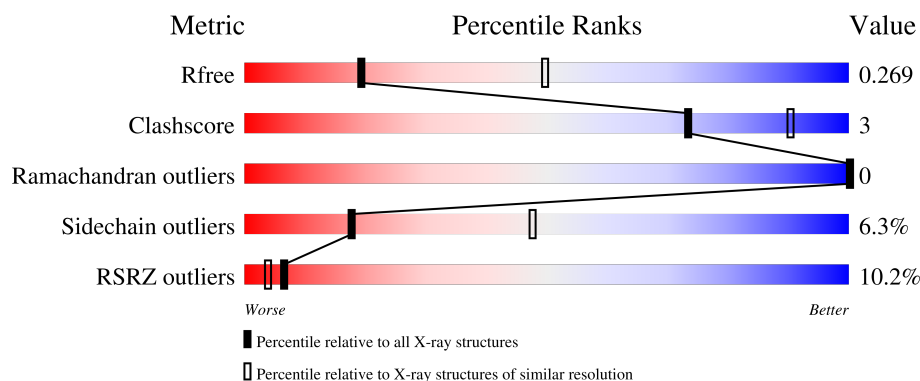
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	425	<div> <div>10%</div> <div>80%</div> <div>7%</div> <div>12%</div> </div>
1	B	425	<div> <div>8%</div> <div>78%</div> <div>9%</div> <div>12%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CMO	A	503	-	-	-	X
4	CMO	B	503	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6115 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2978	1913	508	540	17			
1	B	372	Total	C	N	O	S	0	0	0
			2954	1900	504	533	17			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP P14902
A	404	LYS	-	expression tag	UNP P14902
A	405	GLY	-	expression tag	UNP P14902
A	406	GLU	-	expression tag	UNP P14902
A	407	LEU	-	expression tag	UNP P14902
A	408	ASN	-	expression tag	UNP P14902
A	409	SER	-	expression tag	UNP P14902
A	410	LYS	-	expression tag	UNP P14902
A	411	LEU	-	expression tag	UNP P14902
A	412	GLU	-	expression tag	UNP P14902
A	413	GLY	-	expression tag	UNP P14902
A	414	LYS	-	expression tag	UNP P14902
A	415	PRO	-	expression tag	UNP P14902
A	416	ILE	-	expression tag	UNP P14902
A	417	PRO	-	expression tag	UNP P14902
A	418	ASN	-	expression tag	UNP P14902
A	419	PRO	-	expression tag	UNP P14902
A	420	LEU	-	expression tag	UNP P14902
A	421	LEU	-	expression tag	UNP P14902
A	422	GLY	-	expression tag	UNP P14902
A	423	LEU	-	expression tag	UNP P14902
A	424	ASP	-	expression tag	UNP P14902
A	425	SER	-	expression tag	UNP P14902
A	426	THR	-	expression tag	UNP P14902
A	427	ARG	-	expression tag	UNP P14902

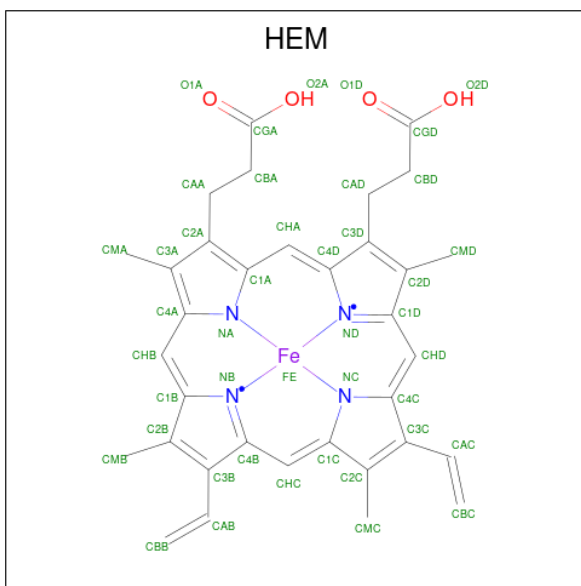
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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	THR	-	expression tag	UNP P14902
A	429	GLY	-	expression tag	UNP P14902
A	430	HIS	-	expression tag	UNP P14902
A	431	HIS	-	expression tag	UNP P14902
A	432	HIS	-	expression tag	UNP P14902
A	433	HIS	-	expression tag	UNP P14902
A	434	HIS	-	expression tag	UNP P14902
A	435	HIS	-	expression tag	UNP P14902
B	11	MET	-	initiating methionine	UNP P14902
B	404	LYS	-	expression tag	UNP P14902
B	405	GLY	-	expression tag	UNP P14902
B	406	GLU	-	expression tag	UNP P14902
B	407	LEU	-	expression tag	UNP P14902
B	408	ASN	-	expression tag	UNP P14902
B	409	SER	-	expression tag	UNP P14902
B	410	LYS	-	expression tag	UNP P14902
B	411	LEU	-	expression tag	UNP P14902
B	412	GLU	-	expression tag	UNP P14902
B	413	GLY	-	expression tag	UNP P14902
B	414	LYS	-	expression tag	UNP P14902
B	415	PRO	-	expression tag	UNP P14902
B	416	ILE	-	expression tag	UNP P14902
B	417	PRO	-	expression tag	UNP P14902
B	418	ASN	-	expression tag	UNP P14902
B	419	PRO	-	expression tag	UNP P14902
B	420	LEU	-	expression tag	UNP P14902
B	421	LEU	-	expression tag	UNP P14902
B	422	GLY	-	expression tag	UNP P14902
B	423	LEU	-	expression tag	UNP P14902
B	424	ASP	-	expression tag	UNP P14902
B	425	SER	-	expression tag	UNP P14902
B	426	THR	-	expression tag	UNP P14902
B	427	ARG	-	expression tag	UNP P14902
B	428	THR	-	expression tag	UNP P14902
B	429	GLY	-	expression tag	UNP P14902
B	430	HIS	-	expression tag	UNP P14902
B	431	HIS	-	expression tag	UNP P14902
B	432	HIS	-	expression tag	UNP P14902
B	433	HIS	-	expression tag	UNP P14902
B	434	HIS	-	expression tag	UNP P14902
B	435	HIS	-	expression tag	UNP P14902

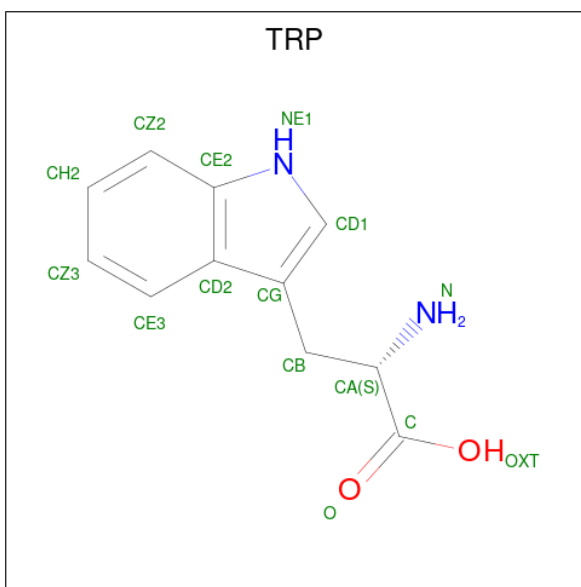
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



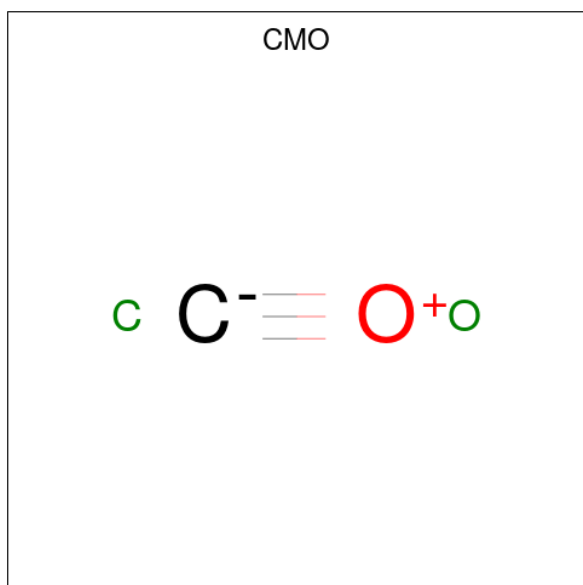
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).



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

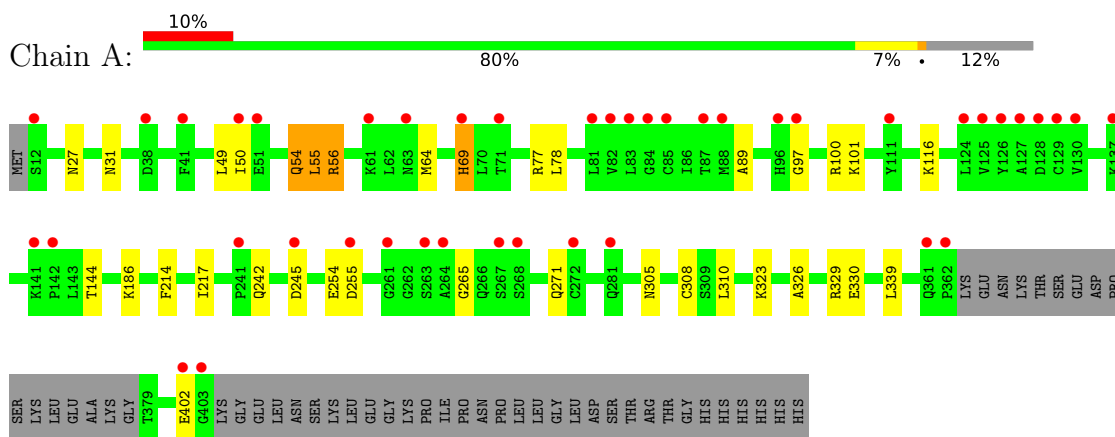
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	27	Total	O	0	0
			27	27		

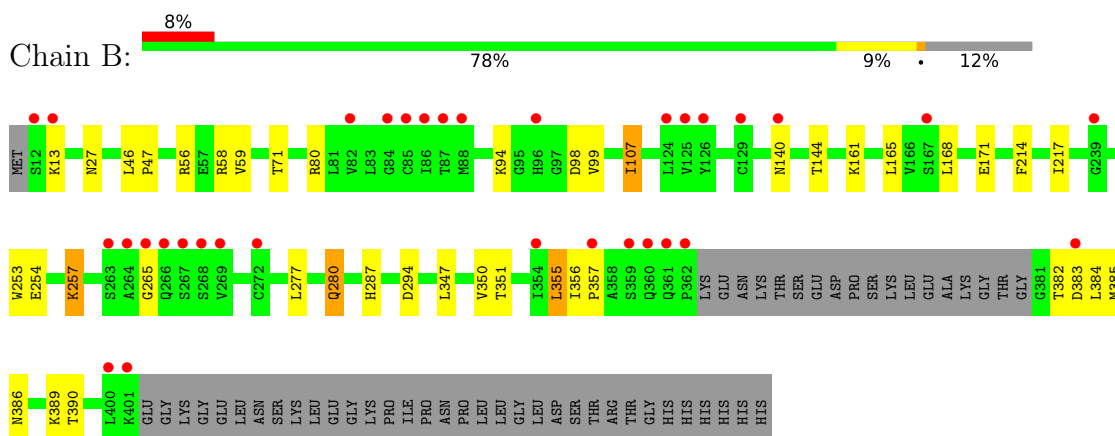
3 Residue-property plots

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

• Molecule 1: Indoleamine 2,3-dioxygenase 1



• Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.94Å 97.73Å 130.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.34 – 2.95 29.34 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.34-2.95) 100.0 (29.34-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.264 0.215 , 0.269	Depositor DCC
R_{free} test set	1165 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	99.9	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6115	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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

5.1 Standard geometry

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	0.66	0/3047	0.70	0/4121
1	B	0.65	0/3023	0.70	0/4089
All	All	0.65	0/6070	0.70	0/8210

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

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	2978	0	2989	14	0
1	B	2954	0	2970	22	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	15	0	9	0	0
3	B	15	0	9	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	36	0	0	0	0
5	B	27	0	0	0	0
All	All	6115	0	6037	40	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 3.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:HD11	2:B:501:HEM:HMA3	1.57	0.84
1:A:50:ILE:HG12	1:A:55:LEU:HD12	1.69	0.73
1:B:384:LEU:HD11	2:B:501:HEM:CMA	2.21	0.70
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.73	0.68
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.79	0.64
1:B:385:MET:HE3	1:B:385:MET:HA	1.83	0.60
1:B:351:THR:HA	1:B:355:LEU:HD23	1.84	0.59
1:B:386:ASN:O	1:B:390:THR:OG1	2.10	0.56
1:A:329:ARG:HH12	1:A:402:GLU:HG2	1.72	0.55
1:B:385:MET:CE	1:B:385:MET:HA	2.36	0.55
1:A:329:ARG:NH1	1:A:402:GLU:HG2	2.21	0.55
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	1.89	0.54
1:A:326:ALA:O	1:A:330:GLU:HG3	2.08	0.53
1:B:217:ILE:HD11	2:B:501:HEM:HAB	1.91	0.52
1:A:97:GLY:HA2	1:A:242:GLN:HE22	1.74	0.52
1:B:280:GLN:HE21	1:B:280:GLN:HA	1.75	0.51
1:B:56:ARG:NH2	1:B:98:ASP:O	2.42	0.51
1:B:385:MET:O	1:B:389:LYS:HB2	2.11	0.51
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.93	0.50
1:A:265:GLY:HA2	2:A:501:HEM:C3D	2.46	0.50
1:B:265:GLY:HA2	2:B:501:HEM:C3D	2.47	0.49
1:B:351:THR:HA	1:B:355:LEU:CD2	2.42	0.49
1:A:55:LEU:HD11	1:A:89:ALA:HB1	1.93	0.49
1:A:49:LEU:HD23	1:A:54:GLN:HB3	1.95	0.48
1:B:253:TRP:HB3	1:B:257:LYS:HE3	1.97	0.46
1:B:168:LEU:O	1:B:171:GLU:HB2	2.16	0.46
1:B:59:VAL:HG13	1:B:107:ILE:HD12	1.98	0.45
1:A:326:ALA:HA	1:A:329:ARG:NH1	2.31	0.44
1:B:46:LEU:N	1:B:47:PRO:HD2	2.32	0.44
1:B:384:LEU:CD1	2:B:501:HEM:HMA3	2.38	0.44
1:B:161:LYS:HG2	1:B:165:LEU:HD12	1.99	0.43
1:A:217:ILE:HD11	2:A:501:HEM:HAB	1.99	0.43
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.46	0.43
1:B:350:VAL:HG13	1:B:384:LEU:HD21	2.00	0.43
1:A:305:ASN:O	1:A:308:CYS:HB3	2.19	0.43
1:B:27:ASN:O	1:B:27:ASN:ND2	2.53	0.42
1:A:56:ARG:HH21	1:A:100:ARG:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HA	1:B:46:LEU:HD23	1.94	0.41
1:A:69:HIS:ND1	1:A:69:HIS:N	2.70	0.40
1:A:329:ARG:NH1	1:A:402:GLU:HA	2.36	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	372/425 (88%)	354 (95%)	18 (5%)	0	100	100
1	B	368/425 (87%)	351 (95%)	17 (5%)	0	100	100
All	All	740/850 (87%)	705 (95%)	35 (5%)	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	325/368 (88%)	304 (94%)	21 (6%)	17	46
1	B	323/368 (88%)	303 (94%)	20 (6%)	18	48
All	All	648/736 (88%)	607 (94%)	41 (6%)	18	48

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	31	ASN
1	A	54	GLN
1	A	55	LEU
1	A	56	ARG
1	A	64	MET
1	A	69	HIS
1	A	77	ARG
1	A	78	LEU
1	A	101	LYS
1	A	116	LYS
1	A	144	THR
1	A	186	LYS
1	A	214	PHE
1	A	245	ASP
1	A	254	GLU
1	A	255	ASP
1	A	271	GLN
1	A	310	LEU
1	A	323	LYS
1	A	339	LEU
1	B	13	LYS
1	B	58	ARG
1	B	71	THR
1	B	80	ARG
1	B	94	LYS
1	B	99	VAL
1	B	107	ILE
1	B	140	ASN
1	B	144	THR
1	B	214	PHE
1	B	254	GLU
1	B	257	LYS
1	B	277	LEU
1	B	280	GLN
1	B	287	HIS
1	B	294	ASP
1	B	347	LEU
1	B	355	LEU
1	B	382	THR
1	B	383	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	76	GLN
1	A	242	GLN
1	A	313	ASN
1	B	27	ASN
1	B	29	GLN
1	B	140	ASN
1	B	218	HIS
1	B	280	GLN
1	B	313	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	CMO	A	503	-	0,1,1	0.00	-	-		
2	HEM	A	501	1	27,50,50	0.88	2 (7%)	17,82,82	1.04	1 (5%)
3	TRP	A	502	-	12,16,16	0.70	0	12,22,22	0.90	0
3	TRP	B	502	-	12,16,16	0.72	0	12,22,22	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	501	1	27,50,50	0.87	2 (7%)	17,82,82	1.53	2 (11%)
4	CMO	B	503	-	0,1,1	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	A	502	-	-	1/3/8/8	0/2/2/2
3	TRP	B	502	-	-	1/3/8/8	0/2/2/2
2	HEM	A	501	1	-	0/6/54/54	-
2	HEM	B	501	1	-	0/6/54/54	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C2B	-2.61	1.36	1.40
2	A	501	HEM	C3B-C2B	-2.49	1.36	1.40
2	A	501	HEM	C4D-C3D	2.16	1.47	1.42
2	B	501	HEM	C4D-C3D	2.14	1.47	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CMA-C3A-C4A	-4.12	122.13	128.46
2	B	501	HEM	CMA-C3A-C2A	2.64	129.92	124.94
2	A	501	HEM	CMA-C3A-C4A	-2.31	124.92	128.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

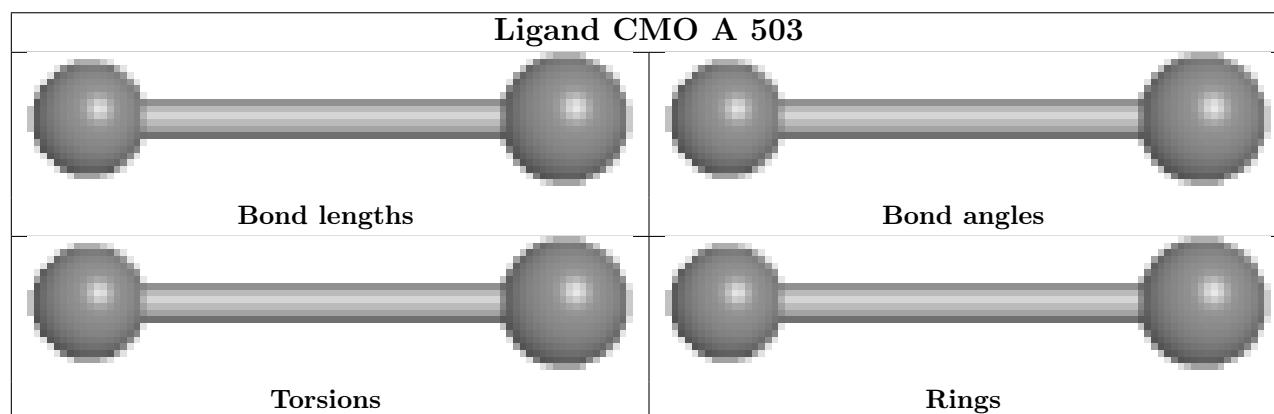
Mol	Chain	Res	Type	Atoms
3	B	502	TRP	CA-CB-CG-CD1
3	A	502	TRP	CA-CB-CG-CD1

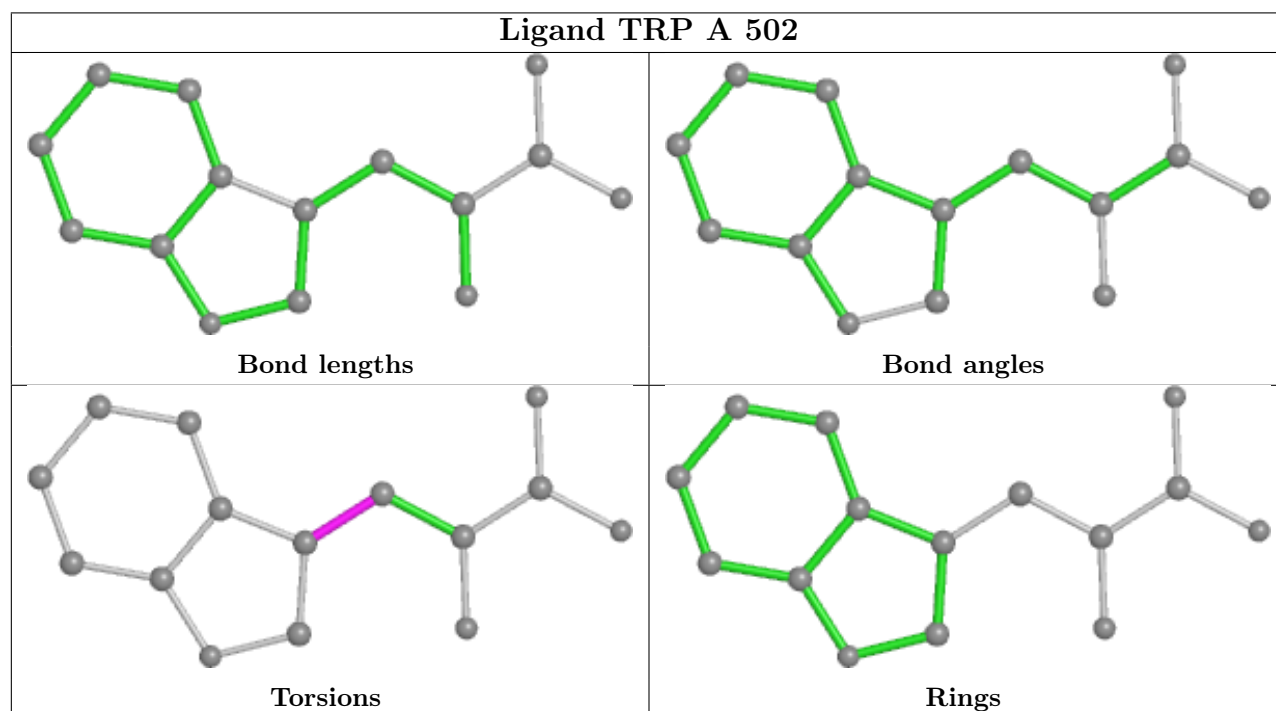
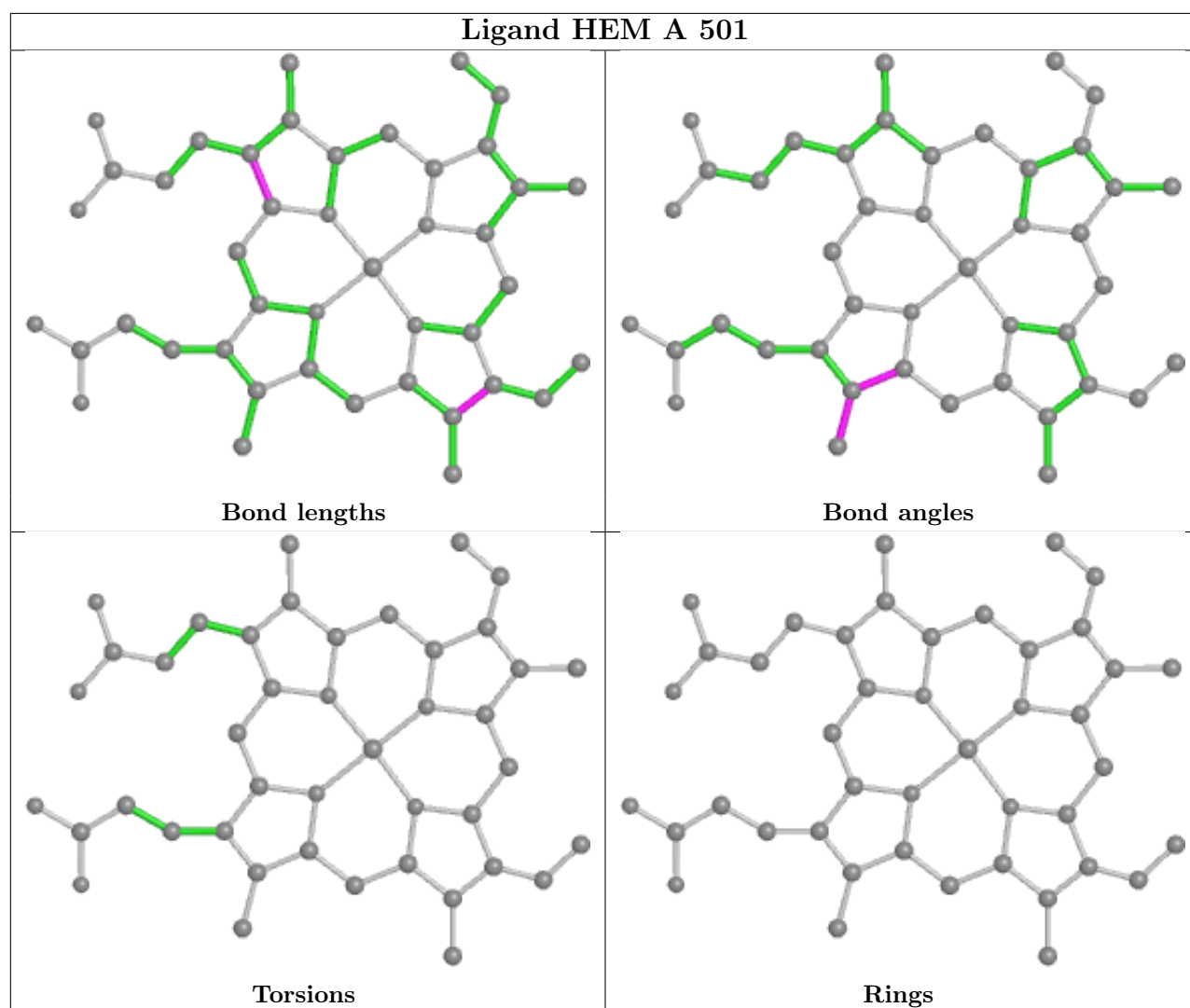
There are no ring outliers.

2 monomers are involved in 11 short contacts:

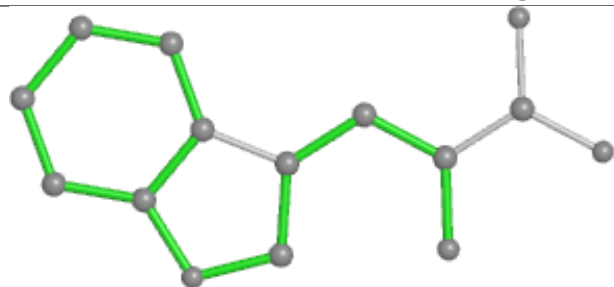
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
2	B	501	HEM	6	0

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.

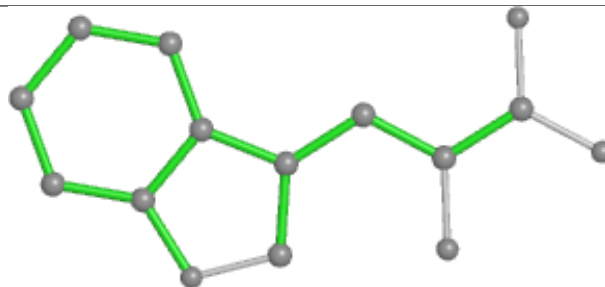




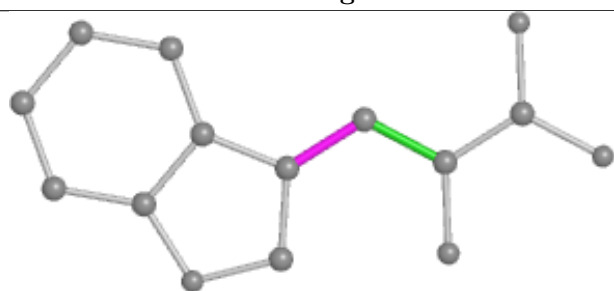
Ligand TRP B 502



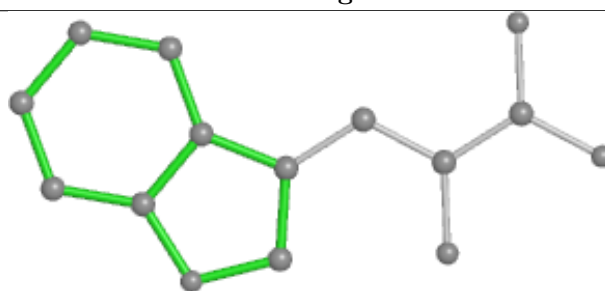
Bond lengths



Bond angles

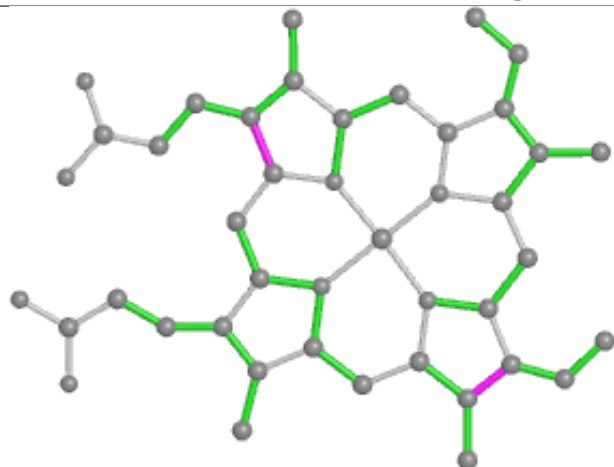


Torsions

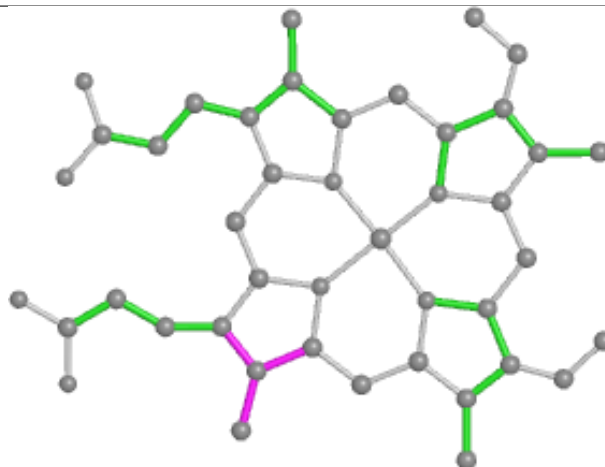


Rings

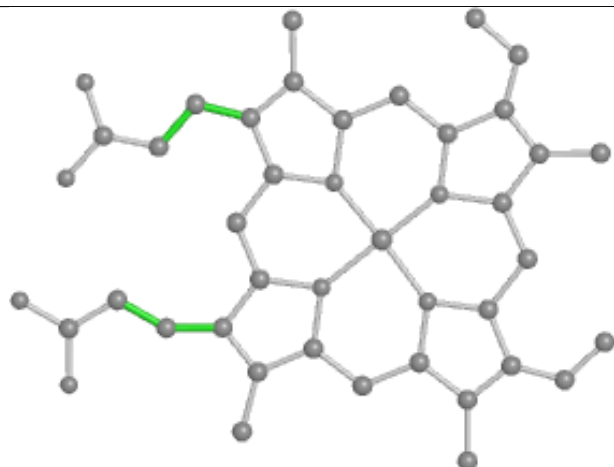
Ligand HEM B 501



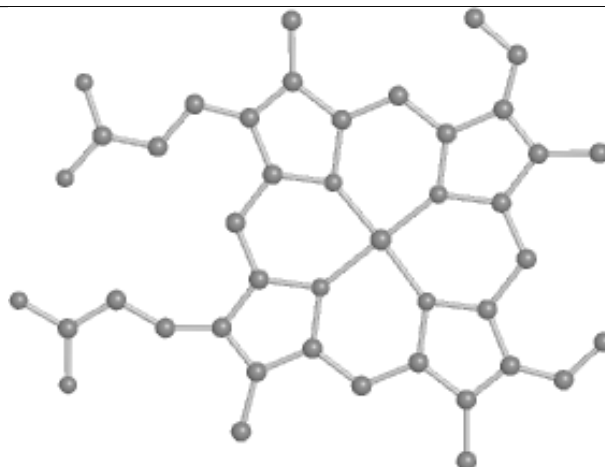
Bond lengths







Bond angles



Torsions



Rings

Ligand CMO B 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	376/425 (88%)	0.61	43 (11%) 5 3	83, 111, 150, 155	0
1	B	372/425 (87%)	0.51	33 (8%) 9 5	82, 106, 139, 170	0
All	All	748/850 (88%)	0.56	76 (10%) 6 4	82, 107, 147, 170	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	SER	7.8
1	B	84	GLY	5.5
1	B	362	PRO	5.3
1	B	263	SER	5.2
1	A	129	CYS	5.1
1	A	85	CYS	4.6
1	B	267	SER	4.5
1	A	142	PRO	4.2
1	A	125	VAL	4.1
1	A	128	ASP	3.9
1	B	264	ALA	3.9
1	B	85	CYS	3.9
1	A	84	GLY	3.8
1	A	71	THR	3.7
1	A	402	GLU	3.7
1	A	127	ALA	3.7
1	A	245	ASP	3.6
1	A	267	SER	3.6
1	A	361	GLN	3.6
1	A	264	ALA	3.4
1	A	41	PHE	3.4
1	B	401	LYS	3.4
1	A	141	LYS	3.4
1	B	87	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	263	SER	3.3
1	A	268	SER	3.3
1	A	12	SER	3.3
1	B	360	GLN	3.3
1	A	403	GLY	3.2
1	A	255	ASP	3.2
1	A	126	TYR	3.1
1	A	81	LEU	3.0
1	A	69	HIS	3.0
1	B	268	SER	3.0
1	A	63	ASN	2.9
1	B	359	SER	2.9
1	B	361	GLN	2.9
1	A	124	LEU	2.8
1	A	97	GLY	2.8
1	B	269	VAL	2.8
1	A	130	VAL	2.7
1	A	87	THR	2.6
1	B	86	ILE	2.6
1	B	124	LEU	2.6
1	B	400	LEU	2.6
1	A	96	HIS	2.6
1	A	51	GLU	2.5
1	B	357	PRO	2.5
1	A	38	ASP	2.5
1	A	241	PRO	2.5
1	B	88	MET	2.5
1	B	265	GLY	2.5
1	B	140	ASN	2.4
1	A	88	MET	2.4
1	B	125	VAL	2.4
1	B	126	TYR	2.3
1	A	362	PRO	2.3
1	B	272	CYS	2.3
1	B	82	VAL	2.2
1	B	96	HIS	2.2
1	A	50	ILE	2.2
1	A	83	LEU	2.2
1	A	272	CYS	2.2
1	A	261	GLY	2.2
1	B	266	GLN	2.2
1	B	129	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	137	LYS	2.2
1	A	61	LYS	2.2
1	B	13	LYS	2.1
1	B	354	ILE	2.1
1	B	383	ASP	2.1
1	A	111	TYR	2.0
1	A	281	GLN	2.0
1	A	82	VAL	2.0
1	B	239	GLY	2.0
1	B	167	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](#)

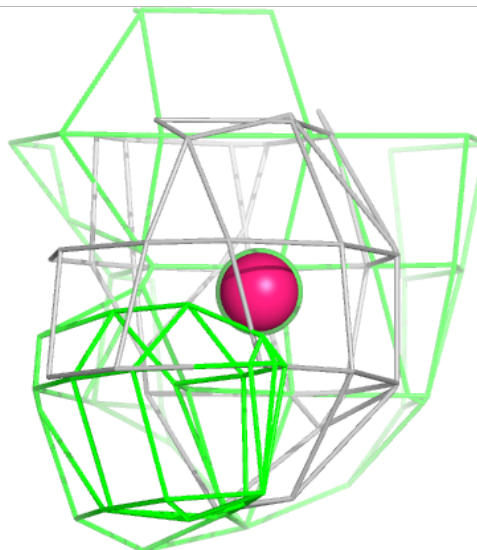
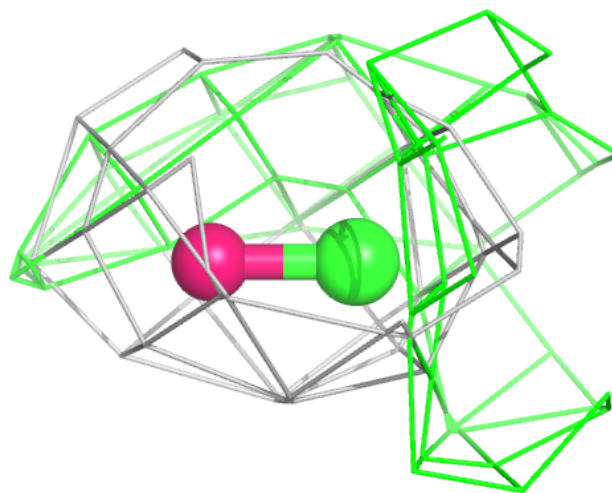
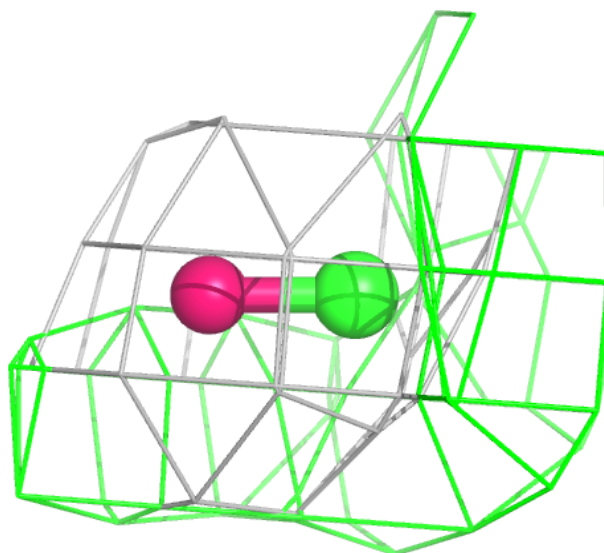
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CMO	B	503	2/2	0.79	0.57	101,101,101,101	0
4	CMO	A	503	2/2	0.80	0.48	90,90,90,91	0
3	TRP	B	502	15/15	0.84	0.35	128,133,136,136	0
3	TRP	A	502	15/15	0.90	0.28	135,141,143,143	0
2	HEM	B	501	43/43	0.96	0.26	94,97,106,111	0
2	HEM	A	501	43/43	0.98	0.23	96,98,100,103	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.

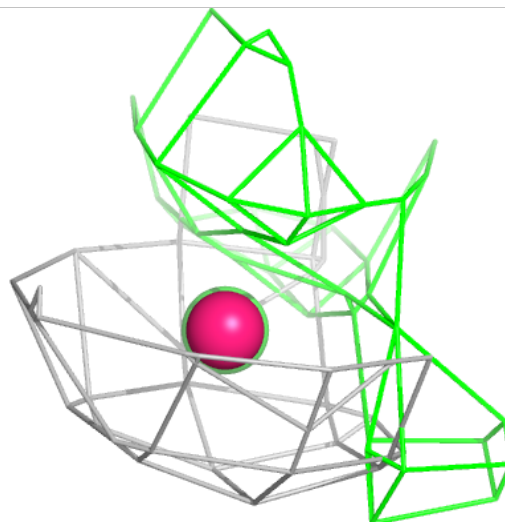
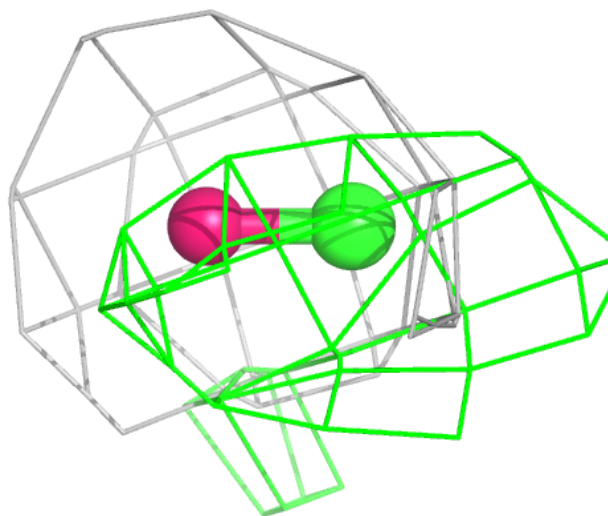
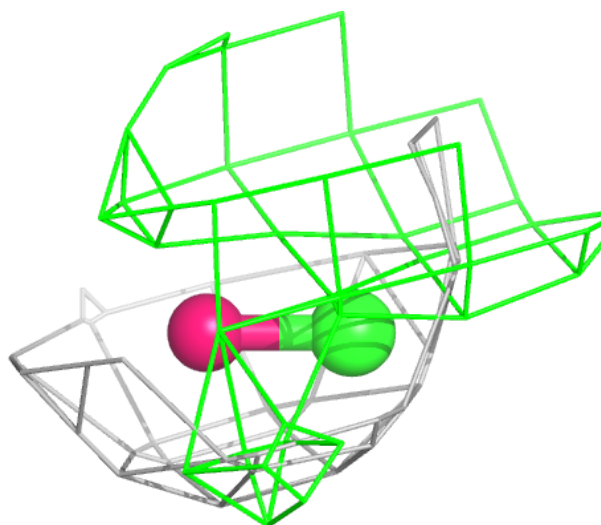
Electron density around CMO B 503:

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



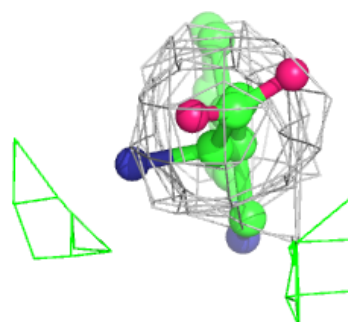
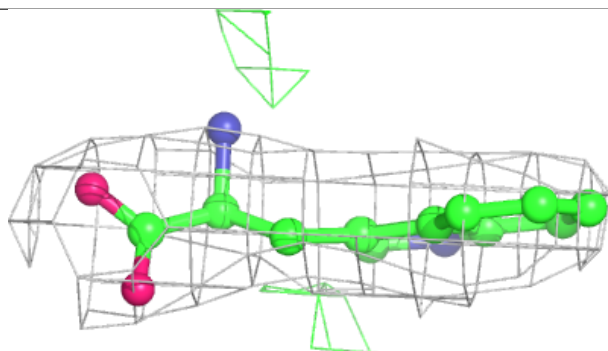
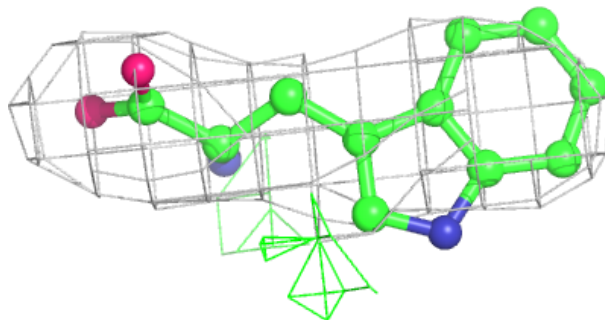
Electron density around CMO A 503:

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

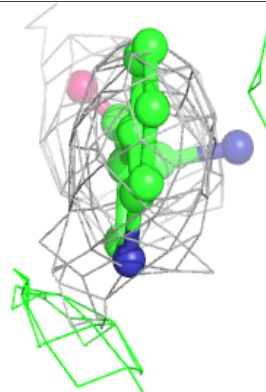
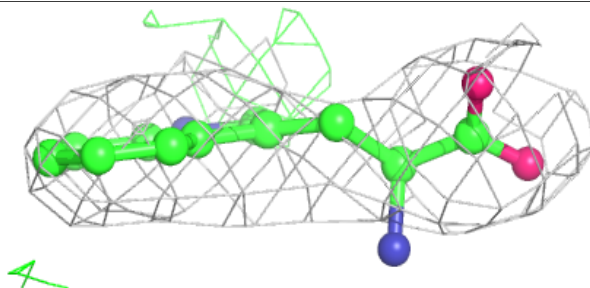
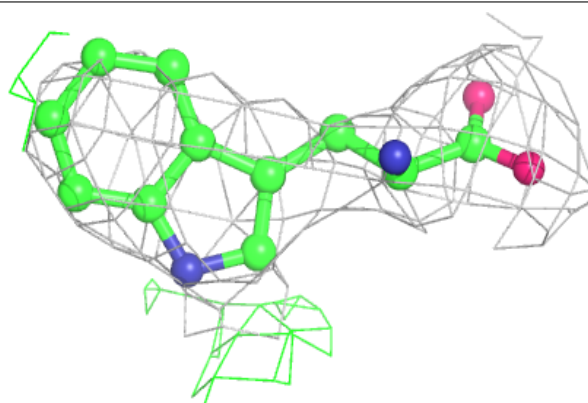


Electron density around TRP B 502:

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

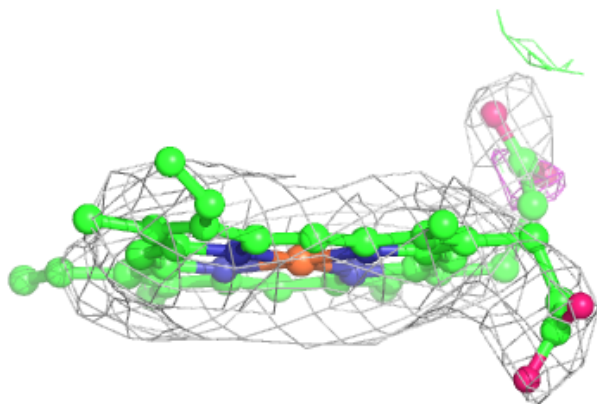
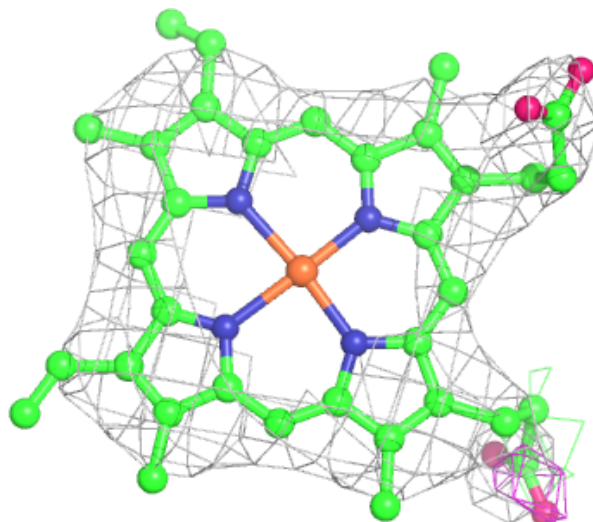
**Electron density around TRP A 502:**

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



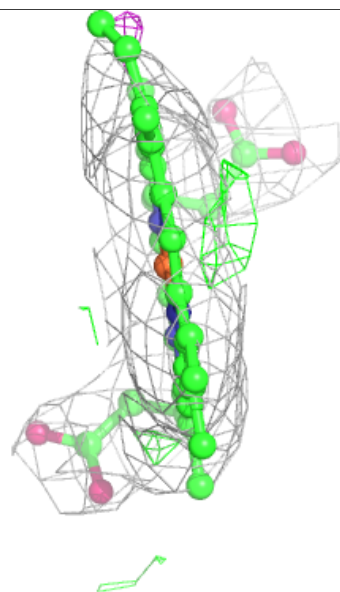
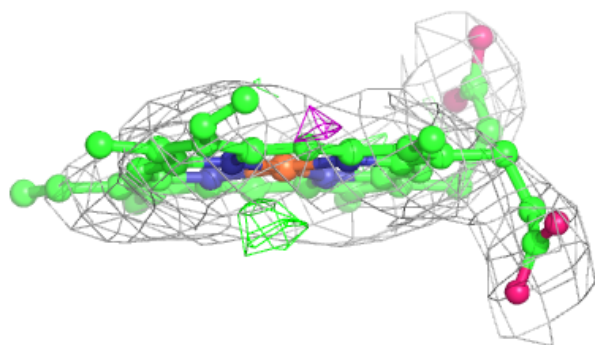
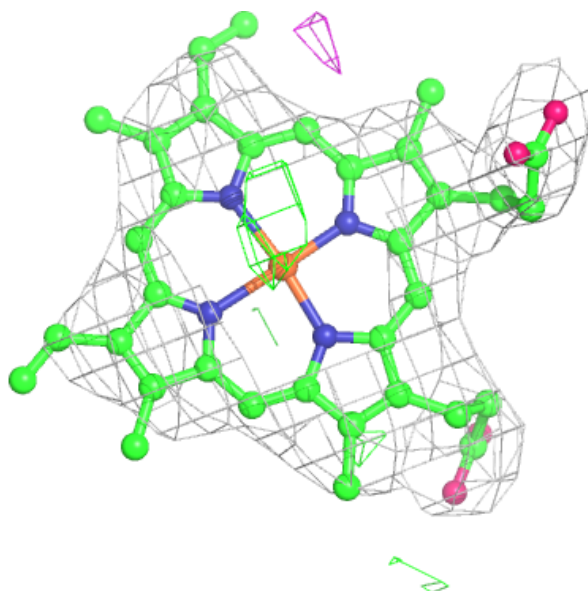
Electron density around HEM B 501:

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



Electron density around HEM A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.