Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 09:26 AM EDT

PDB ID	:	6E46
Title	:	CRYSTAL STRUCTURE OF HUMAN INDOLEAMINE 2,3-DIOXYGENASE 1 (IDO1) in complex with ferrous heme and tryptophan
Authors	:	Luo, S.; Tong, L.
Deposited on	:	2018-07-16
Resolution	:	2.09 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:

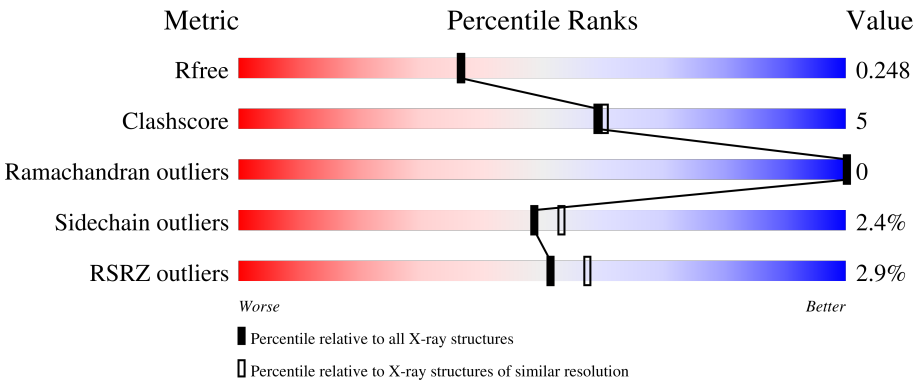
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	405	2%, 81%, 10%, • 8%
1	B	405	3%, 81%, 11%, 8%
1	C	405	4%, 79%, 12%, 8%
1	D	405	2%, 80%, 12%, 7%

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
3	TRP	A	502	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12439 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
			Total	C	N	O	S			
1	A	373	2944	1892	502	533	17	0	0	0
1	B	373	2943	1892	502	531	18	0	1	0
1	C	372	2935	1887	501	530	17	0	0	0
1	D	375	2958	1900	505	536	17	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P14902
A	0	GLY	-	expression tag	UNP P14902
A	1	SER	-	expression tag	UNP P14902
A	2	SER	-	expression tag	UNP P14902
A	3	HIS	-	expression tag	UNP P14902
A	4	HIS	-	expression tag	UNP P14902
A	5	HIS	-	expression tag	UNP P14902
A	6	HIS	-	expression tag	UNP P14902
A	7	HIS	-	expression tag	UNP P14902
A	8	HIS	-	expression tag	UNP P14902
A	9	SER	-	expression tag	UNP P14902
A	10	SER	-	expression tag	UNP P14902
A	11	GLY	-	expression tag	UNP P14902
A	12	SER	-	expression tag	UNP P14902
A	13	ALA	-	expression tag	UNP P14902
A	14	ALA	-	expression tag	UNP P14902
A	116	ALA	LYS	engineered mutation	UNP P14902
A	117	ALA	LYS	engineered mutation	UNP P14902
B	-1	MET	-	initiating methionine	UNP P14902
B	0	GLY	-	expression tag	UNP P14902
B	1	SER	-	expression tag	UNP P14902

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP P14902
B	3	HIS	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
B	5	HIS	-	expression tag	UNP P14902
B	6	HIS	-	expression tag	UNP P14902
B	7	HIS	-	expression tag	UNP P14902
B	8	HIS	-	expression tag	UNP P14902
B	9	SER	-	expression tag	UNP P14902
B	10	SER	-	expression tag	UNP P14902
B	11	GLY	-	expression tag	UNP P14902
B	12	SER	-	expression tag	UNP P14902
B	13	ALA	-	expression tag	UNP P14902
B	14	ALA	-	expression tag	UNP P14902
B	116	ALA	LYS	engineered mutation	UNP P14902
B	117	ALA	LYS	engineered mutation	UNP P14902
C	-1	MET	-	initiating methionine	UNP P14902
C	0	GLY	-	expression tag	UNP P14902
C	1	SER	-	expression tag	UNP P14902
C	2	SER	-	expression tag	UNP P14902
C	3	HIS	-	expression tag	UNP P14902
C	4	HIS	-	expression tag	UNP P14902
C	5	HIS	-	expression tag	UNP P14902
C	6	HIS	-	expression tag	UNP P14902
C	7	HIS	-	expression tag	UNP P14902
C	8	HIS	-	expression tag	UNP P14902
C	9	SER	-	expression tag	UNP P14902
C	10	SER	-	expression tag	UNP P14902
C	11	GLY	-	expression tag	UNP P14902
C	12	SER	-	expression tag	UNP P14902
C	13	ALA	-	expression tag	UNP P14902
C	14	ALA	-	expression tag	UNP P14902
C	116	ALA	LYS	engineered mutation	UNP P14902
C	117	ALA	LYS	engineered mutation	UNP P14902
D	-1	MET	-	initiating methionine	UNP P14902
D	0	GLY	-	expression tag	UNP P14902
D	1	SER	-	expression tag	UNP P14902
D	2	SER	-	expression tag	UNP P14902
D	3	HIS	-	expression tag	UNP P14902
D	4	HIS	-	expression tag	UNP P14902
D	5	HIS	-	expression tag	UNP P14902
D	6	HIS	-	expression tag	UNP P14902
D	7	HIS	-	expression tag	UNP P14902

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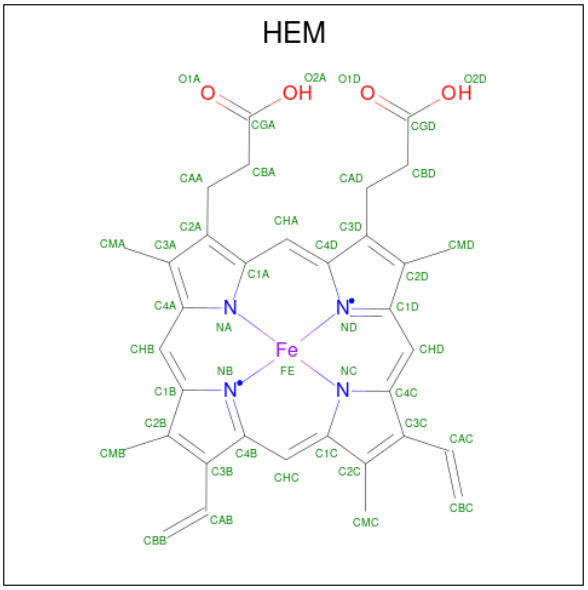
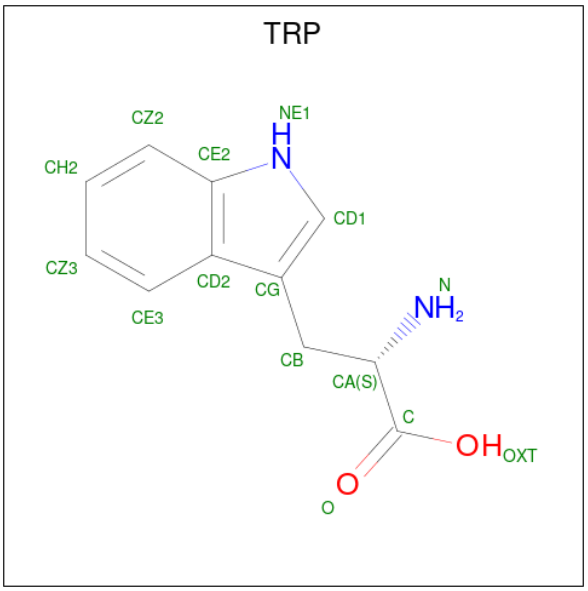
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
D	116	ALA	LYS	engineered mutation	UNP P14902
D	117	ALA	LYS	engineered mutation	UNP P14902

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



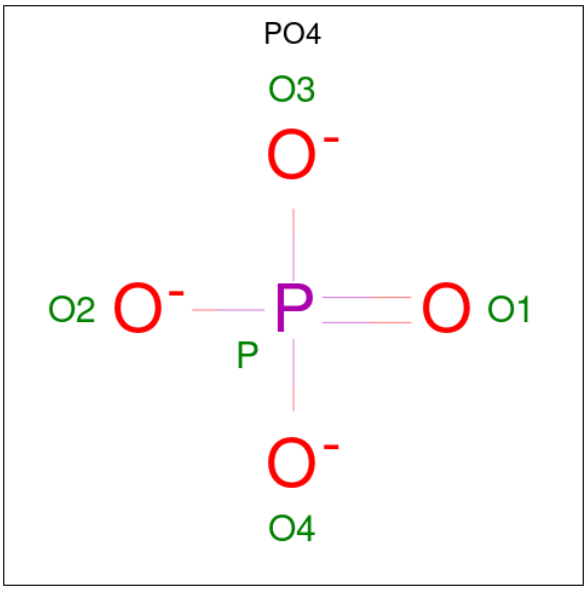
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	C	1	5	4	1	0	0
			Total	O	P		
4	D	1	5	4	1	0	0

- Molecule 5 is water.

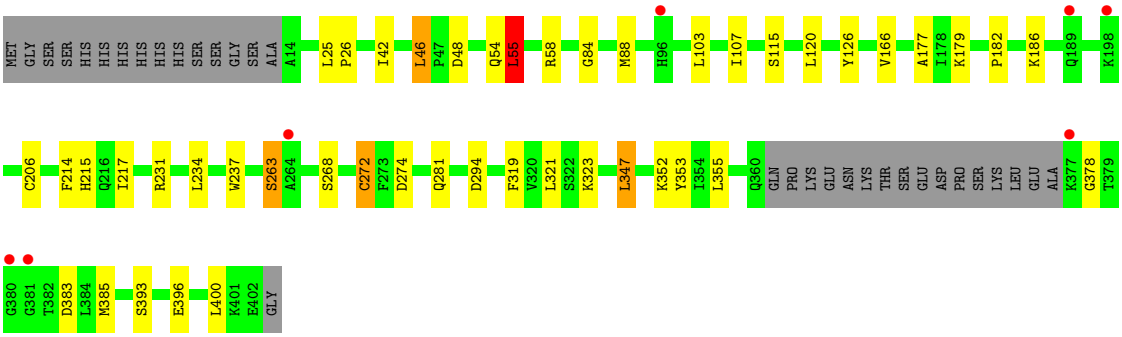
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	109	109	109	0	0
			Total	O		
5	B	115	115	115	0	0
			Total	O		
5	C	86	86	86	0	0
			Total	O		
5	D	107	107	107	0	0

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.

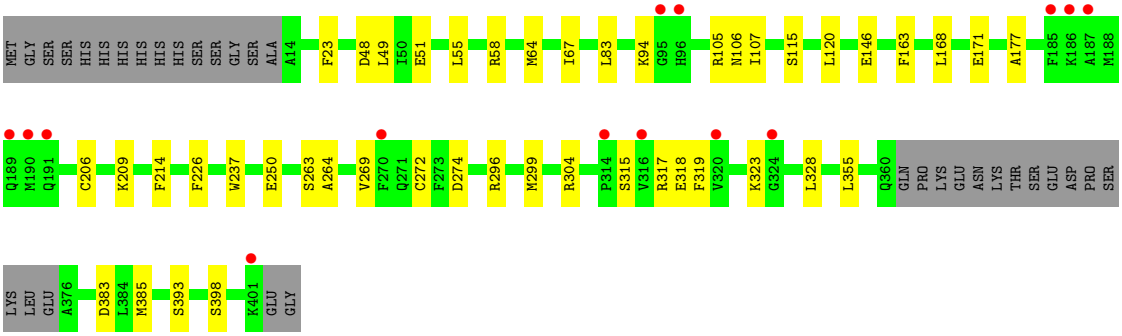
• Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain A:



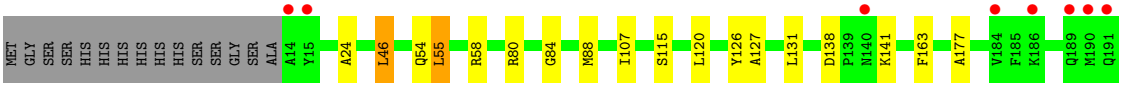
• Molecule 1: Indoleamine 2,3-dioxygenase 1

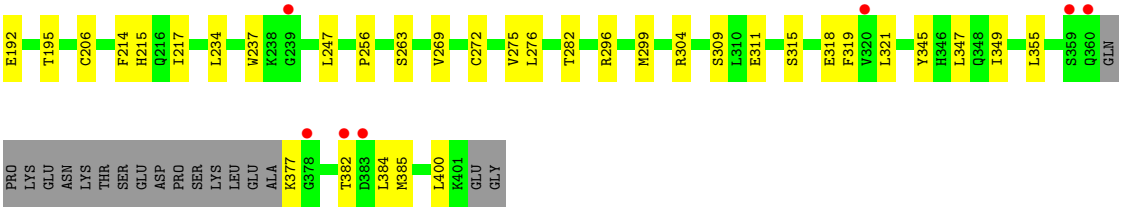
Chain B:



• Molecule 1: Indoleamine 2,3-dioxygenase 1

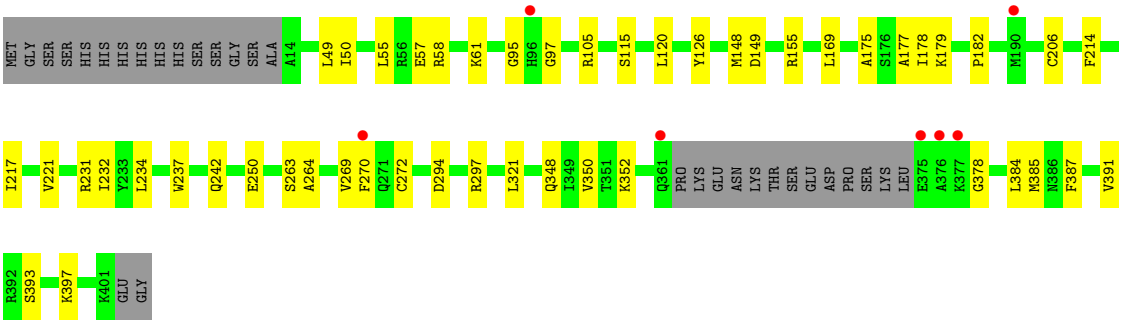
Chain C:





• Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	79.92Å 197.19Å 115.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 2.09 49.30 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.30-2.09) 99.5 (49.30-2.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.207 , 0.247 0.208 , 0.248	Depositor DCC
R_{free} test set	5338 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12439	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6721e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PO4, 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	0.47	0/3012	0.58	1/4076 (0.0%)
1	B	0.43	0/3014	0.59	1/4079 (0.0%)
1	C	0.44	0/3003	0.58	2/4064 (0.0%)
1	D	0.47	0/3026	0.58	2/4095 (0.0%)
All	All	0.45	0/12055	0.58	6/16314 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	LEU	CA-CB-CG	-6.14	101.17	115.30
1	C	276	LEU	CA-CB-CG	6.07	129.27	115.30
1	C	55	LEU	CA-CB-CG	-6.03	101.43	115.30
1	B	55	LEU	CA-CB-CG	-5.92	101.68	115.30
1	D	221	VAL	C-N-CA	-5.45	108.08	121.70
1	D	55	LEU	CA-CB-CG	-5.43	102.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	ASP	Peptide
1	B	383	ASP	Peptide

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	2944	0	2953	26	0
1	B	2943	0	2957	25	0
1	C	2935	0	2947	30	0
1	D	2958	0	2966	26	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	1	0
2	D	43	0	30	3	0
3	A	15	0	9	7	0
3	B	15	0	9	3	0
3	C	15	0	9	5	0
3	D	15	0	9	5	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	109	0	0	3	0
5	B	115	0	0	1	0
5	C	86	0	0	0	0
5	D	107	0	0	1	0
All	All	12439	0	11979	113	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 5.

All (113) 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:C:127:ALA:HA	1:C:131:LEU:HD23	1.54	0.88
1:B:317:ARG:NH1	1:B:398:SER:O	2.11	0.83
1:A:54:GLN:HE21	1:A:58:ARG:NH1	1.79	0.80
1:A:263:SER:HA	3:A:502:TRP:CD2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLY:HA2	1:D:242:GLN:HE22	1.54	0.73
1:D:269:VAL:HG12	1:D:270:PHE:HD1	1.58	0.67
1:C:215:HIS:HD2	1:C:345:TYR:CZ	2.13	0.66
1:B:105:ARG:HG3	1:B:250:GLU:HG2	1.78	0.66
1:A:54:GLN:HE21	1:A:58:ARG:HH12	1.45	0.64
1:C:315:SER:HB3	1:C:318:GLU:HG2	1.79	0.63
1:B:51:GLU:O	1:B:94:LYS:NZ	2.23	0.62
1:C:321:LEU:HD21	1:C:400:LEU:HD22	1.80	0.62
1:A:294:ASP:OD2	5:A:601:HOH:O	2.16	0.61
1:C:177:ALA:HB2	1:C:206:CYS:HB2	1.85	0.59
1:D:179:LYS:O	1:D:182:PRO:HD2	2.03	0.58
1:D:263:SER:HA	3:D:503:TRP:CD2	2.39	0.58
1:C:263:SER:HA	3:C:503:TRP:CD2	2.39	0.57
1:A:234:LEU:HD13	3:A:502:TRP:CE3	2.40	0.57
1:B:115:SER:HB3	1:B:120:LEU:O	2.05	0.57
2:D:501:HEM:CHB	3:D:503:TRP:HA	2.35	0.57
1:C:217:ILE:HG21	1:C:349:ILE:HD12	1.87	0.56
1:A:319:PHE:CE1	1:A:323:LYS:HE2	2.41	0.56
1:C:138:ASP:OD2	1:C:141:LYS:HG3	2.06	0.55
1:C:384:LEU:H	1:C:384:LEU:HD23	1.70	0.55
1:A:115:SER:HB3	1:A:120:LEU:O	2.06	0.55
1:D:177:ALA:HB2	1:D:206:CYS:HB2	1.89	0.55
1:A:25:LEU:HD12	1:A:26:PRO:HD2	1.89	0.55
1:B:319:PHE:O	1:B:323:LYS:HG2	2.07	0.54
1:C:215:HIS:CD2	1:C:345:TYR:CZ	2.94	0.54
2:C:501:HEM:O2A	3:C:503:TRP:N	2.41	0.53
1:A:352:LYS:HD3	1:A:353:TYR:CE1	2.43	0.53
2:A:501:HEM:O2A	3:A:502:TRP:N	2.42	0.53
1:B:315:SER:HB3	1:B:318:GLU:HG2	1.90	0.53
1:C:163:PHE:HZ	3:C:503:TRP:CE2	2.27	0.53
1:C:126:TYR:CD2	1:C:131:LEU:HD21	2.44	0.53
1:A:177:ALA:HB2	1:A:206:CYS:HB2	1.92	0.52
1:C:126:TYR:CE2	1:C:131:LEU:HD21	2.44	0.52
1:C:115:SER:HB3	1:C:120:LEU:O	2.10	0.52
1:B:264:ALA:HB3	2:B:501:HEM:C1D	2.44	0.52
1:A:166:VAL:HG11	1:A:217:ILE:HG12	1.91	0.51
1:B:146:GLU:H	1:B:146:GLU:CD	2.13	0.51
1:D:57:GLU:O	1:D:61:LYS:HG2	2.10	0.51
1:B:263:SER:HA	3:B:502:TRP:CD2	2.46	0.51
1:B:299:MET:O	1:B:304:ARG:NH1	2.44	0.51
1:C:299:MET:O	1:C:304:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:SER:HB2	3:A:502:TRP:N	2.26	0.51
1:D:148:MET:HE1	1:D:169:LEU:HD21	1.93	0.50
1:B:355:LEU:HD11	1:B:385:MET:SD	2.52	0.50
1:C:46:LEU:HD12	1:C:55:LEU:HD13	1.94	0.49
1:C:318:GLU:HG3	1:C:319:PHE:N	2.28	0.49
1:C:192:GLU:HG2	1:C:195:THR:OG1	2.11	0.49
1:A:179:LYS:O	1:A:182:PRO:HD2	2.13	0.49
1:D:352:LYS:NZ	5:D:602:HOH:O	2.33	0.48
1:D:175:ALA:HA	1:D:178:ILE:HD12	1.94	0.48
1:D:350:VAL:HG11	1:D:384:LEU:HD13	1.95	0.48
1:A:231:ARG:NH2	1:A:378:GLY:HA2	2.30	0.47
1:D:234:LEU:HD13	3:D:503:TRP:CE3	2.50	0.47
1:A:268:SER:O	1:A:272:CYS:HB3	2.15	0.46
1:A:355:LEU:HD11	1:A:385:MET:SD	2.55	0.46
1:D:269:VAL:HG12	1:D:270:PHE:CD1	2.45	0.46
1:D:115:SER:HB3	1:D:120:LEU:O	2.16	0.46
1:B:49:LEU:HD22	1:B:58:ARG:HD2	1.97	0.46
1:C:84:GLY:O	1:C:88:MET:HG2	2.16	0.46
1:A:42:ILE:O	1:A:46:LEU:HD13	2.16	0.46
1:A:84:GLY:O	1:A:88:MET:HG2	2.16	0.46
1:A:126:TYR:HD1	3:A:502:TRP:CH2	2.34	0.46
1:A:274:ASP:OD2	1:A:281:GLN:HG3	2.16	0.45
1:B:64:MET:HB2	1:B:106:ASN:OD1	2.16	0.45
1:C:126:TYR:HD1	3:C:503:TRP:CH2	2.34	0.45
1:A:347:LEU:HD22	5:A:623:HOH:O	2.16	0.45
1:D:231:ARG:NH1	1:D:378:GLY:HA2	2.32	0.45
1:B:83:LEU:HD22	1:B:107:ILE:HG13	1.98	0.44
1:B:105:ARG:HG3	1:B:250:GLU:CG	2.47	0.44
1:D:264:ALA:HB3	2:D:501:HEM:C1D	2.52	0.44
1:B:23:PHE:HD2	1:B:269:VAL:HG23	1.83	0.44
1:C:296:ARG:O	1:C:304:ARG:HD3	2.18	0.44
1:B:226:PHE:CE2	2:B:501:HEM:HMB3	2.53	0.43
1:C:275:VAL:HG13	1:C:311:GLU:HG3	2.00	0.43
1:D:384:LEU:HD12	1:D:385:MET:N	2.34	0.43
2:A:501:HEM:CHB	3:A:502:TRP:HA	2.48	0.43
1:D:105:ARG:HB3	1:D:250:GLU:HG2	2.00	0.43
1:D:294:ASP:OD1	1:D:297:ARG:NH2	2.51	0.43
1:B:315:SER:HB3	1:B:318:GLU:CG	2.49	0.42
1:B:163:PHE:HZ	3:B:502:TRP:CE2	2.38	0.42
1:C:269:VAL:O	1:C:272:CYS:HB3	2.19	0.42
1:A:263:SER:HA	3:A:502:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:O	1:C:256:PRO:HA	2.19	0.42
2:D:501:HEM:O2A	3:D:503:TRP:N	2.52	0.42
1:B:177:ALA:HB2	1:B:206:CYS:HB2	2.00	0.42
1:C:355:LEU:HD11	1:C:385:MET:SD	2.60	0.42
1:D:321:LEU:HA	1:D:321:LEU:HD23	1.84	0.42
1:A:321:LEU:HD21	1:A:400:LEU:HD22	2.01	0.42
5:A:663:HOH:O	1:B:67:ILE:HD11	2.20	0.42
1:C:58:ARG:HA	1:C:58:ARG:HD2	1.80	0.42
1:C:377:LYS:HA	1:C:382:THR:O	2.20	0.42
1:D:387:PHE:O	1:D:391:VAL:HG23	2.20	0.41
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.94	0.41
1:C:234:LEU:HD13	3:C:503:TRP:CE3	2.55	0.41
1:A:103:LEU:HG	1:A:107:ILE:HG23	2.01	0.41
1:C:24:ALA:HA	1:C:131:LEU:HD12	2.03	0.41
1:A:55:LEU:O	1:A:55:LEU:HG	2.17	0.41
1:B:296:ARG:O	1:B:304:ARG:HG3	2.21	0.41
1:D:95:GLY:HA2	1:D:232:ILE:HG21	2.03	0.41
1:D:126:TYR:HD1	3:D:503:TRP:CZ2	2.39	0.41
1:A:393:SER:HA	1:A:396:GLU:HG2	2.03	0.40
2:B:501:HEM:CHB	3:B:502:TRP:HA	2.51	0.40
1:D:50:ILE:HG21	1:D:155:ARG:HD3	2.03	0.40
1:B:168:LEU:O	1:B:171:GLU:HB2	2.21	0.40
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.96	0.40
1:D:393:SER:O	1:D:397:LYS:HG3	2.20	0.40
1:B:274:ASP:OD2	5:B:601:HOH:O	2.22	0.40
1:C:54:GLN:O	1:C:58:ARG:HG2	2.21	0.40
1:D:148:MET:HB2	1:D:148:MET:HE2	1.77	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	369/405 (91%)	362 (98%)	7 (2%)	0	100	100
1	B	370/405 (91%)	362 (98%)	8 (2%)	0	100	100
1	C	368/405 (91%)	357 (97%)	11 (3%)	0	100	100
1	D	371/405 (92%)	362 (98%)	9 (2%)	0	100	100
All	All	1478/1620 (91%)	1443 (98%)	35 (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	319/346 (92%)	309 (97%)	10 (3%)	40	43
1	B	319/346 (92%)	312 (98%)	7 (2%)	52	57
1	C	318/346 (92%)	310 (98%)	8 (2%)	47	52
1	D	320/346 (92%)	313 (98%)	7 (2%)	52	57
All	All	1276/1384 (92%)	1244 (98%)	32 (2%)	49	52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	48	ASP
1	A	55	LEU
1	A	186	LYS
1	A	214	PHE
1	A	215	HIS
1	A	237	TRP
1	A	263	SER
1	A	272	CYS
1	A	347	LEU
1	B	48	ASP
1	B	209	LYS
1	B	214	PHE

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Mol	Chain	Res	Type
1	B	237	TRP
1	B	272[A]	CYS
1	B	272[B]	CYS
1	B	393	SER
1	C	46	LEU
1	C	80	ARG
1	C	107	ILE
1	C	214	PHE
1	C	237	TRP
1	C	282	THR
1	C	309	SER
1	C	347	LEU
1	D	58	ARG
1	D	149	ASP
1	D	214	PHE
1	D	217	ILE
1	D	237	TRP
1	D	272	CYS
1	D	348	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	290	GLN
1	A	360	GLN
1	A	386	ASN
1	B	27	ASN
1	B	360	GLN
1	C	215	HIS
1	C	386	ASN
1	D	54	GLN
1	D	242	GLN
1	D	360	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	TRP	A	502	-	14,16,16	1.09	1 (7%)	13,22,22	0.79	0
4	PO4	C	502	-	4,4,4	0.70	0	6,6,6	0.74	0
3	TRP	C	503	-	14,16,16	0.92	1 (7%)	13,22,22	0.95	0
4	PO4	D	502	-	4,4,4	0.59	0	6,6,6	1.00	0
2	HEM	B	501	1	42,50,50	1.55	5 (11%)	46,82,82	1.45	8 (17%)
2	HEM	D	501	1	42,50,50	1.54	5 (11%)	46,82,82	1.46	7 (15%)
2	HEM	C	501	1	42,50,50	1.50	5 (11%)	46,82,82	1.48	7 (15%)
2	HEM	A	501	1	42,50,50	1.53	5 (11%)	46,82,82	1.50	9 (19%)
3	TRP	D	503	-	14,16,16	0.92	1 (7%)	13,22,22	1.02	1 (7%)
3	TRP	B	502	-	14,16,16	0.90	1 (7%)	13,22,22	1.08	1 (7%)

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	-	-	1/7/8/8	0/2/2/2
3	TRP	C	503	-	-	1/7/8/8	0/2/2/2
2	HEM	B	501	1	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	501	1	-	2/12/54/54	-
2	HEM	C	501	1	-	2/12/54/54	-
2	HEM	A	501	1	-	2/12/54/54	-
3	TRP	D	503	-	-	3/7/8/8	0/2/2/2
3	TRP	B	502	-	-	2/7/8/8	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-4.74	1.33	1.40
2	B	501	HEM	C3C-C2C	-4.50	1.34	1.40
2	A	501	HEM	C3C-C2C	-4.15	1.34	1.40
2	C	501	HEM	C3C-C2C	-4.00	1.34	1.40
2	B	501	HEM	C3C-C4C	3.56	1.46	1.41
2	D	501	HEM	C3C-C4C	3.39	1.46	1.41
2	C	501	HEM	C3C-CAC	3.29	1.55	1.47
2	A	501	HEM	CAB-C3B	3.23	1.56	1.47
2	D	501	HEM	C3C-CAC	3.21	1.54	1.47
2	C	501	HEM	CAB-C3B	3.12	1.55	1.47
2	B	501	HEM	CAB-C3B	2.99	1.55	1.47
2	B	501	HEM	C3C-CAC	2.91	1.54	1.47
2	A	501	HEM	C3C-CAC	2.85	1.54	1.47
2	D	501	HEM	CAB-C3B	2.84	1.55	1.47
2	A	501	HEM	C3C-C4C	2.71	1.45	1.41
2	A	501	HEM	CMB-C2B	2.55	1.56	1.50
2	C	501	HEM	C3C-C4C	2.52	1.45	1.41
2	C	501	HEM	CMB-C2B	2.23	1.55	1.50
2	B	501	HEM	CMB-C2B	2.19	1.55	1.50
3	C	503	TRP	OXT-C	-2.17	1.23	1.30
3	A	502	TRP	OXT-C	-2.16	1.23	1.30
3	D	503	TRP	OXT-C	-2.13	1.23	1.30
3	B	502	TRP	OXT-C	-2.13	1.23	1.30
2	D	501	HEM	CMB-C2B	2.12	1.55	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	C4C-CHD-C1D	4.06	127.92	122.56
2	A	501	HEM	C4C-CHD-C1D	3.26	126.86	122.56
2	C	501	HEM	C4C-CHD-C1D	3.14	126.71	122.56
2	C	501	HEM	C4D-ND-C1D	2.83	108.56	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C3B-C2B-C1B	2.79	108.50	106.41
2	C	501	HEM	CAA-CBA-CGA	-2.76	106.39	113.83
2	B	501	HEM	CMA-C3A-C4A	-2.75	124.43	128.46
2	A	501	HEM	C1B-NB-C4B	2.72	108.43	105.21
2	B	501	HEM	C4C-CHD-C1D	2.66	126.07	122.56
2	C	501	HEM	C2D-C1D-ND	-2.62	106.88	109.90
2	A	501	HEM	C2C-C3C-C4C	2.57	108.69	106.90
2	B	501	HEM	CAA-CBA-CGA	-2.54	106.99	113.83
2	B	501	HEM	C4A-C3A-C2A	2.54	108.76	107.00
3	B	502	TRP	OXT-C-O	-2.51	118.38	124.08
2	A	501	HEM	C4D-ND-C1D	2.49	108.16	105.21
2	D	501	HEM	C4D-ND-C1D	2.48	108.14	105.21
2	C	501	HEM	C1B-NB-C4B	2.43	108.09	105.21
2	B	501	HEM	C2C-C3C-C4C	2.39	108.56	106.90
2	D	501	HEM	C2D-C1D-ND	-2.36	107.17	109.90
2	C	501	HEM	C2C-C3C-C4C	2.30	108.50	106.90
2	D	501	HEM	C4A-C3A-C2A	2.26	108.57	107.00
2	A	501	HEM	CBA-CAA-C2A	-2.25	108.75	112.54
2	B	501	HEM	C4D-ND-C1D	2.24	107.86	105.21
2	B	501	HEM	C3B-C2B-C1B	2.24	108.09	106.41
2	D	501	HEM	CMA-C3A-C4A	-2.24	125.18	128.46
2	D	501	HEM	CBD-CAD-C3D	-2.20	106.46	112.53
2	C	501	HEM	CMC-C2C-C3C	2.17	129.01	124.68
2	B	501	HEM	CBD-CAD-C3D	-2.16	106.56	112.53
2	D	501	HEM	CAA-CBA-CGA	-2.14	108.05	113.83
3	D	503	TRP	OXT-C-O	-2.11	119.29	124.08
2	A	501	HEM	C3D-C4D-ND	-2.08	107.89	110.17
2	A	501	HEM	CBD-CAD-C3D	-2.04	106.88	112.53
2	A	501	HEM	C2B-C1B-NB	-2.00	107.54	109.84

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	TRP	CA-CB-CG-CD1
3	D	503	TRP	CA-CB-CG-CD1
3	A	502	TRP	CA-CB-CG-CD1
3	C	503	TRP	CA-CB-CG-CD1
2	D	501	HEM	CAA-CBA-CGA-O1A
3	D	503	TRP	O-C-CA-CB
2	D	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O2A
3	D	503	TRP	OXT-C-CA-CB
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O1A
3	B	502	TRP	O-C-CA-N

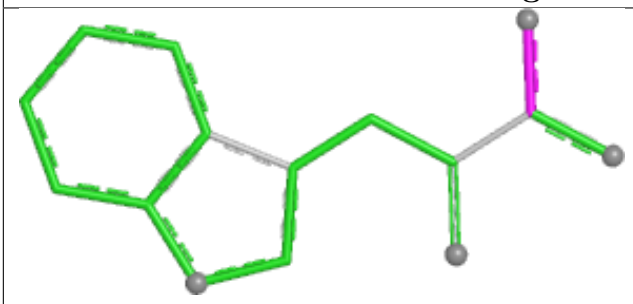
There are no ring outliers.

8 monomers are involved in 23 short contacts:

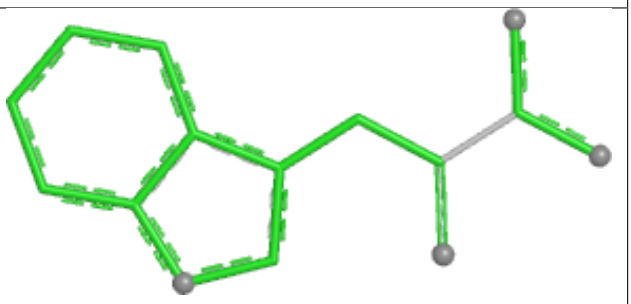
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	TRP	7	0
3	C	503	TRP	5	0
2	B	501	HEM	3	0
2	D	501	HEM	3	0
2	C	501	HEM	1	0
2	A	501	HEM	2	0
3	D	503	TRP	5	0
3	B	502	TRP	3	0

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.

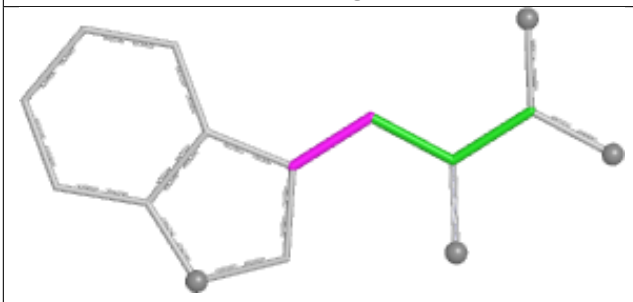
Ligand TRP A 502



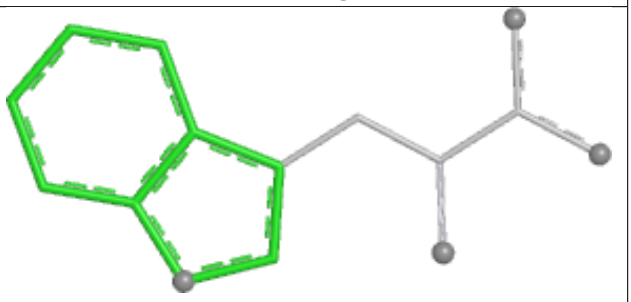
Bond lengths



Bond angles

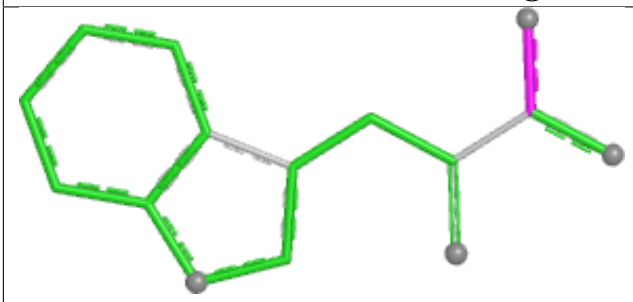


Torsions

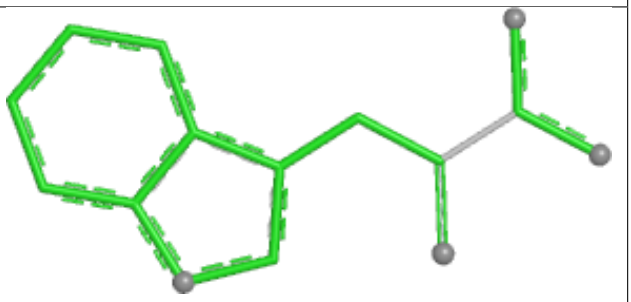


Rings

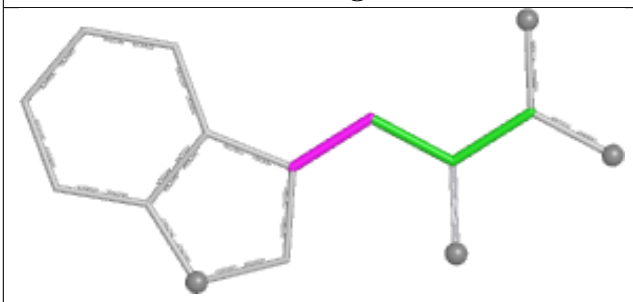
Ligand TRP C 503



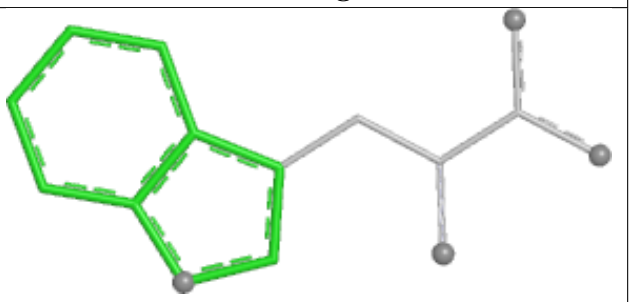
Bond lengths



Bond angles

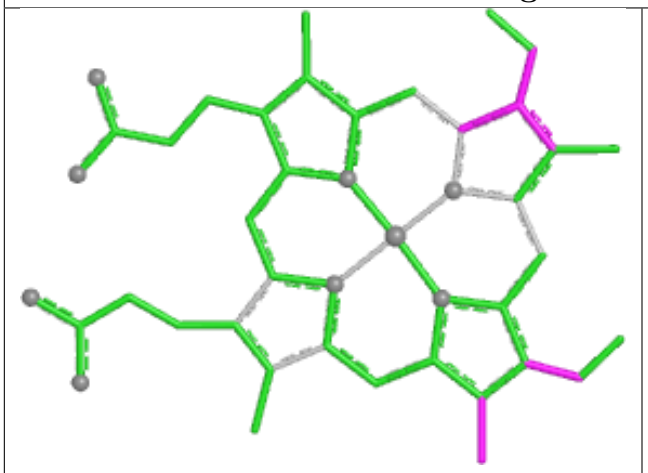


Torsions

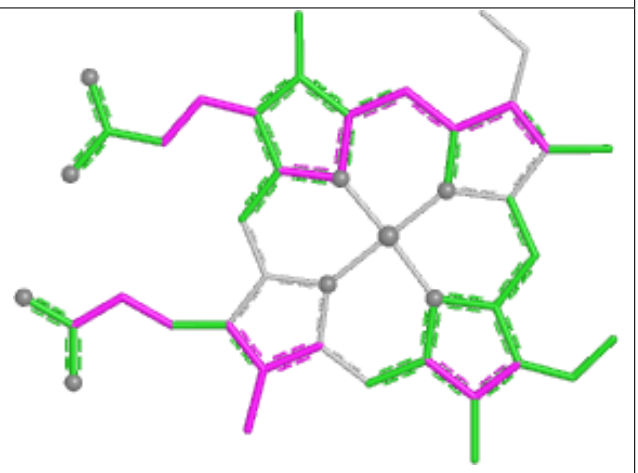


Rings

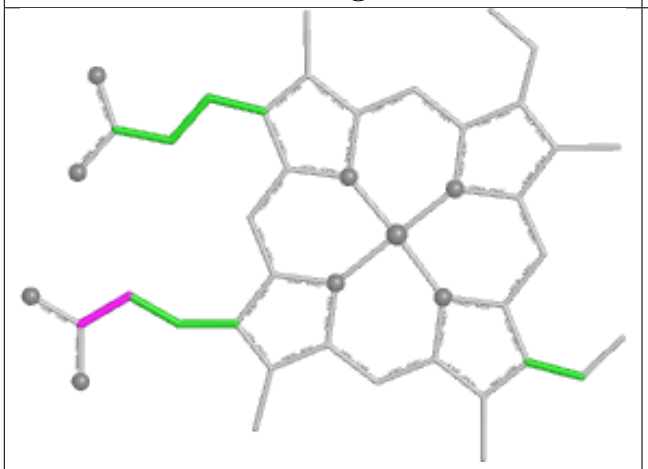
Ligand HEM B 501



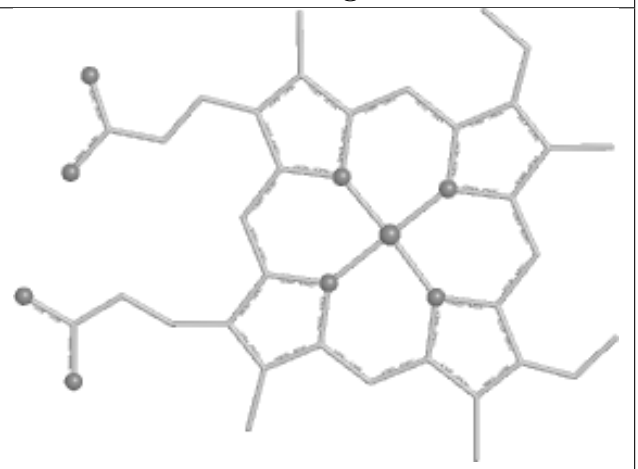
Bond lengths



Bond angles

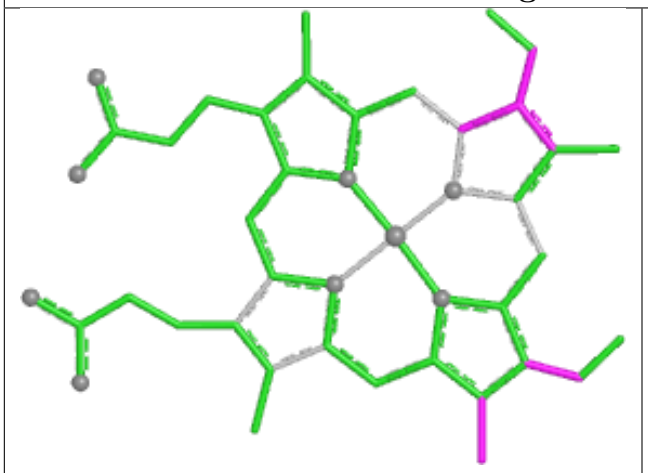


Torsions



Rings

Ligand HEM D 501



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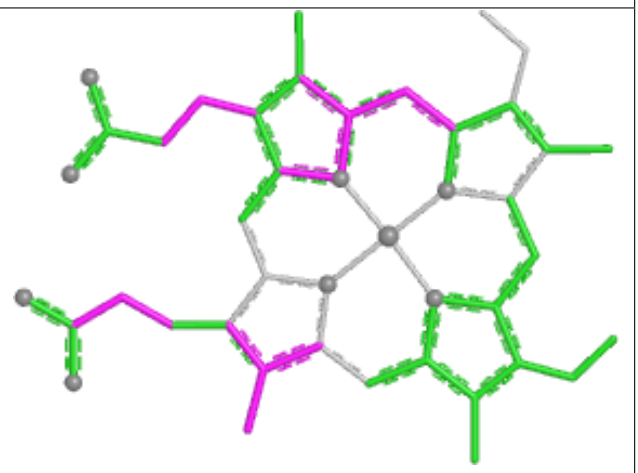

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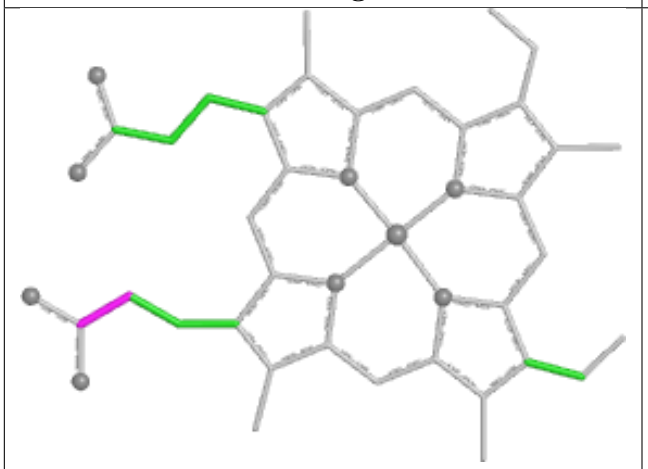

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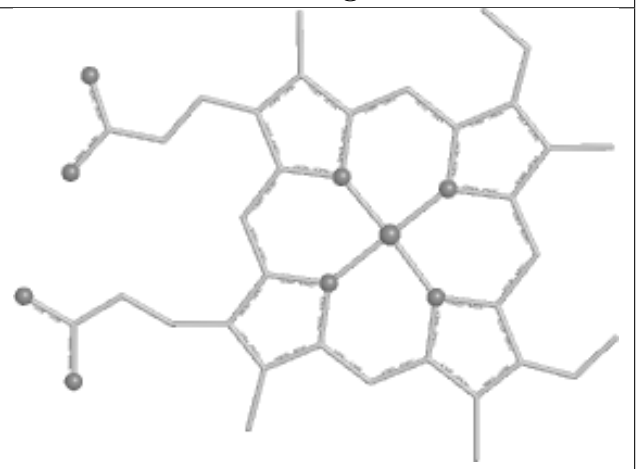
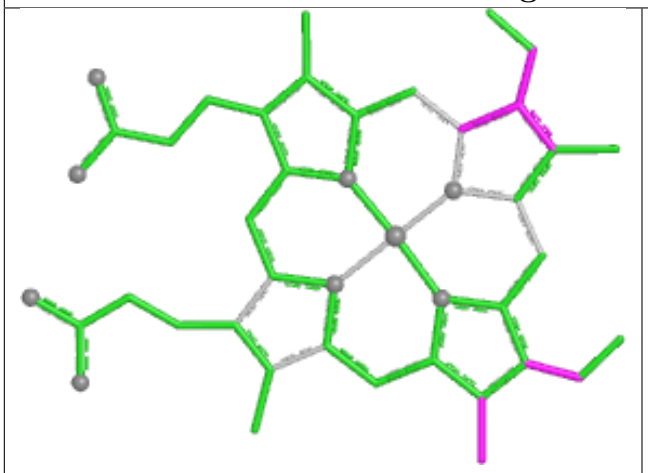
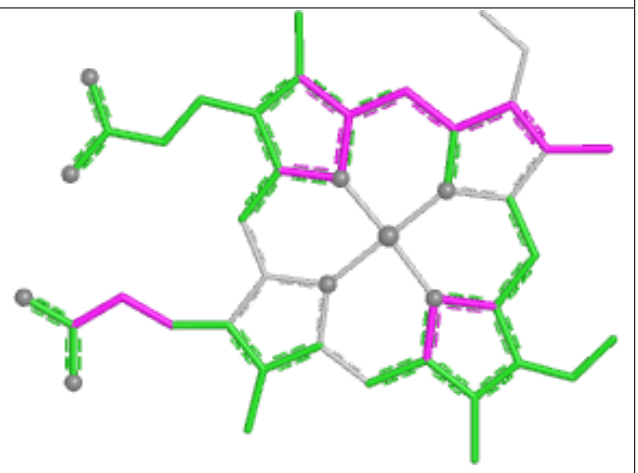


Rings

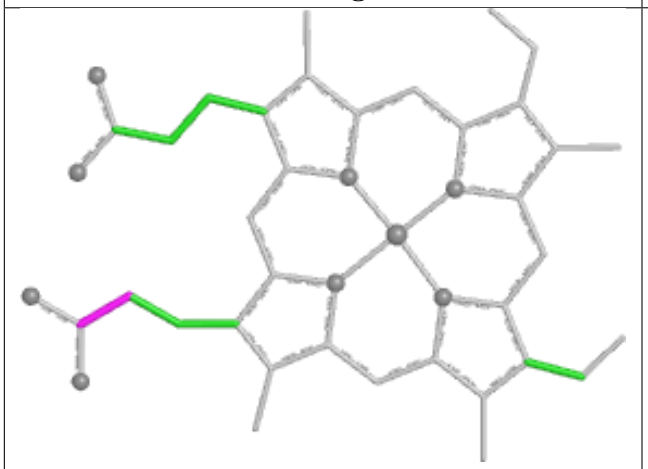
Ligand HEM C 501



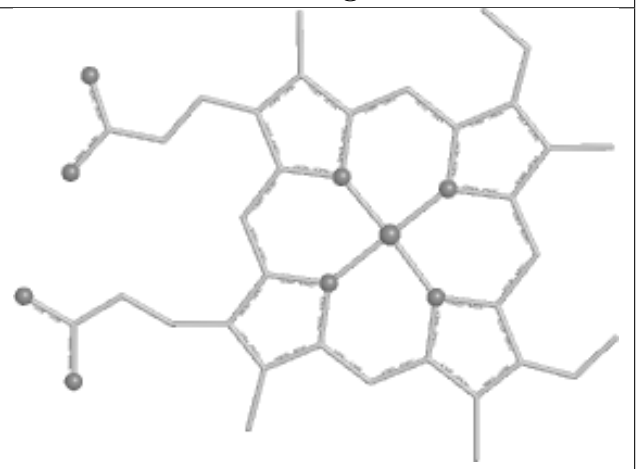
Bond lengths



Bond angles

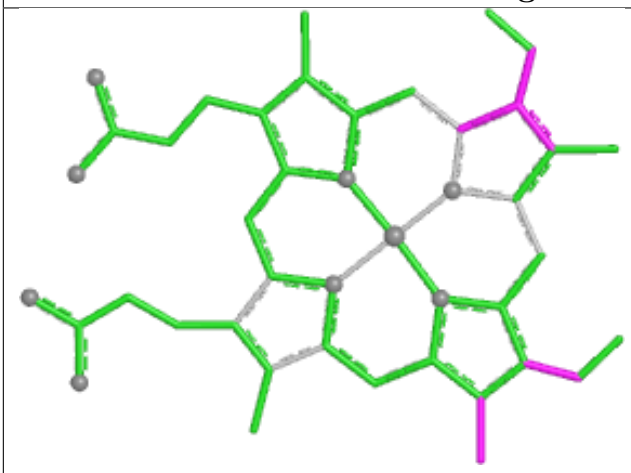


Torsions

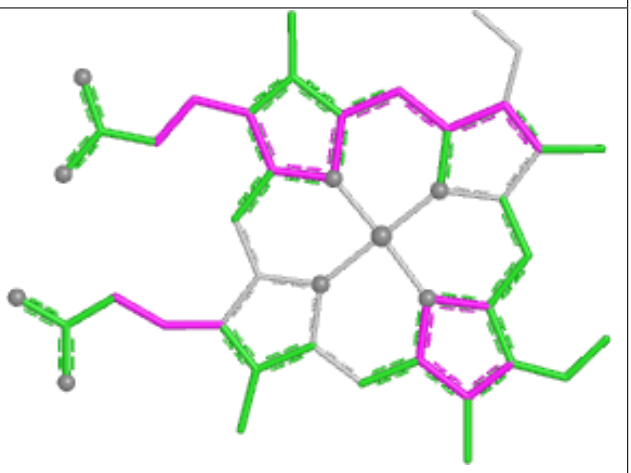


Rings

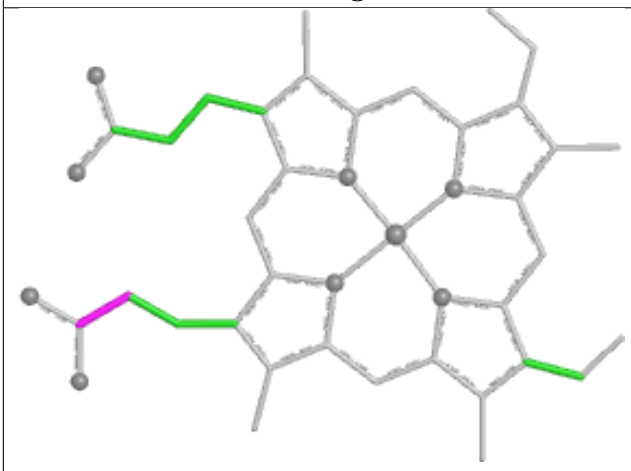
Ligand HEM A 501



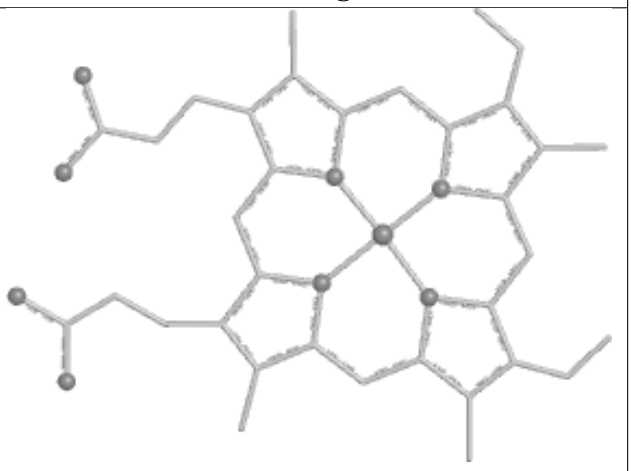
Bond lengths



Bond angles

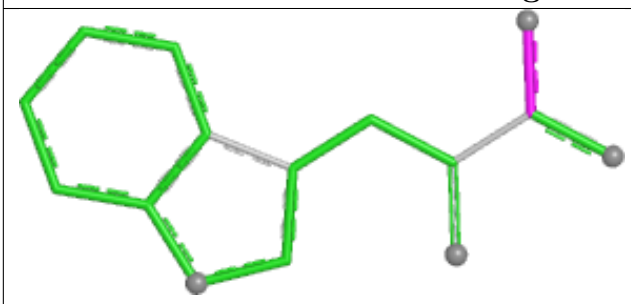


Torsions

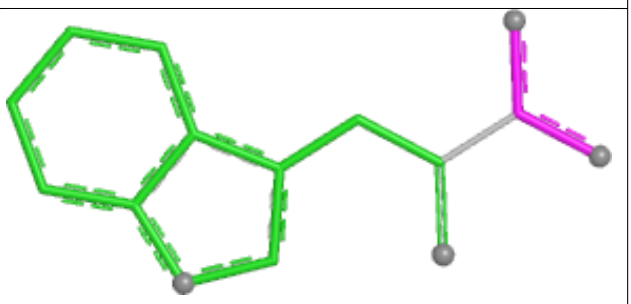


Rings

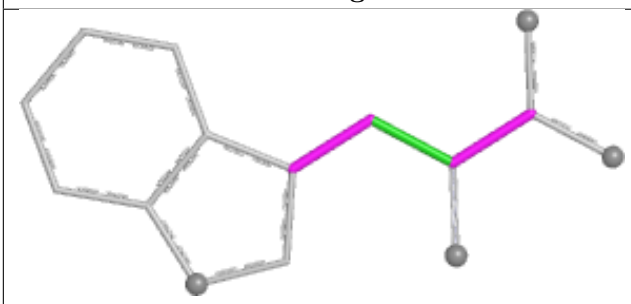
Ligand TRP D 503



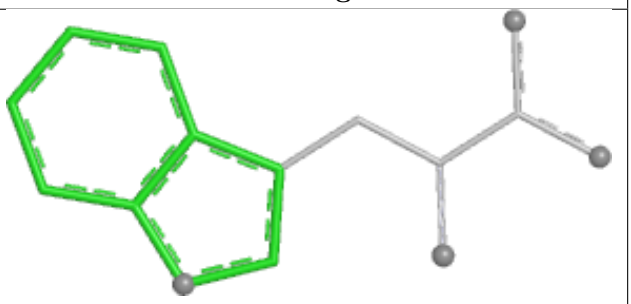
Bond lengths



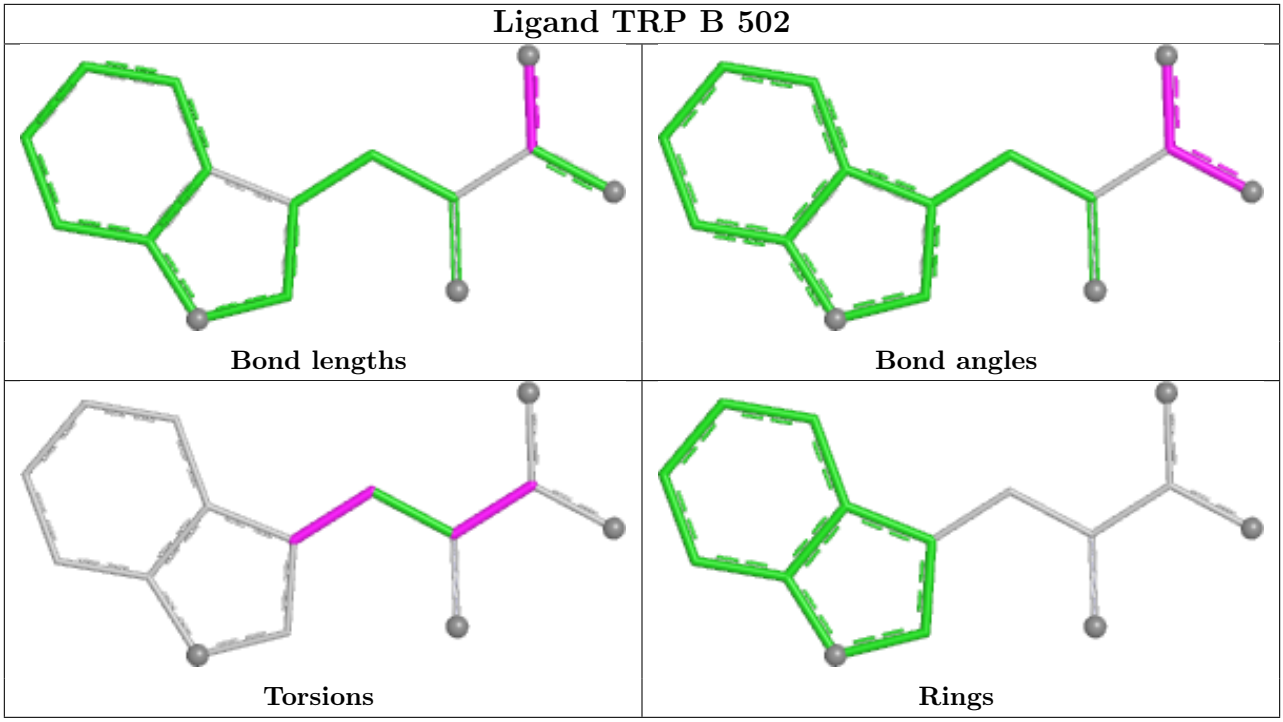
Bond angles



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 (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	373/405 (92%)	0.04	7 (1%)	66	71	28, 42, 60, 69	0
1	B	373/405 (92%)	0.19	14 (3%)	40	46	26, 42, 61, 77	0
1	C	372/405 (91%)	0.24	15 (4%)	38	44	29, 48, 67, 83	0
1	D	375/405 (92%)	0.11	7 (1%)	66	71	27, 44, 61, 79	0
All	All	1493/1620 (92%)	0.14	43 (2%)	51	57	26, 44, 63, 83	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	GLN	6.3
1	B	189	GLN	4.8
1	A	381	GLY	4.0
1	C	186	LYS	3.9
1	D	270	PHE	3.6
1	C	378	GLY	3.6
1	B	187	ALA	3.3
1	D	376	ALA	3.2
1	B	190	MET	3.2
1	D	361	GLN	3.1
1	B	96	HIS	3.1
1	C	359	SER	3.0
1	A	189	GLN	3.0
1	B	185	PHE	3.0
1	B	186	LYS	3.0
1	B	314	PRO	3.0
1	A	380	GLY	2.9
1	C	360	GLN	2.8
1	C	190	MET	2.8
1	B	191	GLN	2.7
1	C	191	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	382	THR	2.7
1	A	96	HIS	2.6
1	D	375	GLU	2.6
1	B	316	VAL	2.5
1	B	320	VAL	2.5
1	C	239	GLY	2.5
1	C	140	ASN	2.4
1	A	377	LYS	2.4
1	A	198	LYS	2.3
1	C	383	ASP	2.2
1	C	320	VAL	2.2
1	C	14	ALA	2.2
1	B	95	GLY	2.2
1	B	401	LYS	2.2
1	D	190	MET	2.2
1	A	264	ALA	2.2
1	B	270	PHE	2.1
1	B	324	GLY	2.1
1	C	15	TYR	2.1
1	C	184	VAL	2.1
1	D	96	HIS	2.0
1	D	377	LYS	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
3	TRP	A	502	15/15	0.83	0.34	41,47,50,51	0

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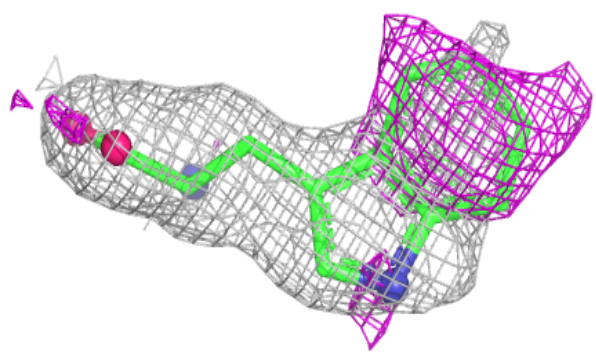
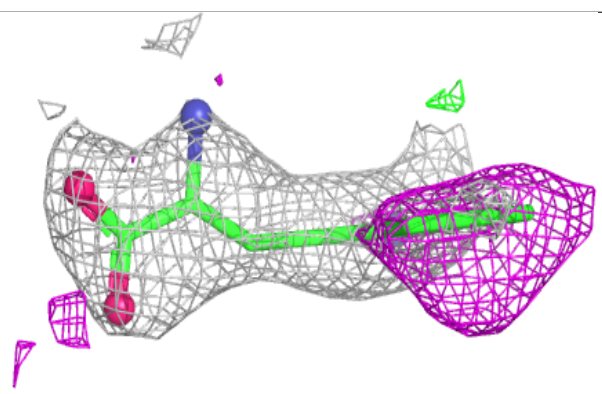
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	D	502	5/5	0.85	0.16	49,53,65,73	0
3	TRP	D	503	15/15	0.88	0.22	41,47,50,52	0
3	TRP	C	503	15/15	0.89	0.25	47,51,55,55	0
3	TRP	B	502	15/15	0.91	0.17	39,41,43,43	0
4	PO4	C	502	5/5	0.92	0.34	59,61,68,75	0
2	HEM	B	501	43/43	0.97	0.14	31,35,42,45	0
2	HEM	C	501	43/43	0.97	0.13	38,43,50,58	0
2	HEM	A	501	43/43	0.98	0.13	32,36,44,49	0
2	HEM	D	501	43/43	0.98	0.13	33,38,45,52	0

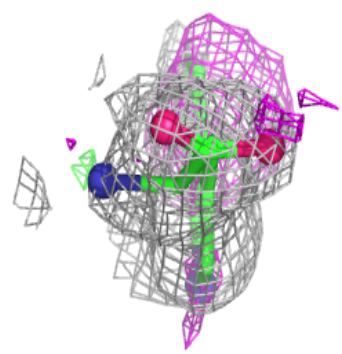
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRP 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)

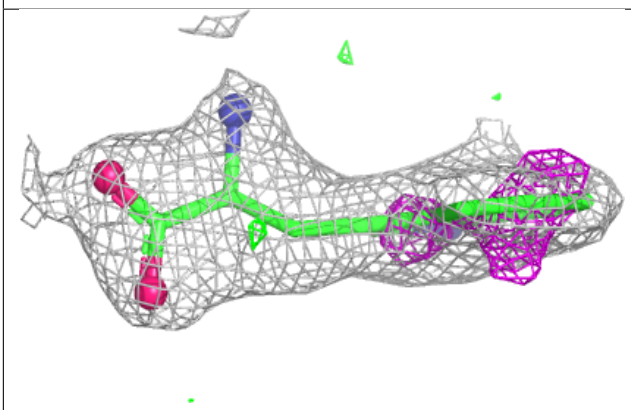


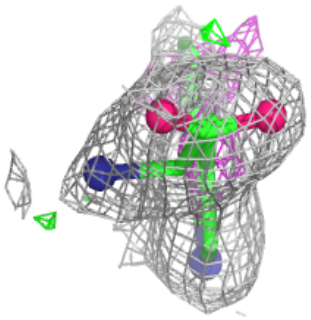




Electron density around TRP D 503:

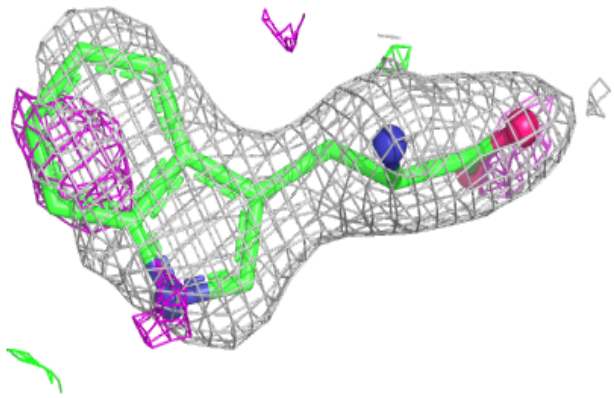
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

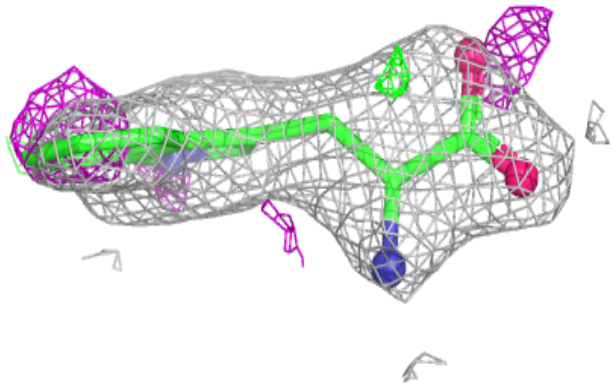


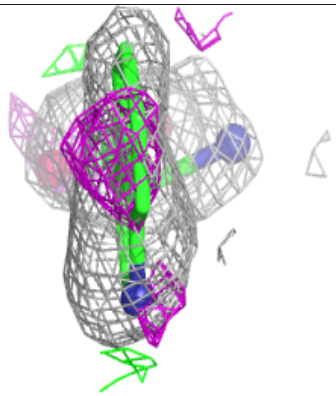


Electron density around TRP C 503:

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

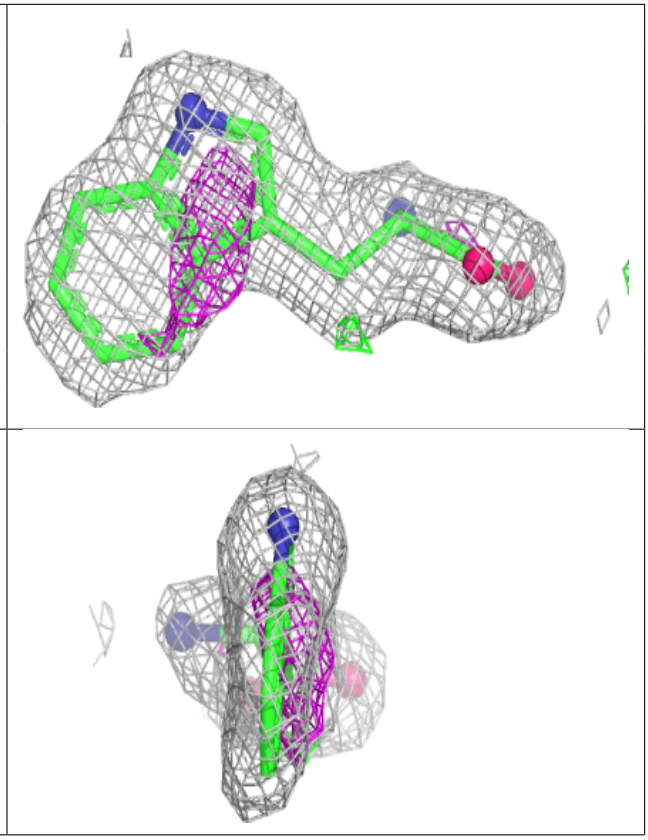






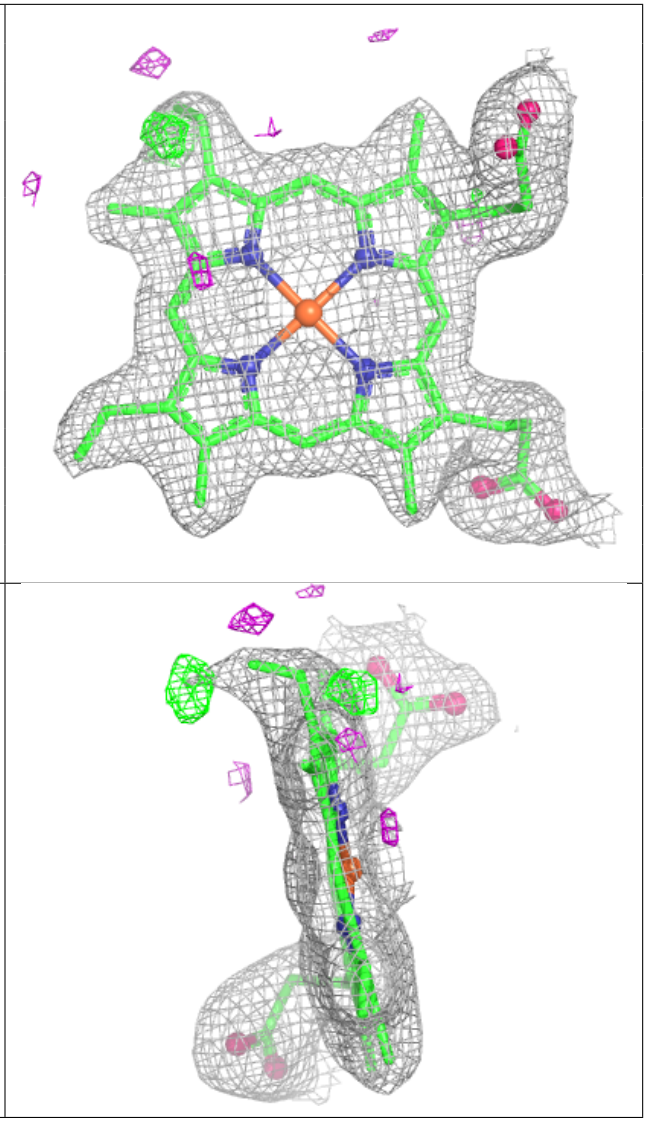
Electron density around TRP B 502:

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



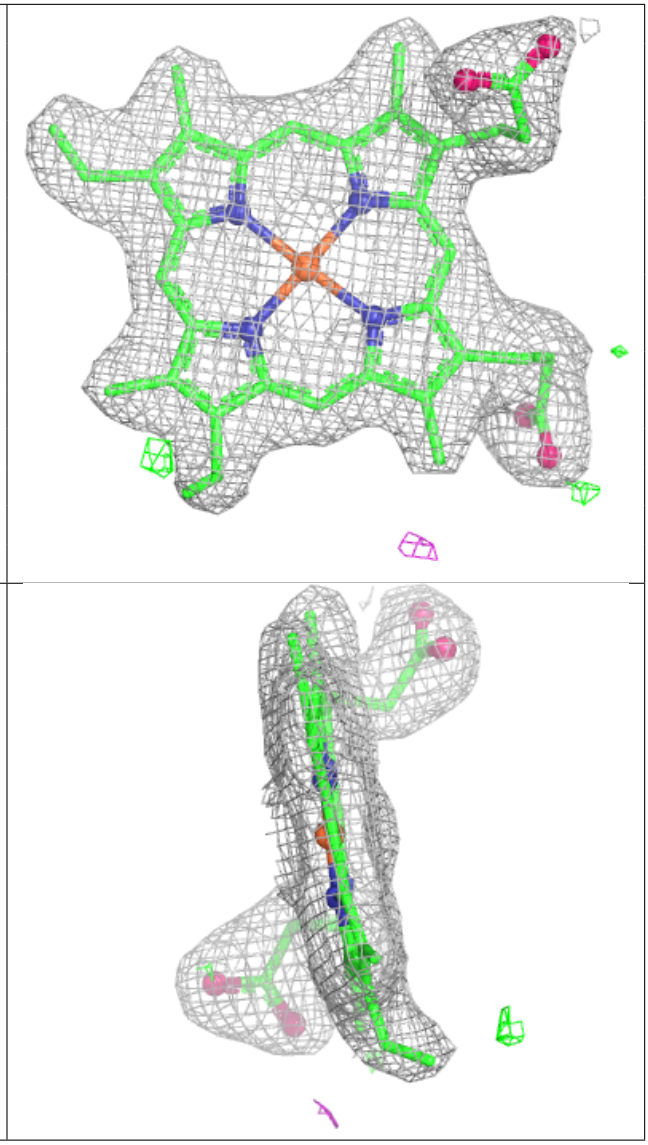
Electron density around HEM B 501:

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



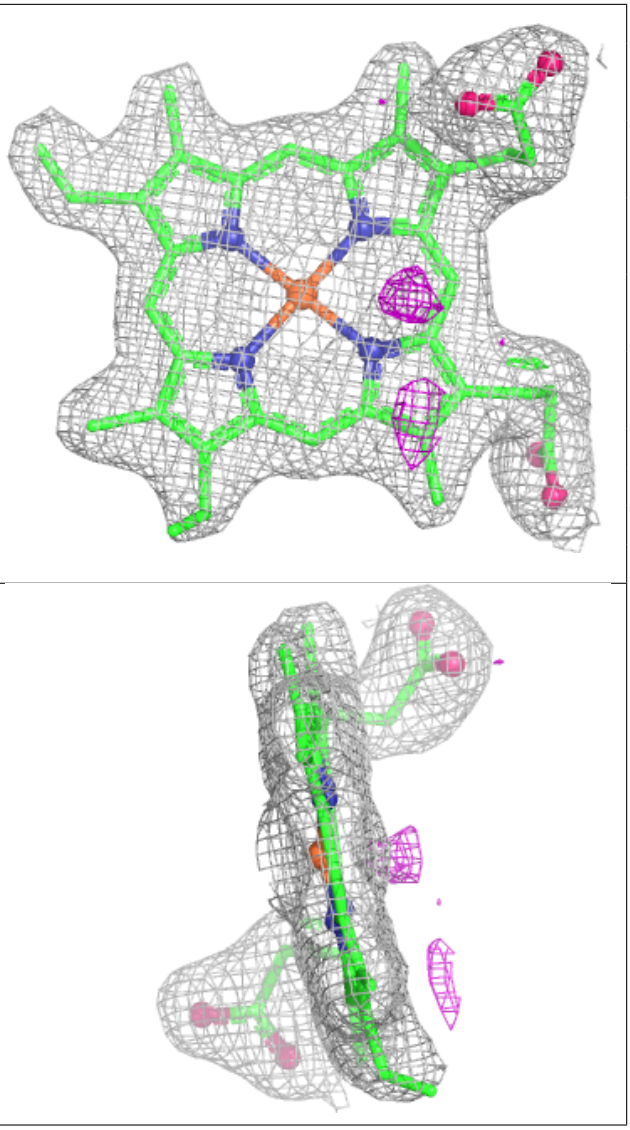
Electron density around HEM C 501:

$2mF_o$-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)



Electron density around HEM D 501:

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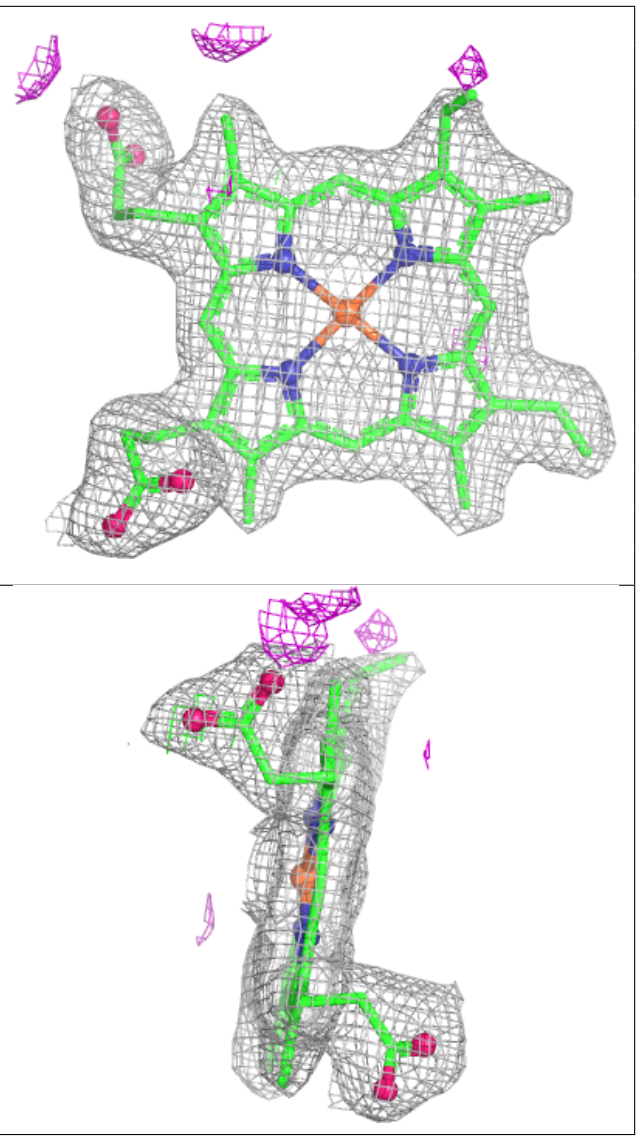
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.