Full wwPDB X-ray Structure Validation Report (i)

Dec 21, 2021 – 12:09 pm GMT

PDB ID	:	7P0R
Title	:	Crystal structure of L-Trp/Indoleamine 2,3-dioxygenase (hIDO1) complex with the JK-loop refined in the intermediate conformation
Authors	:	Mirgaux, M.; Wouters, J.
Deposited on	:	2021-06-30
Resolution	:	2.50 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 following versions of software and data (see references (i)) were used in the production of this report:

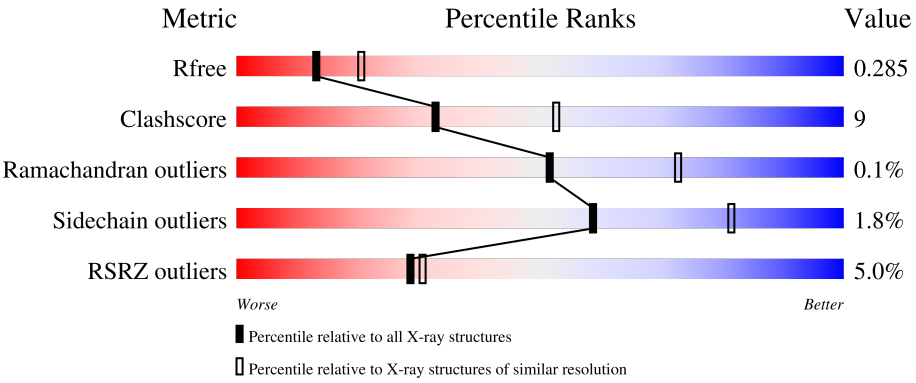
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	4% 77% 15% · 7%
1	B	405	5% 74% 19% 6%
1	C	405	5% 76% 17% 6%
1	D	405	4% 74% 19% 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	GOL	B	507	-	X	-	-
4	NFK	A	506	-	-	-	X
4	NFK	C	507	-	-	-	X
6	TRP	B	502	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12750 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
			2963	1903	506	537	17			
1	B	379	Total	C	N	O	S	0	0	0
			2989	1920	510	542	17			
1	C	380	Total	C	N	O	S	0	0	0
			2983	1912	509	545	17			
1	D	375	Total	C	N	O	S	0	0	0
			2956	1897	504	538	17			

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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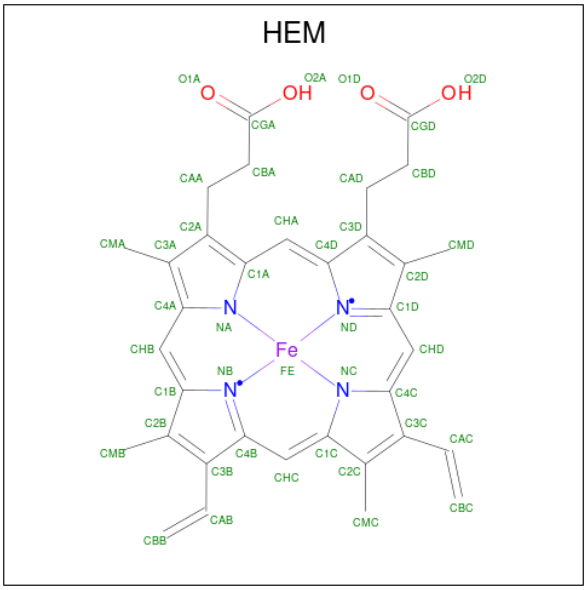
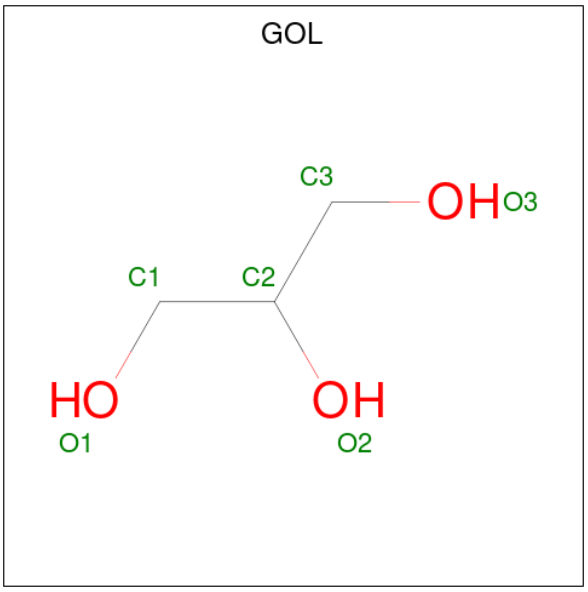
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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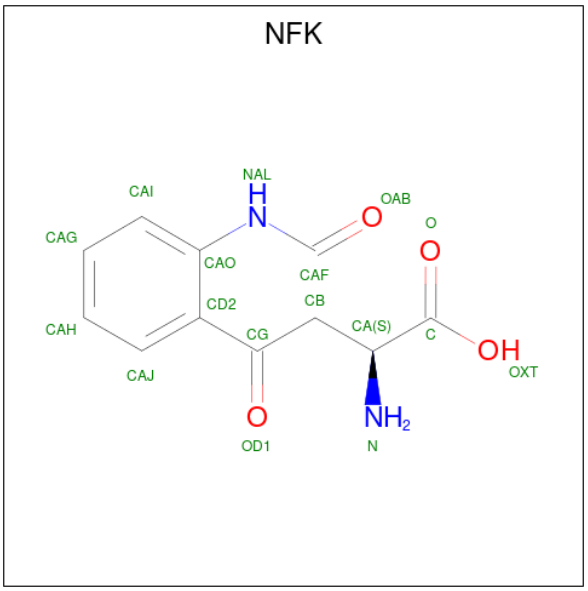
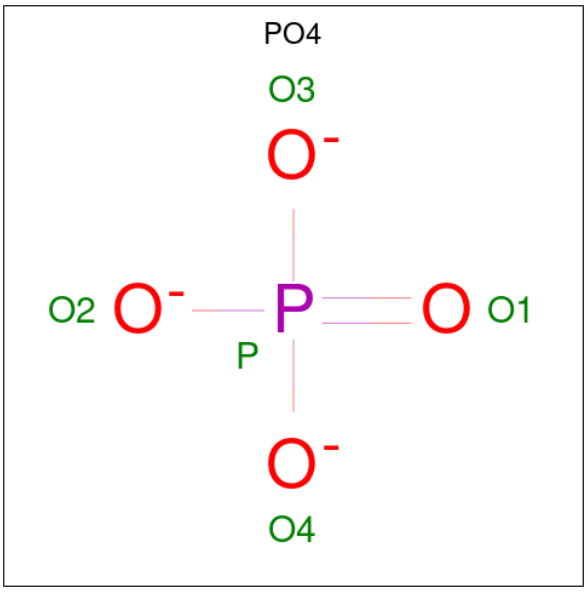
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is N'-Formylkynurenine (three-letter code: NFK) (formula: $C_{11}H_{12}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



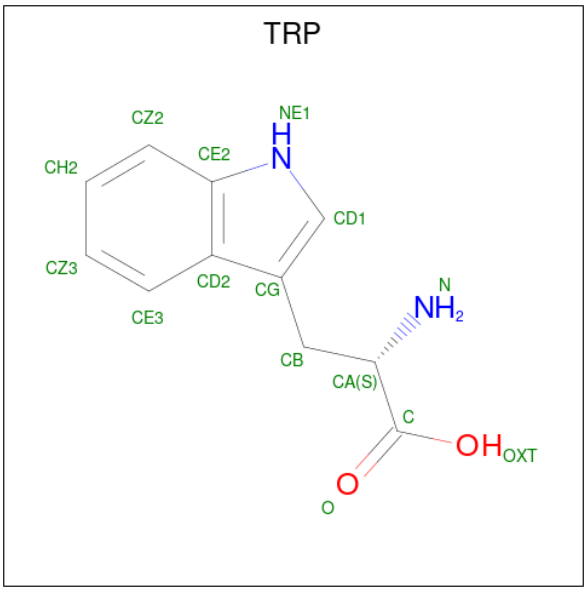
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 17 11 2 4	0	0
4	C	1	Total C N O 17 11 2 4	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 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
6	B	1	Total C N O 15 11 2 2	0	0
6	B	1	Total C N O 15 11 2 2	0	0
6	D	1	Total C N O 15 11 2 2	0	0

- Molecule 7 is water.

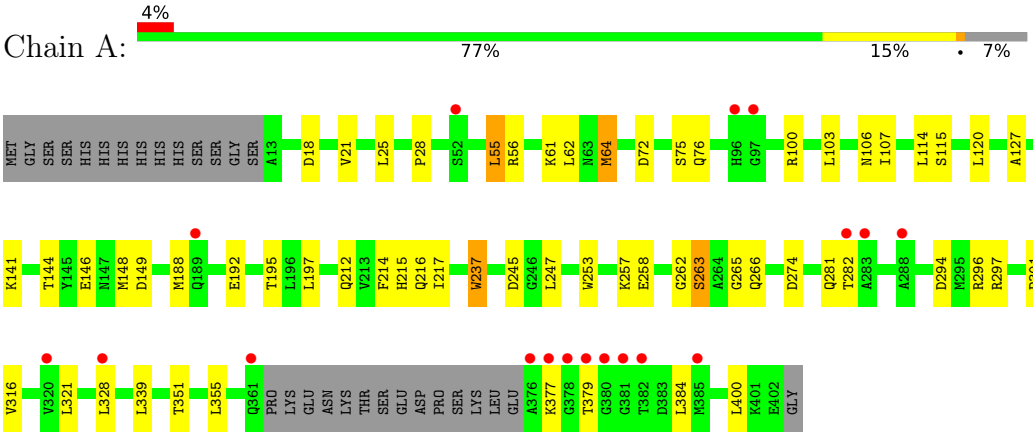
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	135	Total O 135 135	0	0
7	B	119	Total O 119 119	0	0
7	C	125	Total O 125 125	0	0
7	D	118	Total O 118 118	0	0

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.

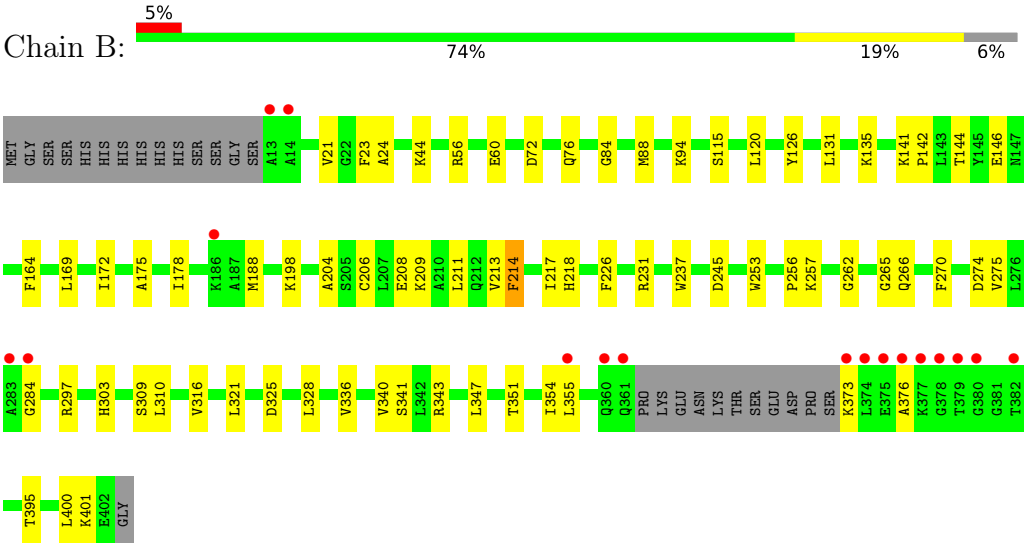
• Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain A:



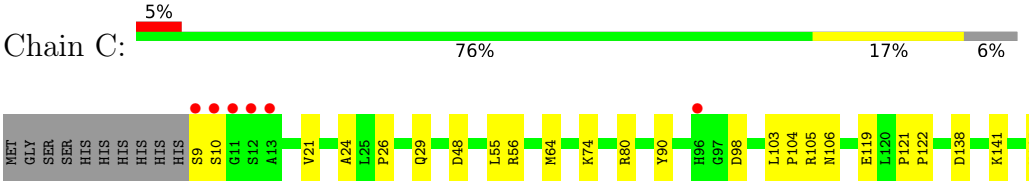
• Molecule 1: Indoleamine 2,3-dioxygenase 1

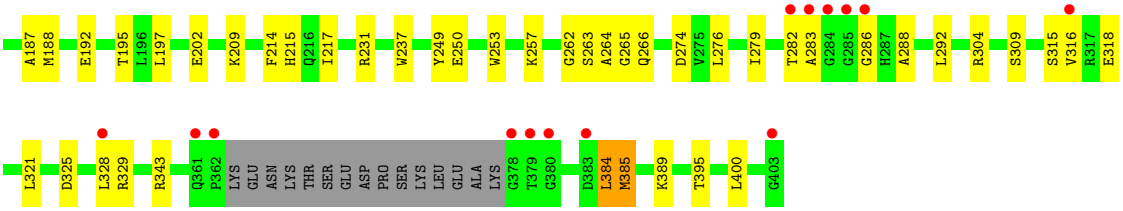
Chain B:



• Molecule 1: Indoleamine 2,3-dioxygenase 1

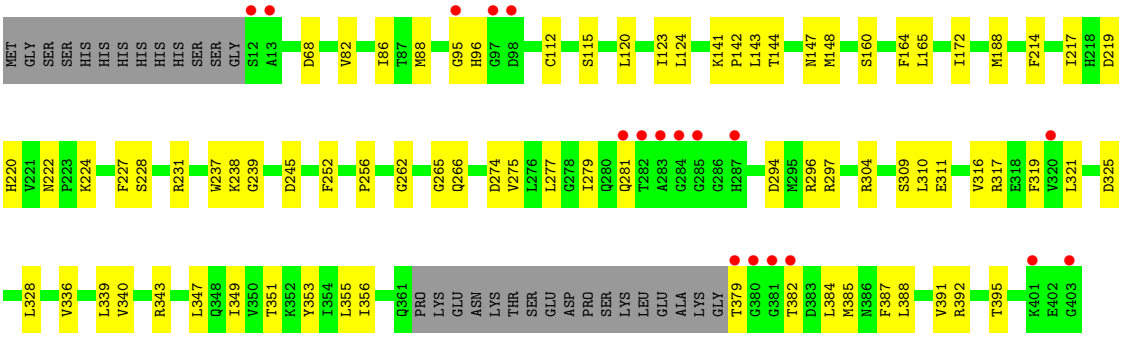
Chain C:





• 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	80.89Å 115.72Å 217.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 2.50 49.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.22-2.50) 99.4 (49.22-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.218 , 0.285 0.217 , 0.285	Depositor DCC
R_{free} test set	3562 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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 47.43 % 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 9.9362e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GOL, NFK, PO4

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	0/3031	0.62	2/4102 (0.0%)
1	B	0.47	0/3057	0.63	0/4136
1	C	0.47	0/3052	0.62	1/4130 (0.0%)
1	D	0.45	0/3024	0.63	0/4092
All	All	0.47	0/12164	0.62	3/16460 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	LEU	CA-CB-CG	-6.21	101.02	115.30
1	A	64	MET	CG-SD-CE	-5.17	91.92	100.20
1	C	55	LEU	CA-CB-CG	-5.07	103.64	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	297	ARG	Sidechain

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	2963	0	2969	47	0
1	B	2989	0	2999	54	0
1	C	2983	0	2979	44	0
1	D	2956	0	2956	58	0
2	A	43	0	30	8	0
2	B	43	0	30	8	0
2	C	43	0	30	4	0
2	D	43	0	30	6	0
3	A	24	0	32	2	0
3	B	24	0	32	3	0
3	C	30	0	40	1	0
3	D	18	0	24	0	0
4	A	17	0	0	0	0
4	C	17	0	0	1	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
6	B	30	0	18	3	0
6	D	15	0	9	5	0
7	A	135	0	0	5	0
7	B	119	0	0	4	0
7	C	125	0	0	3	0
7	D	118	0	0	6	0
All	All	12750	0	12178	213	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 9.

All (213) 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:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.47	0.95
1:A:351:THR:HA	1:A:355:LEU:HB2	1.65	0.79
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.66	0.77
1:B:218:HIS:HB3	3:B:505:GOL:H32	1.67	0.75
1:B:141:LYS:HD3	1:B:142:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:NZ	7:A:602:HOH:O	2.22	0.72
1:A:146:GLU:OE2	7:A:601:HOH:O	2.08	0.71
1:D:144:THR:O	1:D:148:MET:HG3	1.90	0.71
6:B:502:TRP:N	7:B:601:HOH:O	2.23	0.71
1:C:188:MET:CE	1:C:316:VAL:HA	2.21	0.70
1:D:347:LEU:HD11	1:D:388:LEU:HB3	1.73	0.69
1:A:212:GLN:HA	1:A:215:HIS:HD2	1.59	0.68
1:C:385:MET:SD	1:C:389:LYS:NZ	2.67	0.68
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.76	0.68
1:B:274:ASP:OD2	1:B:343:ARG:NH2	2.26	0.67
1:A:274:ASP:OD2	1:A:281:GLN:HG3	1.94	0.67
1:D:340:VAL:HG22	1:D:395:THR:HG22	1.74	0.67
1:C:80:ARG:NH2	1:C:121:PRO:O	2.28	0.67
1:B:384:LEU:HD11	2:B:501:HEM:HAA1	1.77	0.66
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.77	0.66
1:C:188:MET:HE1	1:C:316:VAL:HA	1.76	0.66
1:A:377:LYS:HE2	1:A:384:LEU:HD21	1.78	0.65
1:C:197:LEU:HD12	1:C:328:LEU:HD23	1.80	0.64
1:C:9:SER:N	1:C:309:SER:HG	1.94	0.64
1:B:21:VAL:HB	1:B:24:ALA:HB3	1.78	0.64
1:C:26:PRO:O	1:C:74:LYS:NZ	2.28	0.64
1:B:144:THR:O	1:B:148:MET:HG3	1.99	0.63
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.78	0.63
1:D:277:LEU:HB2	1:D:279:ILE:HD12	1.81	0.63
1:B:56:ARG:HB2	6:B:503:TRP:CZ2	2.34	0.62
1:B:84:GLY:O	1:B:88:MET:HG2	1.99	0.62
1:C:282:THR:HG22	1:C:283:ALA:H	1.64	0.62
2:B:501:HEM:HBB2	2:B:501:HEM:CHC	2.24	0.62
1:D:384:LEU:HD11	2:D:501:HEM:HAA1	1.82	0.62
1:D:387:PHE:O	1:D:391:VAL:HG23	1.99	0.62
1:C:265:GLY:HA2	2:C:501:HEM:C3D	2.35	0.61
1:D:217:ILE:HD11	2:D:501:HEM:HBB1	1.81	0.61
1:D:231:ARG:NH2	1:D:379:THR:HG22	2.16	0.61
1:C:315:SER:HB3	1:C:318:GLU:HB2	1.84	0.60
1:D:262:GLY:HA2	1:D:266:GLN:NE2	2.16	0.60
1:D:68:ASP:OD2	7:D:601:HOH:O	2.17	0.59
1:A:321:LEU:HD21	1:A:400:LEU:HD22	1.85	0.59
1:A:262:GLY:HA2	1:A:266:GLN:HE22	1.68	0.59
1:B:60:GLU:HG2	3:B:504:GOL:H12	1.85	0.59
1:B:340:VAL:HG23	1:B:395:THR:HG22	1.85	0.58
1:B:347:LEU:HD21	1:B:389:LYS:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:HG12	2:A:501:HEM:HBB1	1.84	0.57
1:A:265:GLY:HA2	2:A:501:HEM:C3D	2.38	0.57
1:B:351:THR:HA	1:B:355:LEU:HB2	1.86	0.57
1:C:262:GLY:HA2	1:C:266:GLN:NE2	2.20	0.57
1:C:282:THR:HG22	1:C:283:ALA:N	2.18	0.57
1:B:141:LYS:NZ	7:B:602:HOH:O	2.27	0.57
1:B:265:GLY:HA2	2:B:501:HEM:C2D	2.39	0.57
1:B:142:PRO:HB2	1:B:144:THR:HG23	1.86	0.56
1:D:336:VAL:O	1:D:340:VAL:HG23	2.06	0.56
1:A:282:THR:HG21	1:A:296:ARG:NH1	2.20	0.56
1:C:192:GLU:HB3	1:C:195:THR:HB	1.88	0.56
1:D:224:LYS:O	1:D:228:SER:OG	2.23	0.56
1:A:56:ARG:HH11	3:A:504:GOL:H11	1.69	0.56
1:C:321:LEU:HD21	1:C:400:LEU:HD22	1.88	0.56
1:D:325:ASP:HB3	1:D:328:LEU:HB2	1.87	0.56
1:B:262:GLY:HA2	1:B:266:GLN:NE2	2.22	0.55
1:A:188:MET:CE	1:A:316:VAL:HA	2.36	0.55
1:D:294:ASP:HA	1:D:297:ARG:HH11	1.73	0.54
1:D:279:ILE:HG22	1:D:281:GLN:HG2	1.89	0.54
1:C:231:ARG:HD2	7:C:626:HOH:O	2.07	0.54
1:A:192:GLU:HB3	1:A:195:THR:HB	1.90	0.54
1:D:142:PRO:HB2	1:D:144:THR:HG23	1.89	0.54
1:B:373:LYS:HZ3	1:B:376:ALA:H	1.56	0.53
4:C:507:NFK:NAL	4:C:507:NFK:OD1	2.42	0.53
1:D:317:ARG:O	1:D:321:LEU:HG	2.08	0.53
1:D:143:LEU:HD13	1:D:172:ILE:HD13	1.90	0.53
1:D:82:VAL:O	1:D:86:ILE:HG13	2.08	0.53
1:B:23:PHE:O	1:B:131:LEU:HD13	2.09	0.53
1:A:197:LEU:HD12	1:A:328:LEU:HD23	1.91	0.52
1:C:146:GLU:OE2	1:C:146:GLU:HA	2.10	0.52
1:A:188:MET:HE3	1:A:316:VAL:HA	1.91	0.52
1:B:303:HIS:ND1	7:B:606:HOH:O	2.34	0.52
1:D:222:ASN:HB3	6:D:502:TRP:CE3	2.45	0.52
1:B:169:LEU:HA	1:B:172:ILE:HD12	1.92	0.52
1:C:188:MET:HE3	1:C:316:VAL:HA	1.91	0.51
1:D:296:ARG:O	1:D:304:ARG:HD3	2.09	0.51
1:D:382:THR:HG22	7:D:696:HOH:O	2.10	0.51
1:B:277:LEU:HD13	1:B:336:VAL:HG22	1.92	0.51
1:D:231:ARG:HD2	7:D:651:HOH:O	2.09	0.51
1:B:262:GLY:HA2	1:B:266:GLN:HE22	1.76	0.51
1:B:206:CYS:HA	1:B:209:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:CD1	2:B:501:HEM:HBB1	2.41	0.50
1:B:94:LYS:H	6:B:503:TRP:HB3	1.76	0.50
1:D:351:THR:O	1:D:356:ILE:HG13	2.11	0.50
1:A:64:MET:HB2	1:A:106:ASN:OD1	2.11	0.50
1:C:274:ASP:OD2	1:C:343:ARG:NH2	2.45	0.50
1:C:202:GLU:OE2	1:C:202:GLU:HA	2.12	0.50
1:A:263:SER:OG	1:A:265:GLY:N	2.42	0.50
1:C:21:VAL:HB	1:C:24:ALA:HB3	1.93	0.50
1:C:187:ALA:HB2	1:C:195:THR:HG22	1.94	0.49
1:D:275:VAL:HG13	1:D:311:GLU:HG3	1.92	0.49
1:B:175:ALA:HA	1:B:178:ILE:HD12	1.93	0.49
1:B:204:ALA:O	1:B:208:GLU:HG3	2.12	0.49
1:A:76:GLN:HB3	1:A:114:LEU:HD11	1.94	0.49
1:B:275:VAL:CG1	1:B:310:LEU:HB3	2.42	0.49
1:B:226:PHE:HE2	1:B:354:ILE:HD11	1.78	0.49
1:B:146:GLU:HB2	7:B:602:HOH:O	2.13	0.48
1:D:141:LYS:HB3	1:D:147:ASN:ND2	2.28	0.48
1:D:339:LEU:HD22	1:D:395:THR:HG21	1.95	0.48
1:B:115:SER:HB3	1:B:120:LEU:O	2.14	0.48
1:D:188:MET:HG2	1:D:319:PHE:CD2	2.47	0.48
1:C:10:SER:HA	1:C:182:PRO:HG3	1.96	0.48
1:D:95:GLY:O	1:D:96:HIS:ND1	2.46	0.47
1:C:181:ILE:HG23	1:C:276:LEU:HD13	1.96	0.47
1:D:384:LEU:CD1	2:D:501:HEM:HAA1	2.45	0.47
6:D:502:TRP:HD1	7:D:686:HOH:O	1.98	0.47
1:A:215:HIS:HB3	6:D:502:TRP:CZ3	2.49	0.47
1:B:277:LEU:HB2	1:B:279:ILE:HG13	1.97	0.47
1:A:25:LEU:HD23	1:A:28:PRO:HB3	1.96	0.47
1:B:325:ASP:HB3	1:B:328:LEU:HB2	1.96	0.47
1:D:219:ASP:O	6:D:502:TRP:HZ2	1.97	0.47
1:B:275:VAL:HG12	1:B:310:LEU:HB3	1.97	0.47
3:B:505:GOL:H31	1:C:215:HIS:NE2	2.31	0.46
1:C:9:SER:N	1:C:309:SER:OG	2.48	0.46
1:C:384:LEU:O	1:C:385:MET:CB	2.63	0.46
1:C:98:ASP:HB3	7:C:606:HOH:O	2.15	0.46
1:C:122:PRO:HB2	1:C:249:TYR:CE2	2.50	0.46
1:D:88:MET:HE1	1:D:123:ILE:HG13	1.97	0.46
1:A:56:ARG:HD2	3:A:504:GOL:H32	1.97	0.46
1:D:274:ASP:OD2	1:D:343:ARG:NH2	2.49	0.46
1:D:351:THR:HA	1:D:355:LEU:HB2	1.96	0.46
1:C:217:ILE:CD1	2:C:501:HEM:HBB1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:O	1:A:148:MET:HG3	2.16	0.45
1:B:245:ASP:O	1:B:256:PRO:HB2	2.16	0.45
1:A:55:LEU:O	1:A:55:LEU:HG	2.10	0.45
7:A:608:HOH:O	1:D:220:HIS:HD2	2.00	0.45
1:D:115:SER:HB3	1:D:120:LEU:O	2.17	0.45
1:B:209:LYS:O	1:B:213:VAL:HG23	2.16	0.45
1:D:112:CYS:HB3	1:D:252:PHE:CE2	2.51	0.45
1:A:237:TRP:O	1:A:258:GLU:HG2	2.17	0.45
1:A:265:GLY:HA2	2:A:501:HEM:C2D	2.51	0.45
1:D:355:LEU:HA	1:D:355:LEU:HD23	1.76	0.45
1:A:212:GLN:HA	1:A:215:HIS:CD2	2.47	0.45
1:A:216:GLN:HG2	6:D:502:TRP:N	2.32	0.45
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.73	0.45
1:B:160:SER:HB2	1:B:164:PHE:CE2	2.53	0.44
1:B:188:MET:SD	1:B:316:VAL:HG22	2.57	0.44
1:B:231:ARG:HH22	1:B:376:ALA:HB1	1.81	0.44
1:D:328:LEU:HD23	1:D:328:LEU:HA	1.76	0.44
1:D:277:LEU:HB2	1:D:279:ILE:CD1	2.44	0.44
1:A:377:LYS:HB3	1:A:384:LEU:HD23	1.99	0.44
1:C:48:ASP:HB3	7:C:681:HOH:O	2.18	0.44
1:D:310:LEU:HD23	1:D:310:LEU:HA	1.75	0.44
1:D:188:MET:HE3	1:D:316:VAL:HA	2.00	0.44
1:A:301:PRO:HD2	7:A:679:HOH:O	2.17	0.44
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.80	0.44
1:A:62:LEU:HD13	1:A:107:ILE:HD11	1.99	0.43
1:A:138:ASP:HB3	1:A:141:LYS:HG3	2.00	0.43
1:C:145:TYR:OH	3:C:503:GOL:H2	2.17	0.43
1:D:265:GLY:HA2	2:D:501:HEM:C3D	2.53	0.43
1:A:294:ASP:O	1:A:297:ARG:HB3	2.18	0.43
1:A:103:LEU:HB2	1:A:247:LEU:HD21	2.01	0.43
1:D:239:GLY:HA2	7:D:673:HOH:O	2.18	0.43
2:A:501:HEM:HMD1	2:A:501:HEM:O1D	2.19	0.43
1:C:253:TRP:CD2	1:C:257:LYS:HD2	2.53	0.43
1:D:343:ARG:O	1:D:347:LEU:HD13	2.18	0.43
1:A:100:ARG:HD3	1:A:100:ARG:HA	1.79	0.43
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.90	0.43
1:C:103:LEU:HD12	1:C:104:PRO:HD2	2.01	0.43
1:D:217:ILE:HD11	2:D:501:HEM:CBB	2.46	0.43
1:B:44:LYS:HE2	1:B:152:PHE:CE1	2.54	0.42
1:B:373:LYS:NZ	1:B:376:ALA:H	2.17	0.42
1:C:325:ASP:O	1:C:329:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:HG3	1:C:90:TYR:CE1	2.54	0.42
1:D:88:MET:HE3	1:D:124:LEU:H	1.84	0.42
1:A:18:ASP:OD2	1:A:21:VAL:HG22	2.19	0.42
1:A:217:ILE:CG1	2:A:501:HEM:HBB1	2.50	0.42
1:B:217:ILE:HG12	2:B:501:HEM:HBB1	2.01	0.42
1:A:379:THR:HA	7:A:668:HOH:O	2.18	0.42
1:D:262:GLY:HA2	1:D:266:GLN:HE22	1.83	0.42
1:B:72:ASP:O	1:B:76:GLN:HG3	2.20	0.42
1:B:211:LEU:HD22	1:B:341:SER:HB3	2.01	0.42
1:D:165:LEU:HD23	1:D:165:LEU:HA	1.77	0.42
1:C:64:MET:HB2	1:C:106:ASN:OD1	2.20	0.42
1:B:253:TRP:CE3	1:B:257:LYS:HD2	2.55	0.42
1:D:294:ASP:O	1:D:297:ARG:HB2	2.20	0.42
1:A:115:SER:HB3	1:A:120:LEU:O	2.19	0.42
1:B:265:GLY:HA2	2:B:501:HEM:C3D	2.55	0.42
1:C:263:SER:HB3	1:C:264:ALA:H	1.73	0.42
1:D:188:MET:CE	1:D:316:VAL:HA	2.49	0.42
1:B:355:LEU:HA	1:B:355:LEU:HD23	1.79	0.42
1:B:400:LEU:O	1:B:401:LYS:HG2	2.19	0.42
1:B:135:LYS:HE3	1:B:135:LYS:HB2	1.90	0.41
1:D:141:LYS:NZ	7:D:612:HOH:O	2.53	0.41
1:B:126:TYR:HB2	1:B:266:GLN:HB2	2.02	0.41
1:B:214:PHE:HD1	1:B:214:PHE:O	2.04	0.41
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.92	0.41
2:A:501:HEM:HBB2	2:A:501:HEM:CHC	2.39	0.41
1:D:88:MET:HE1	1:D:123:ILE:CG1	2.51	0.41
1:D:274:ASP:CG	1:D:281:GLN:HG3	2.40	0.41
1:C:279:ILE:HD13	1:C:395:THR:HG23	2.03	0.41
1:D:160:SER:HB2	1:D:164:PHE:CE2	2.55	0.41
1:D:227:PHE:HB2	1:D:353:TYR:O	2.21	0.41
1:A:253:TRP:CD2	1:A:257:LYS:HD2	2.56	0.41
1:C:138:ASP:OD2	1:C:141:LYS:HE3	2.21	0.41
1:C:119:GLU:HB3	1:C:304:ARG:HH22	1.86	0.41
1:D:245:ASP:O	1:D:256:PRO:HB2	2.20	0.41
1:A:72:ASP:OD1	1:A:75:SER:OG	2.39	0.41
1:D:349:ILE:HD13	1:D:349:ILE:HA	1.89	0.40
1:B:270:PHE:CD2	2:B:501:HEM:HMD2	2.56	0.40
1:C:217:ILE:HD11	2:C:501:HEM:HBB1	2.03	0.40
1:A:188:MET:HE1	1:A:316:VAL:HA	2.03	0.40
1:C:105:ARG:N	1:C:250:GLU:OE1	2.54	0.40
1:A:127:ALA:HA	1:A:131:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:CD1	2:A:501:HEM:HBB1	2.52	0.40
1:A:262:GLY:HA2	1:A:266:GLN:NE2	2.35	0.40
1:C:286:GLY:O	1:C:288:ALA:N	2.46	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	372/405 (92%)	351 (94%)	21 (6%)	0	100	100
1	B	375/405 (93%)	351 (94%)	23 (6%)	1 (0%)	41	61
1	C	376/405 (93%)	350 (93%)	25 (7%)	1 (0%)	41	61
1	D	371/405 (92%)	355 (96%)	16 (4%)	0	100	100
All	All	1494/1620 (92%)	1407 (94%)	85 (6%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	385	MET
1	B	284	GLY

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	320/346 (92%)	314 (98%)	6 (2%)	57 80
1	B	323/346 (93%)	319 (99%)	4 (1%)	71 88
1	C	323/346 (93%)	318 (98%)	5 (2%)	65 85
1	D	320/346 (92%)	314 (98%)	6 (2%)	57 80
All	All	1286/1384 (93%)	1265 (98%)	21 (2%)	59 84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	A	214	PHE
1	A	237	TRP
1	A	245	ASP
1	A	263	SER
1	A	309	SER
1	B	198	LYS
1	B	214	PHE
1	B	237	TRP
1	B	309	SER
1	C	29	GLN
1	C	209	LYS
1	C	214	PHE
1	C	237	TRP
1	C	384	LEU
1	D	214	PHE
1	D	237	TRP
1	D	238	LYS
1	D	309	SER
1	D	385	MET
1	D	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	B	293	GLN
1	C	386	ASN
1	D	16	HIS
1	D	313	ASN

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

28 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	$\#\|Z\| > 2$
5	PO4	B	509	-	4,4,4	0.75	0	6,6,6	0.51	0
3	GOL	C	505	-	5,5,5	1.16	0	5,5,5	0.95	0
6	TRP	D	502	-	12,16,16	1.35	1 (8%)	12,22,22	0.91	0
2	HEM	A	501	1	27,50,50	1.78	5 (18%)	17,82,82	1.94	7 (41%)
3	GOL	C	504	-	5,5,5	1.29	1 (20%)	5,5,5	0.96	0
3	GOL	A	503	-	5,5,5	1.00	0	5,5,5	0.91	0
3	GOL	D	504	-	5,5,5	1.04	0	5,5,5	0.83	0
3	GOL	B	504	-	5,5,5	0.77	0	5,5,5	1.14	0
4	NFK	C	507	-	14,17,17	2.90	5 (35%)	16,22,22	1.17	2 (12%)
3	GOL	C	502	-	5,5,5	1.02	0	5,5,5	1.02	0
4	NFK	A	506	-	14,17,17	2.98	3 (21%)	16,22,22	0.87	0
3	GOL	A	502	-	5,5,5	0.99	0	5,5,5	0.89	0
2	HEM	B	501	1	27,50,50	1.79	4 (14%)	17,82,82	2.25	8 (47%)
3	GOL	C	506	-	5,5,5	1.15	0	5,5,5	0.97	0
2	HEM	D	501	1	27,50,50	1.80	5 (18%)	17,82,82	1.97	6 (35%)
6	TRP	B	502	-	12,16,16	1.39	1 (8%)	12,22,22	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	C	503	-	5,5,5	1.06	0	5,5,5	0.93	0
3	GOL	A	505	-	5,5,5	0.75	0	5,5,5	1.02	0
3	GOL	D	505	-	5,5,5	0.98	0	5,5,5	0.85	0
3	GOL	B	505	-	5,5,5	1.07	0	5,5,5	0.87	0
3	GOL	A	504	-	5,5,5	1.07	1 (20%)	5,5,5	0.89	0
6	TRP	B	503	-	12,16,16	1.43	1 (8%)	12,22,22	0.82	0
5	PO4	B	508	-	4,4,4	0.65	0	6,6,6	0.62	0
3	GOL	B	507	-	5,5,5	1.23	1 (20%)	5,5,5	1.06	1 (20%)
3	GOL	D	503	-	5,5,5	1.28	1 (20%)	5,5,5	0.74	0
3	GOL	B	506	-	5,5,5	0.68	0	5,5,5	1.07	0
2	HEM	C	501	1	27,50,50	1.81	5 (18%)	17,82,82	2.15	6 (35%)
5	PO4	A	507	-	4,4,4	0.82	0	6,6,6	0.64	0

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	GOL	C	505	-	-	2/4/4/4	-
6	TRP	D	502	-	-	2/3/8/8	0/2/2/2
2	HEM	A	501	1	-	2/6/54/54	-
3	GOL	C	504	-	-	0/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	D	504	-	-	1/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
4	NFK	C	507	-	-	0/11/15/15	0/1/1/1
3	GOL	C	502	-	-	4/4/4/4	-
4	NFK	A	506	-	-	9/11/15/15	0/1/1/1
3	GOL	A	502	-	-	2/4/4/4	-
2	HEM	B	501	1	-	4/6/54/54	-
3	GOL	C	506	-	-	0/4/4/4	-
2	HEM	D	501	1	-	0/6/54/54	-
6	TRP	B	502	-	-	3/3/8/8	0/2/2/2
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-
3	GOL	D	505	-	-	2/4/4/4	-
3	GOL	B	505	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	504	-	-	4/4/4/4	-
6	TRP	B	503	-	-	3/3/8/8	0/2/2/2
3	GOL	B	507	-	-	4/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-
2	HEM	C	501	1	-	1/6/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	NFK	CAF-NAL	9.57	1.47	1.34
4	C	507	NFK	CAF-NAL	9.12	1.46	1.34
2	B	501	HEM	C3B-C2B	-5.08	1.33	1.40
2	A	501	HEM	C3B-C2B	-4.64	1.33	1.40
2	C	501	HEM	C3B-C2B	-4.38	1.34	1.40
2	D	501	HEM	C3B-C2B	-4.15	1.34	1.40
2	D	501	HEM	C3C-C2C	-3.90	1.35	1.40
2	A	501	HEM	C3C-CAC	3.75	1.55	1.47
2	C	501	HEM	C3C-CAC	3.65	1.55	1.47
4	C	507	NFK	CAO-NAL	3.62	1.46	1.41
4	A	506	NFK	CAO-NAL	3.55	1.46	1.41
2	B	501	HEM	C3C-CAC	3.36	1.54	1.47
2	C	501	HEM	C3C-C2C	-3.27	1.35	1.40
2	D	501	HEM	C3C-CAC	3.25	1.54	1.47
2	D	501	HEM	C3B-CAB	3.24	1.54	1.47
6	B	502	TRP	CB-CG	3.23	1.60	1.51
2	B	501	HEM	C3C-C2C	-3.12	1.36	1.40
2	C	501	HEM	C3B-CAB	3.12	1.54	1.47
4	A	506	NFK	CD2-CG	2.99	1.54	1.48
4	C	507	NFK	CD2-CG	2.98	1.54	1.48
6	B	503	TRP	CB-CG	2.96	1.59	1.51
2	A	501	HEM	C3C-C2C	-2.90	1.36	1.40
2	A	501	HEM	C3B-CAB	2.77	1.53	1.47
2	C	501	HEM	CAA-C2A	2.66	1.55	1.52
6	D	502	TRP	CB-CG	2.63	1.58	1.51
2	A	501	HEM	CAA-C2A	2.63	1.55	1.52
2	B	501	HEM	C3B-CAB	2.48	1.53	1.47
3	C	504	GOL	C1-C2	2.48	1.61	1.51
4	C	507	NFK	CB-CG	2.32	1.54	1.51
2	D	501	HEM	CAA-C2A	2.25	1.55	1.52
3	B	507	GOL	C1-C2	2.19	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507	NFK	OD1-CG	-2.14	1.18	1.22
3	D	503	GOL	C3-C2	2.13	1.60	1.51
3	A	504	GOL	C1-C2	2.03	1.60	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CAA-CBA-CGA	-4.98	104.31	112.67
2	D	501	HEM	CAD-CBD-CGD	-4.12	105.76	112.67
2	A	501	HEM	C3B-C4B-NB	-3.58	104.58	109.21
2	B	501	HEM	CBA-CAA-C2A	-3.24	106.51	112.49
2	B	501	HEM	CBD-CAD-C3D	3.24	118.44	112.48
2	B	501	HEM	CMA-C3A-C4A	-3.20	123.55	128.46
2	A	501	HEM	CBD-CAD-C3D	-3.15	106.68	112.48
2	B	501	HEM	C2C-C3C-C4C	3.11	109.07	106.90
2	C	501	HEM	CBD-CAD-C3D	-3.08	106.81	112.48
2	B	501	HEM	CAA-CBA-CGA	-3.01	107.63	112.67
2	C	501	HEM	C3B-C4B-NB	-2.95	105.39	109.21
2	B	501	HEM	C3B-C4B-NB	-2.91	105.45	109.21
2	D	501	HEM	C2C-C3C-C4C	2.87	108.91	106.90
2	D	501	HEM	CMA-C3A-C4A	-2.72	124.28	128.46
2	D	501	HEM	C3C-C4C-NC	-2.64	105.97	110.94
2	C	501	HEM	CMA-C3A-C4A	-2.63	124.42	128.46
2	B	501	HEM	C3C-C4C-NC	-2.59	106.05	110.94
2	C	501	HEM	CAD-CBD-CGD	-2.56	108.37	112.67
2	A	501	HEM	C4A-C3A-C2A	2.46	108.71	107.00
2	B	501	HEM	CMC-C2C-C3C	2.41	129.19	124.68
2	A	501	HEM	CAD-CBD-CGD	-2.39	108.66	112.67
2	D	501	HEM	C1D-C2D-C3D	2.36	108.64	107.00
2	D	501	HEM	CBD-CAD-C3D	-2.35	108.14	112.48
2	A	501	HEM	CAA-CBA-CGA	-2.33	108.76	112.67
2	A	501	HEM	CBA-CAA-C2A	-2.17	108.48	112.49
4	C	507	NFK	CB-CG-CD2	2.17	122.88	119.86
2	A	501	HEM	C2C-C3C-C4C	2.16	108.41	106.90
4	C	507	NFK	OAB-CAF-NAL	-2.07	123.16	125.80
2	C	501	HEM	CBA-CAA-C2A	-2.02	108.77	112.49
3	B	507	GOL	C3-C2-C1	-2.01	103.89	111.70

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C2D-C3D-CAD-CBD
2	B	501	HEM	C4D-C3D-CAD-CBD
3	B	504	GOL	O1-C1-C2-C3
3	B	506	GOL	O1-C1-C2-C3
3	B	507	GOL	O1-C1-C2-O2
3	B	507	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
3	C	503	GOL	C1-C2-C3-O3
4	A	506	NFK	C-CA-CB-CG
6	B	502	TRP	N-CA-CB-CG
6	B	502	TRP	C-CA-CB-CG
6	B	503	TRP	C-CA-CB-CG
6	D	502	TRP	N-CA-CB-CG
6	D	502	TRP	C-CA-CB-CG
4	A	506	NFK	CAI-CAO-NAL-CAF
3	C	505	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-C3
3	A	504	GOL	O1-C1-C2-C3
3	A	505	GOL	O1-C1-C2-C3
3	B	505	GOL	C1-C2-C3-O3
3	C	505	GOL	C1-C2-C3-O3
3	D	503	GOL	C1-C2-C3-O3
3	D	505	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2
3	B	505	GOL	O2-C2-C3-O3
3	B	506	GOL	O1-C1-C2-O2
3	D	505	GOL	O2-C2-C3-O3
3	A	505	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
2	C	501	HEM	C3D-CAD-CBD-CGD
4	A	506	NFK	CAJ-CD2-CG-OD1
6	B	503	TRP	CA-CB-CG-CD1
3	A	504	GOL	O2-C2-C3-O3
3	B	507	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-O2
4	A	506	NFK	N-CA-CB-CG
4	A	506	NFK	CA-CB-CG-CD2
4	A	506	NFK	CAJ-CD2-CG-CB
4	A	506	NFK	CD2-CAO-NAL-CAF

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Mol	Chain	Res	Type	Atoms
6	B	503	TRP	N-CA-CB-CG
3	C	503	GOL	O2-C2-C3-O3
3	D	503	GOL	O2-C2-C3-O3
4	A	506	NFK	CA-CB-CG-OD1
2	A	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C3D-CAD-CBD-CGD
6	B	502	TRP	CA-CB-CG-CD1
4	A	506	NFK	CAO-CD2-CG-OD1
3	A	504	GOL	O1-C1-C2-O2
3	A	504	GOL	C1-C2-C3-O3
3	B	507	GOL	C1-C2-C3-O3
3	C	502	GOL	O1-C1-C2-C3
2	B	501	HEM	C2A-CAA-CBA-CGA
2	B	501	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

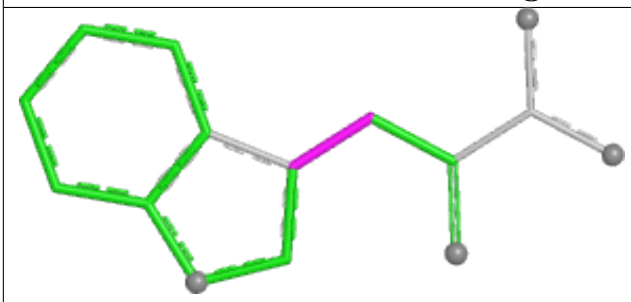
12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	502	TRP	5	0
2	A	501	HEM	8	0
3	B	504	GOL	1	0
4	C	507	NFK	1	0
2	B	501	HEM	8	0
2	D	501	HEM	6	0
6	B	502	TRP	1	0
3	C	503	GOL	1	0
3	B	505	GOL	2	0
3	A	504	GOL	2	0
6	B	503	TRP	2	0
2	C	501	HEM	4	0

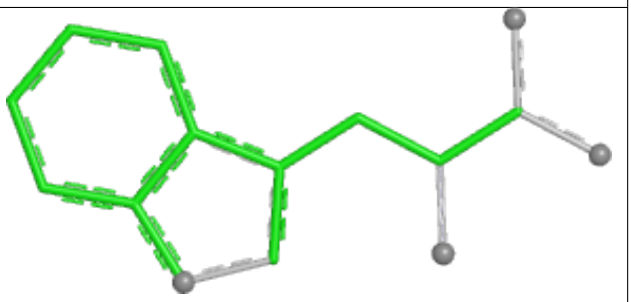
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

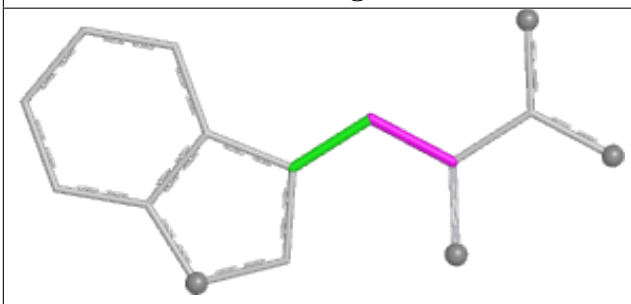
Ligand TRP D 502



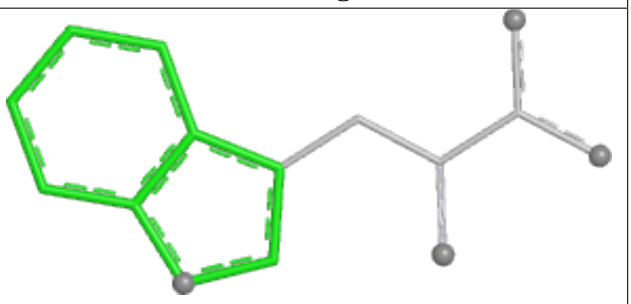
Bond lengths



Bond angles

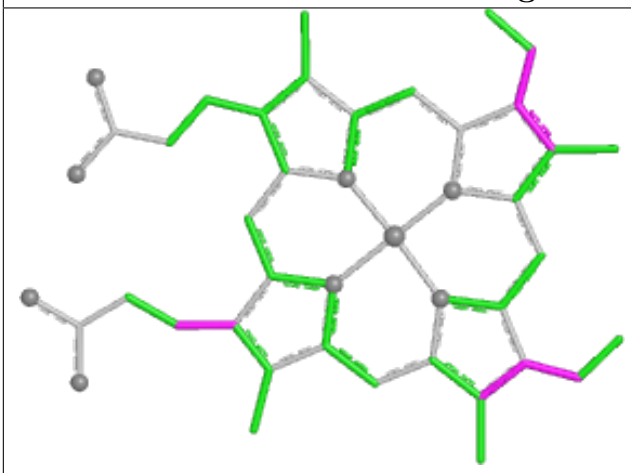


Torsions



Rings

Ligand HEM A 501



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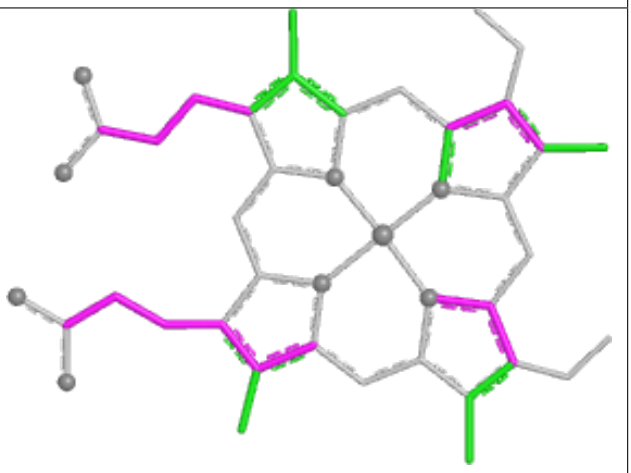

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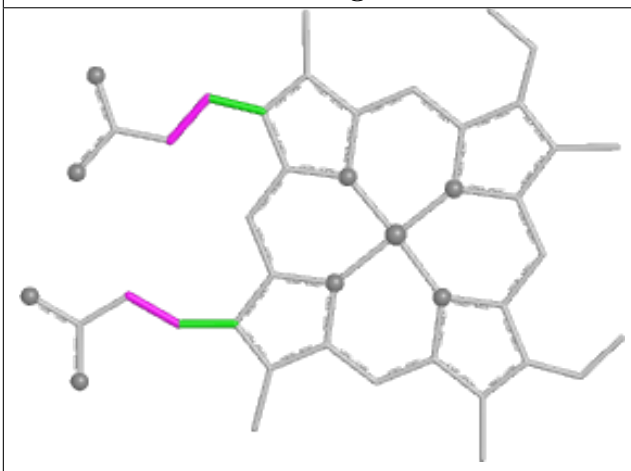

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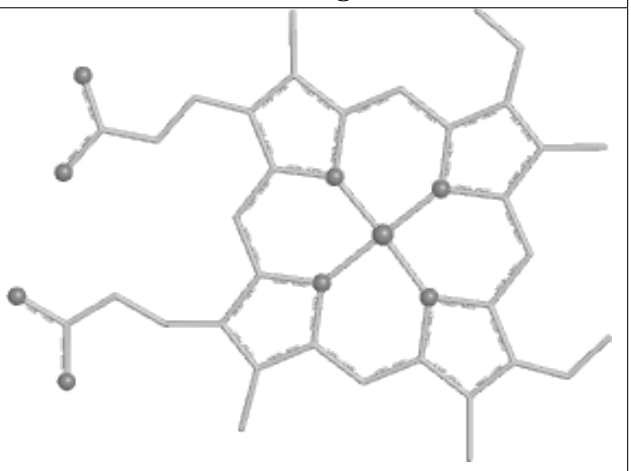
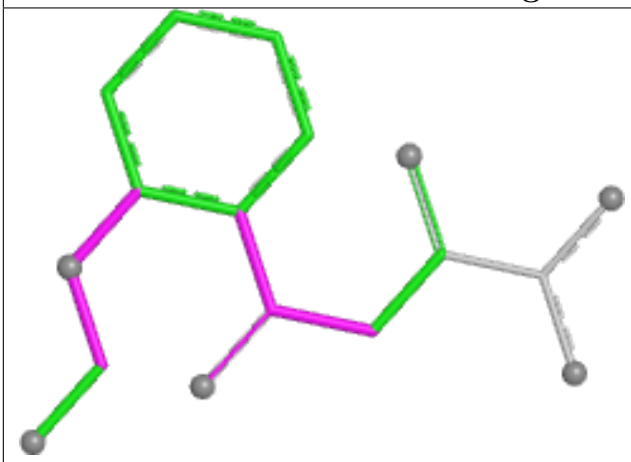
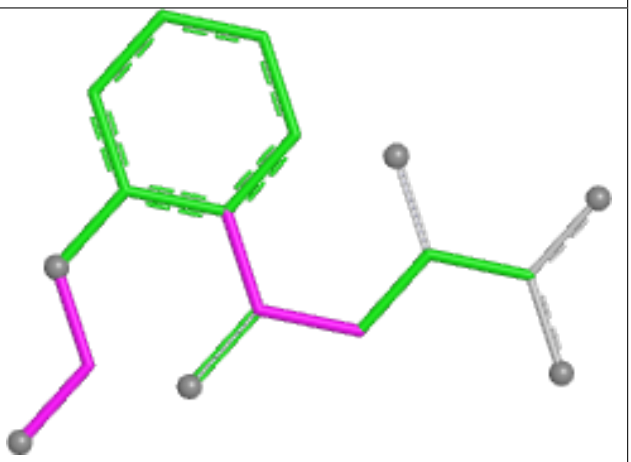


Rings

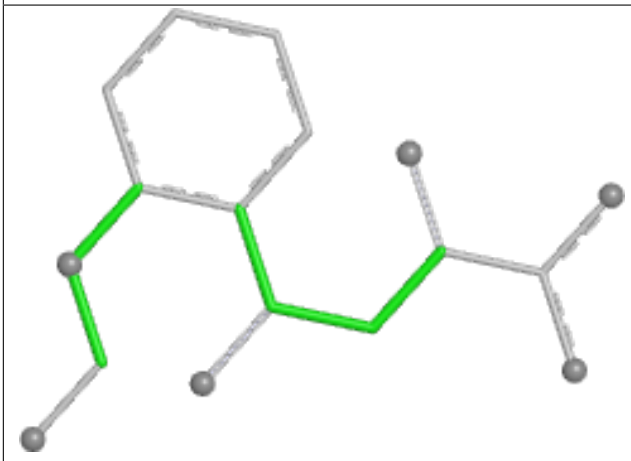
Ligand NFK C 507



Bond lengths



Bond angles



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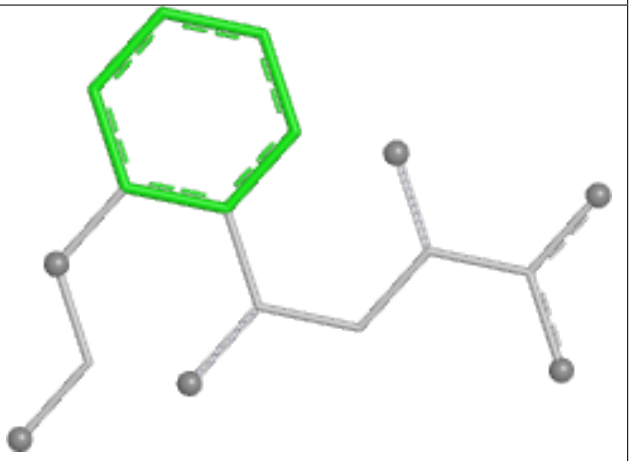
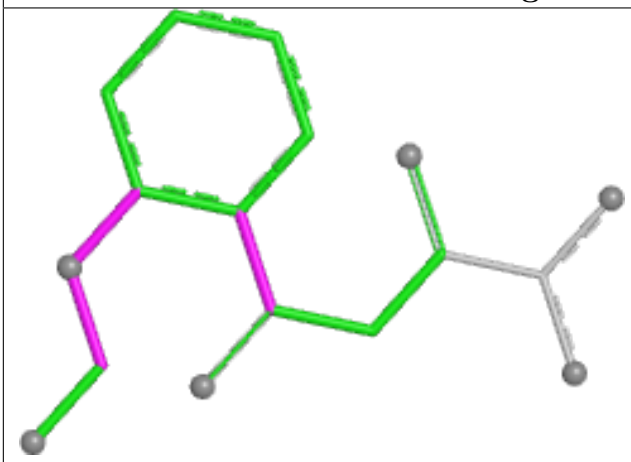


Rings

Ligand NFK A 506



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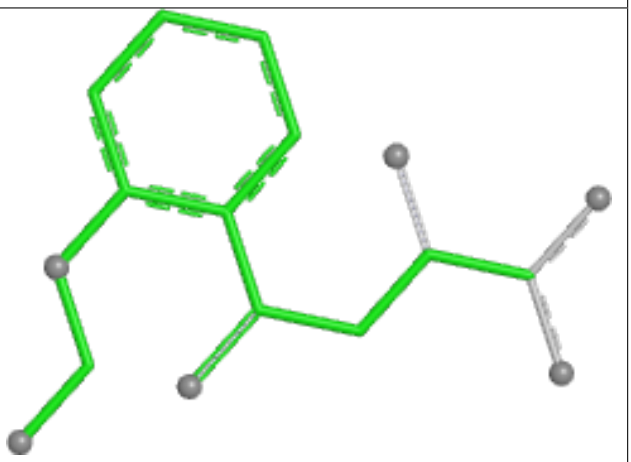
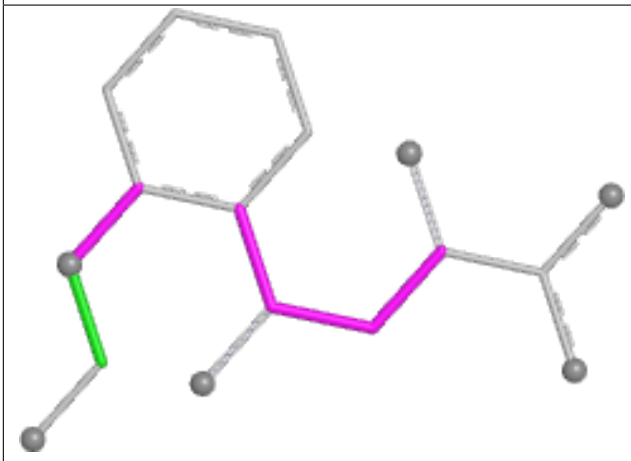


Bond angles



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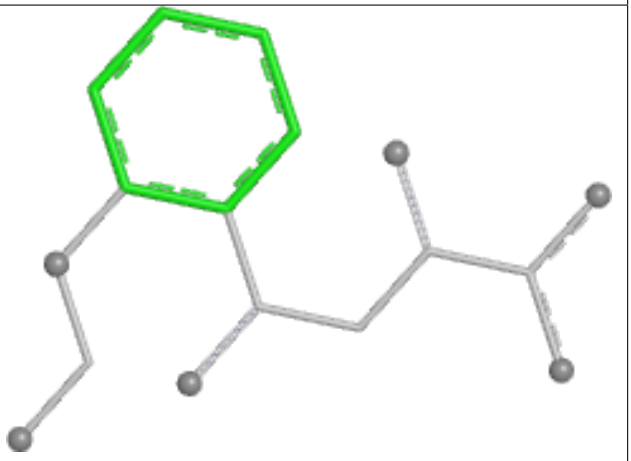
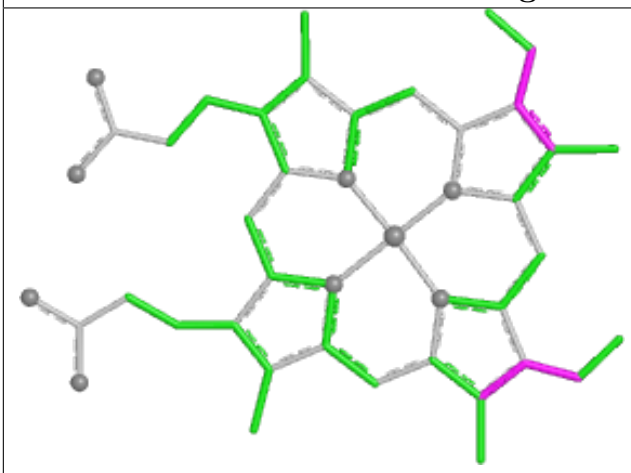
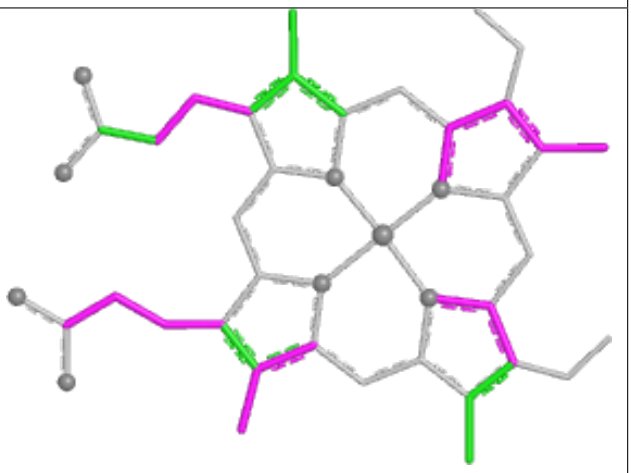


Rings

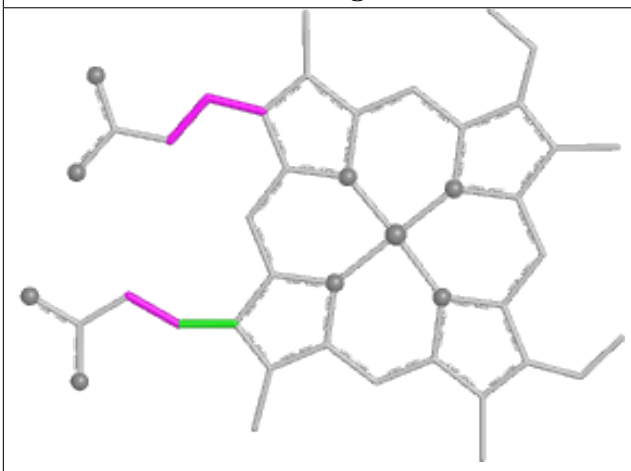
Ligand HEM B 501



Bond lengths



Bond angles



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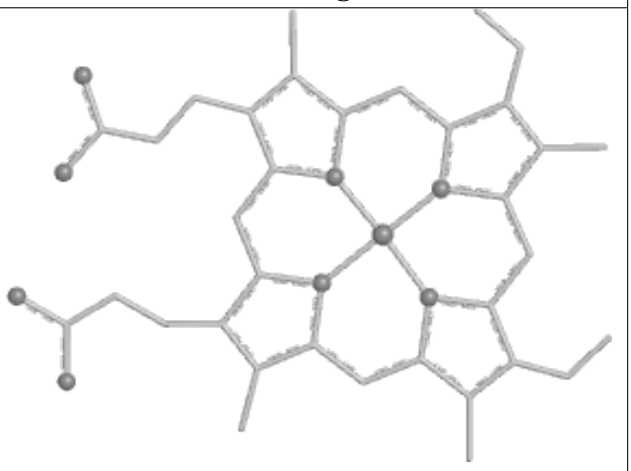
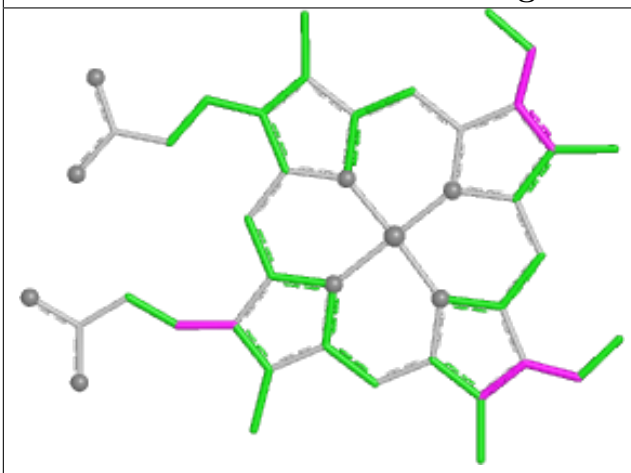


Rings

Ligand HEM D 501



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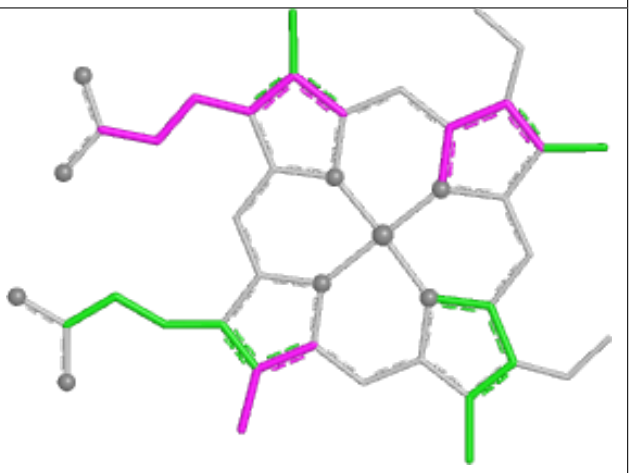
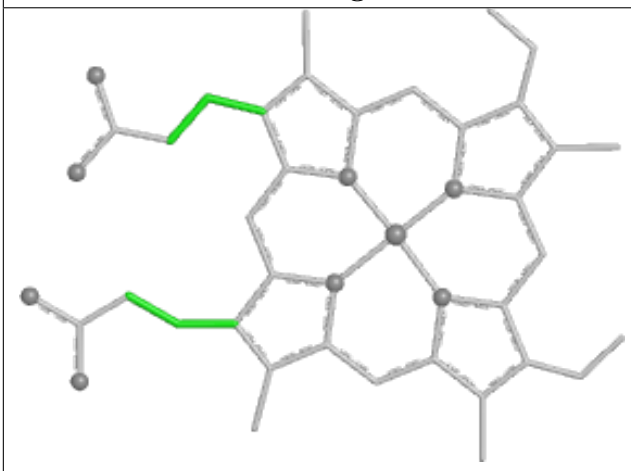
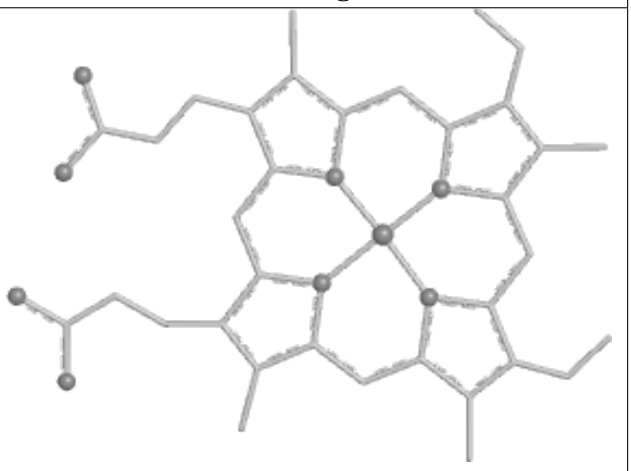


Bond angles

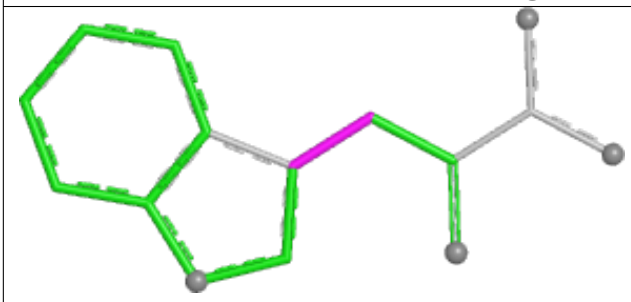


Torsions

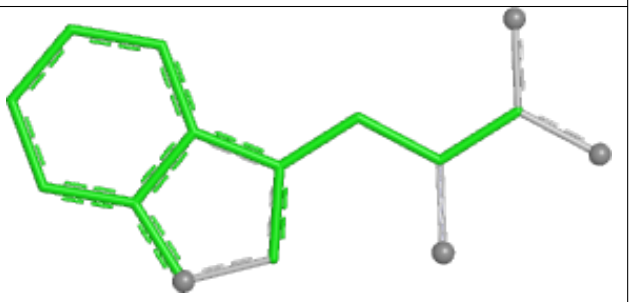


Rings

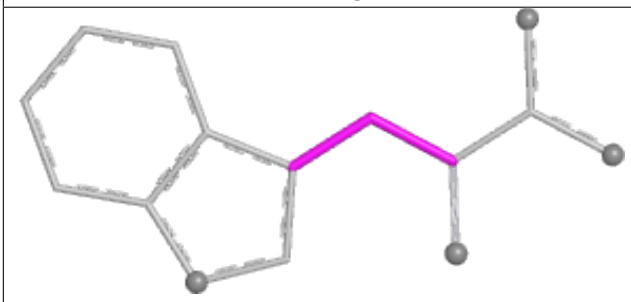
Ligand TRP B 502



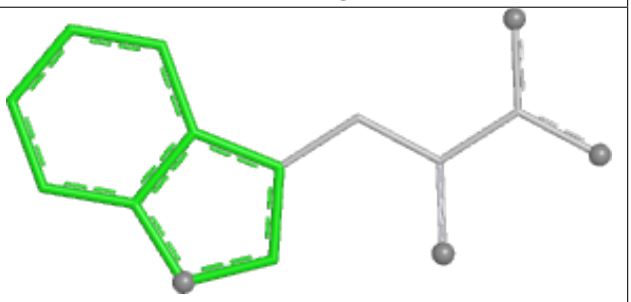
Bond lengths



Bond angles

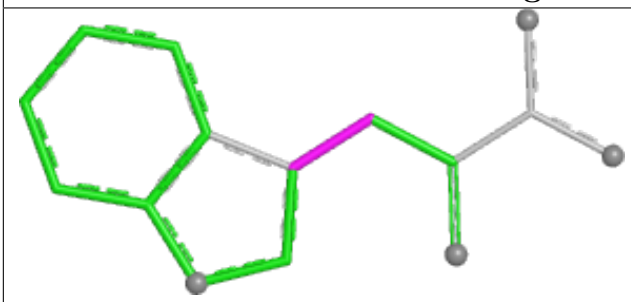


Torsions

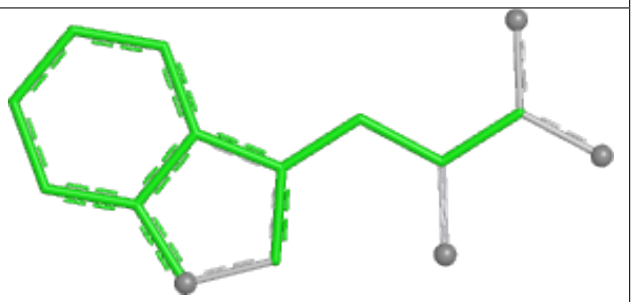


Rings

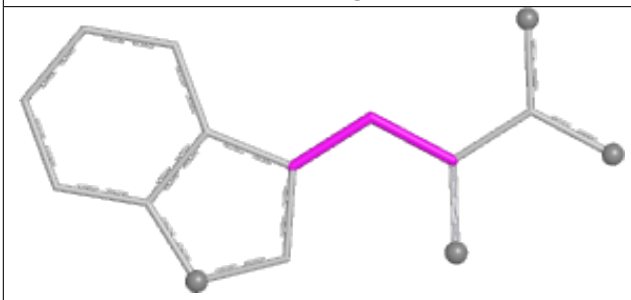
Ligand TRP B 503



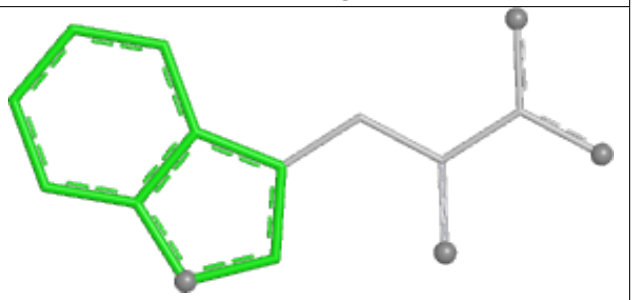
Bond lengths



Bond angles

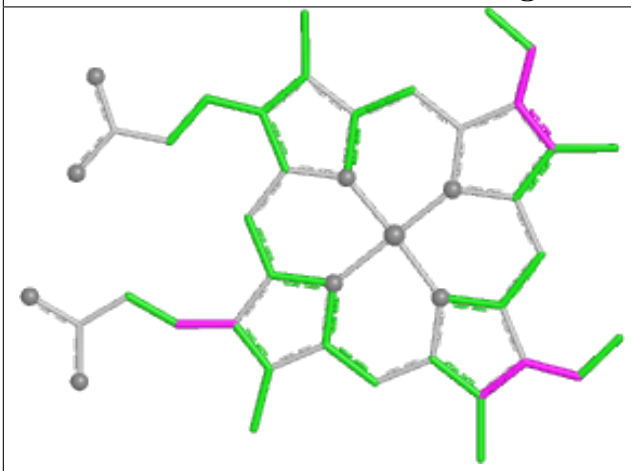


Torsions

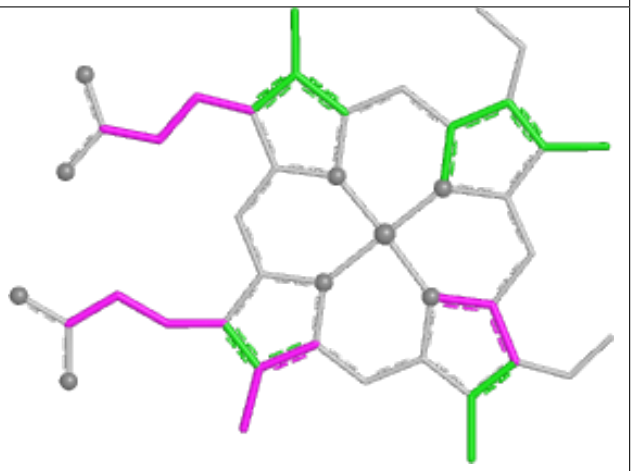


Rings

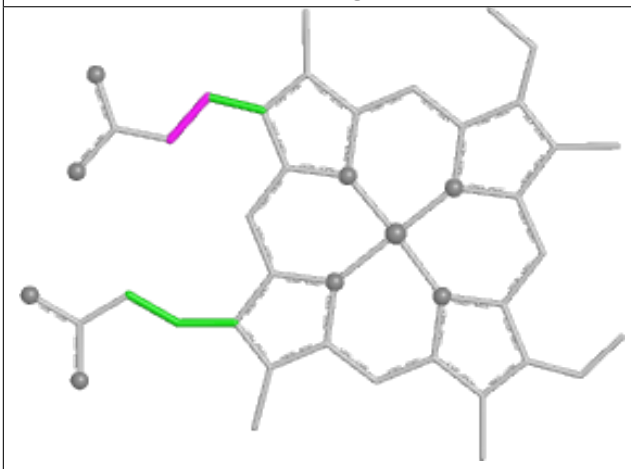
Ligand HEM C 501



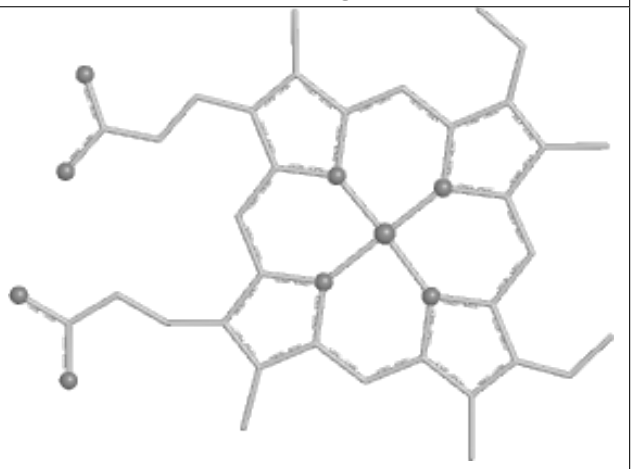
Bond lengths



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, 95^{th} 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	376/405 (92%)	0.44	18 (4%)	30	32	41, 59, 85, 112	0
1	B	379/405 (93%)	0.51	20 (5%)	26	28	42, 59, 94, 121	0
1	C	380/405 (93%)	0.52	20 (5%)	26	28	40, 59, 92, 116	0
1	D	375/405 (92%)	0.49	18 (4%)	30	32	42, 60, 92, 112	0
All	All	1510/1620 (93%)	0.49	76 (5%)	28	30	40, 59, 92, 121	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	378	GLY	11.5
1	C	379	THR	9.7
1	B	376	ALA	9.1
1	C	10	SER	8.9
1	C	11	GLY	7.5
1	A	283	ALA	7.4
1	D	12	SER	7.0
1	A	381	GLY	6.6
1	B	374	LEU	6.6
1	B	283	ALA	6.4
1	B	378	GLY	6.3
1	A	376	ALA	6.3
1	D	379	THR	6.2
1	D	403	GLY	6.2
1	D	382	THR	6.1
1	B	379	THR	6.1
1	C	283	ALA	6.0
1	B	282	THR	5.9
1	B	380	GLY	5.8
1	B	377	LYS	5.7
1	D	13	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	362	PRO	5.4
1	A	380	GLY	5.1
1	B	373	LYS	5.1
1	C	12	SER	4.9
1	D	380	GLY	4.9
1	C	361	GLN	4.8
1	D	282	THR	4.6
1	C	285	GLY	4.5
1	D	284	GLY	4.4
1	C	13	ALA	4.3
1	C	380	GLY	4.3
1	C	403	GLY	4.3
1	C	9	SER	4.2
1	C	282	THR	4.2
1	C	383	ASP	4.2
1	A	382	THR	4.2
1	A	385	MET	4.1
1	B	375	GLU	4.0
1	D	283	ALA	3.9
1	A	379	THR	3.8
1	A	189	GLN	3.7
1	C	284	GLY	3.6
1	B	382	THR	3.4
1	C	328	LEU	3.3
1	B	13	ALA	3.2
1	A	361	GLN	3.1
1	A	282	THR	3.1
1	B	361	GLN	3.1
1	D	285	GLY	3.0
1	A	52	SER	2.8
1	A	377	LYS	2.8
1	A	96	HIS	2.7
1	D	381	GLY	2.6
1	A	97	GLY	2.5
1	C	286	GLY	2.4
1	B	284	GLY	2.4
1	C	96	HIS	2.4
1	D	320	VAL	2.4
1	D	401	LYS	2.4
1	B	355	LEU	2.3
1	B	186	LYS	2.3
1	D	97	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	384	LEU	2.3
1	B	14	ALA	2.2
1	A	328	LEU	2.2
1	D	287	HIS	2.2
1	B	360	GLN	2.1
1	B	385	MET	2.1
1	C	316	VAL	2.1
1	A	378	GLY	2.1
1	D	281	GLN	2.1
1	D	98	ASP	2.1
1	D	95	GLY	2.1
1	A	288	ALA	2.0
1	A	320	VAL	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, 95^{th} 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	GOL	C	506	6/6	0.59	0.30	60,65,67,69	0
3	GOL	C	504	6/6	0.66	0.29	68,76,78,78	0
3	GOL	C	505	6/6	0.69	0.36	48,56,58,60	6
3	GOL	B	505	6/6	0.69	0.23	64,71,73,73	0
6	TRP	B	502	15/15	0.70	0.44	70,79,91,93	15
3	GOL	B	507	6/6	0.71	0.32	52,65,69,71	6
4	NFK	A	506	17/17	0.72	0.47	69,80,91,91	17
4	NFK	C	507	17/17	0.73	0.42	62,70,86,87	17
6	TRP	D	502	15/15	0.74	0.33	56,65,70,72	15
3	GOL	B	504	6/6	0.76	0.32	63,65,72,74	6

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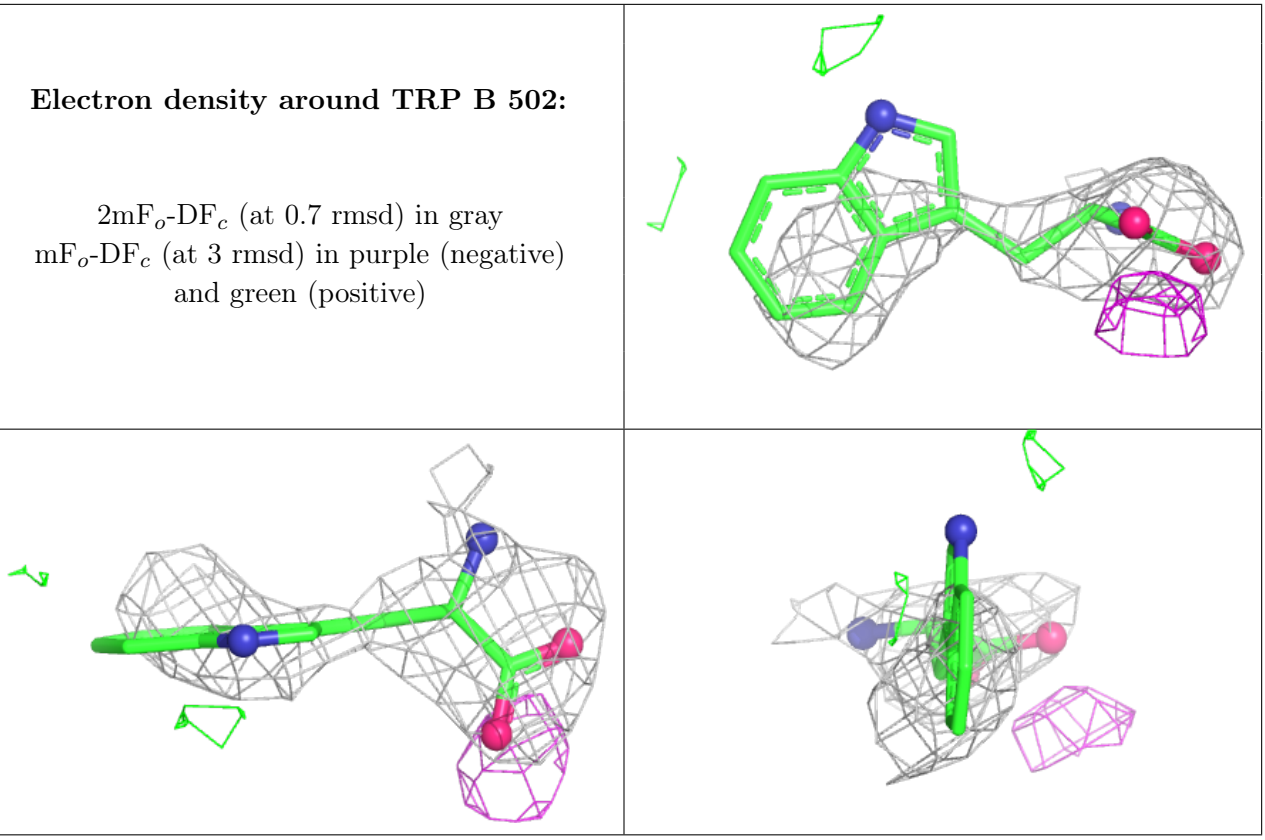
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	503	6/6	0.77	0.17	63,67,70,75	0
5	PO4	B	509	5/5	0.79	0.29	70,70,84,89	5
3	GOL	A	505	6/6	0.79	0.33	61,62,66,67	6
5	PO4	A	507	5/5	0.79	0.35	50,53,59,59	5
3	GOL	D	504	6/6	0.80	0.23	74,76,80,83	0
3	GOL	D	505	6/6	0.82	0.42	66,67,69,74	0
3	GOL	A	503	6/6	0.83	0.48	69,71,75,79	0
3	GOL	A	504	6/6	0.84	0.37	62,64,72,73	0
3	GOL	D	503	6/6	0.85	0.31	58,65,73,75	0
6	TRP	B	503	15/15	0.86	0.34	57,65,70,78	15
3	GOL	A	502	6/6	0.86	0.20	61,63,71,72	0
3	GOL	C	502	6/6	0.88	0.18	56,59,61,70	0
5	PO4	B	508	5/5	0.88	0.23	62,62,65,72	5
3	GOL	B	506	6/6	0.89	0.18	49,55,58,61	6
2	HEM	A	501	43/43	0.92	0.19	53,65,80,92	0
2	HEM	B	501	43/43	0.92	0.21	56,74,86,89	0
2	HEM	C	501	43/43	0.95	0.16	53,64,75,78	0
2	HEM	D	501	43/43	0.96	0.14	56,71,82,87	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.

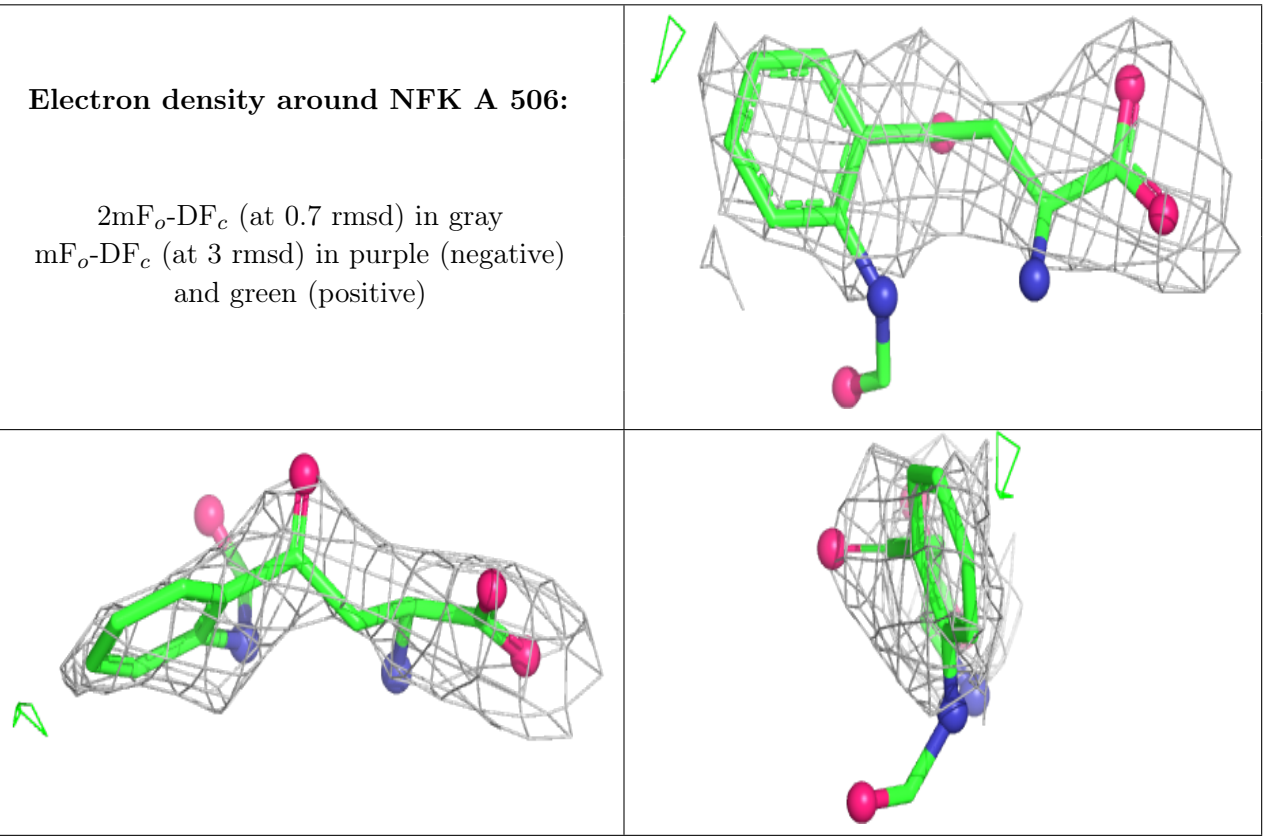
Electron density around TRP B 502:

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



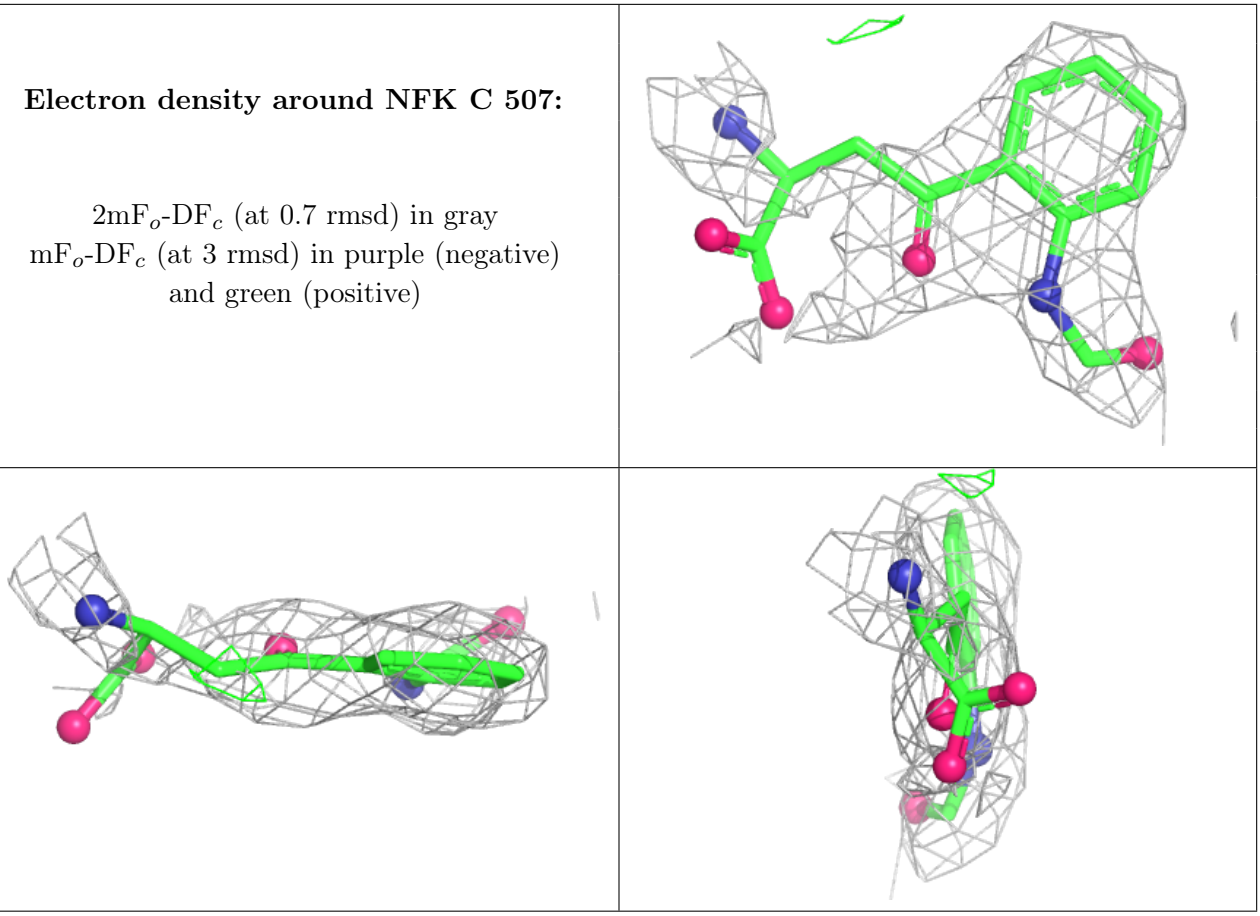
Electron density around NFK A 506:

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



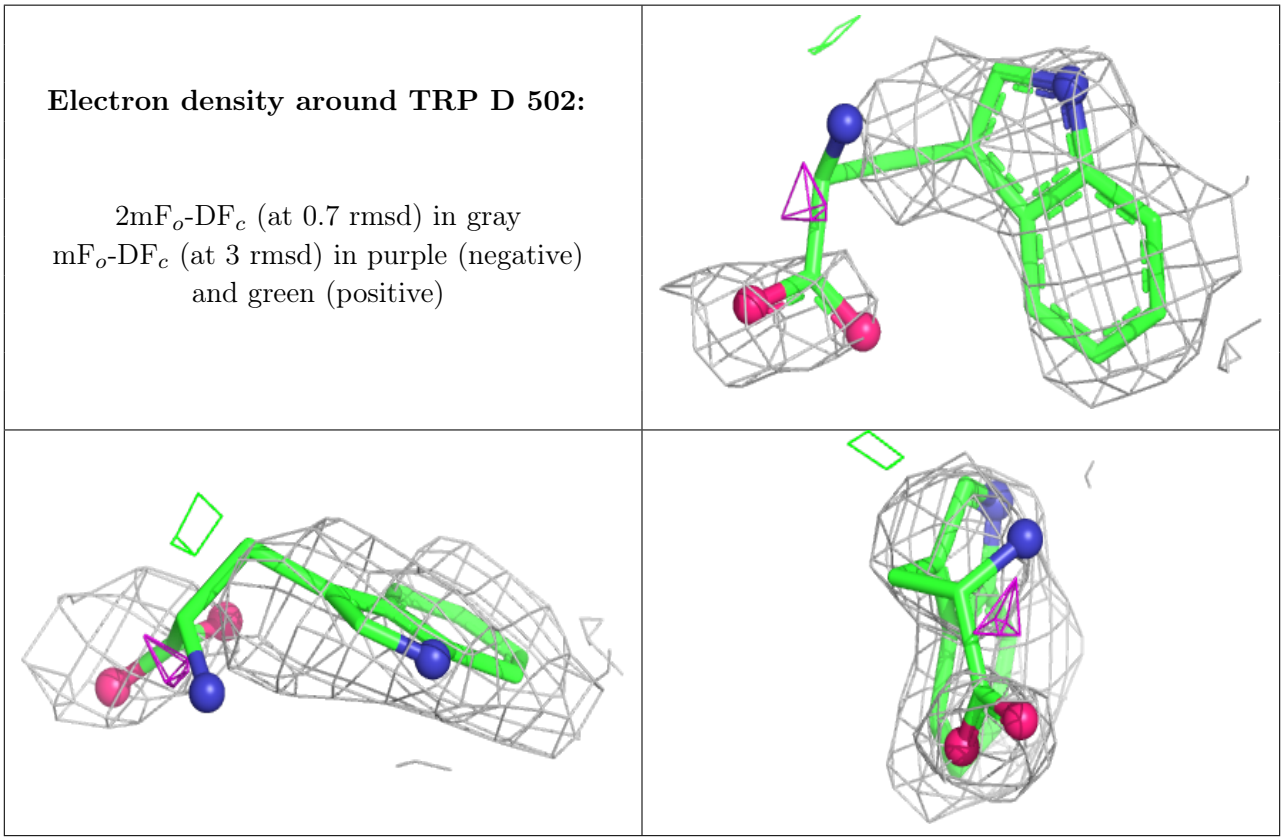
Electron density around NFK C 507:

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



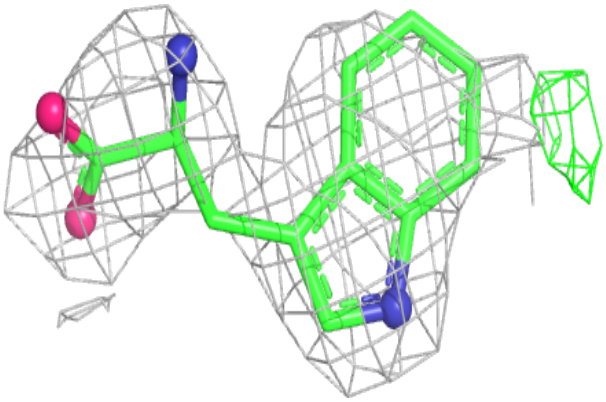
Electron density around TRP D 502:

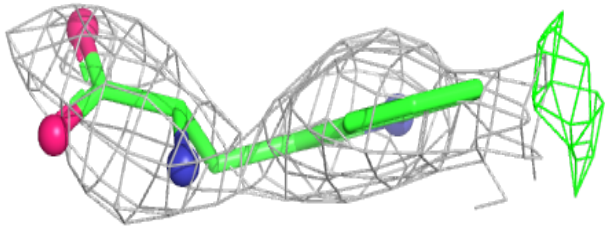
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

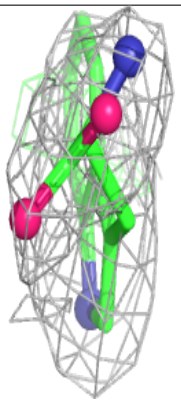


Electron density around TRP B 503:

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

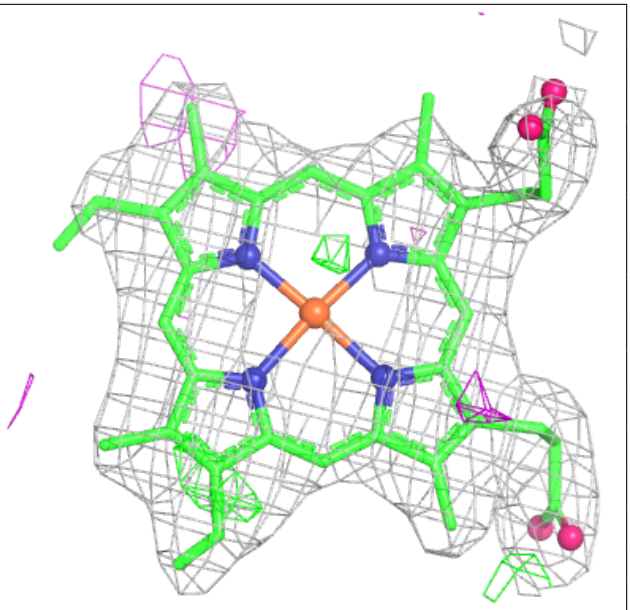


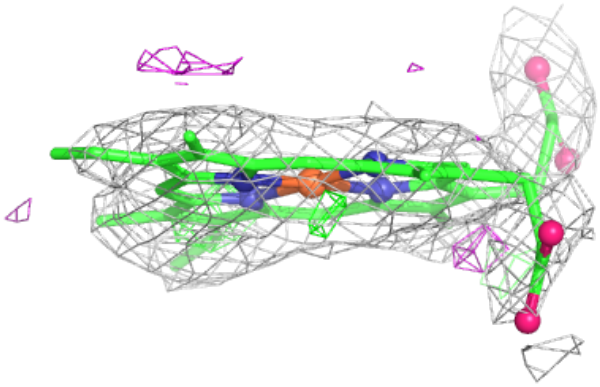


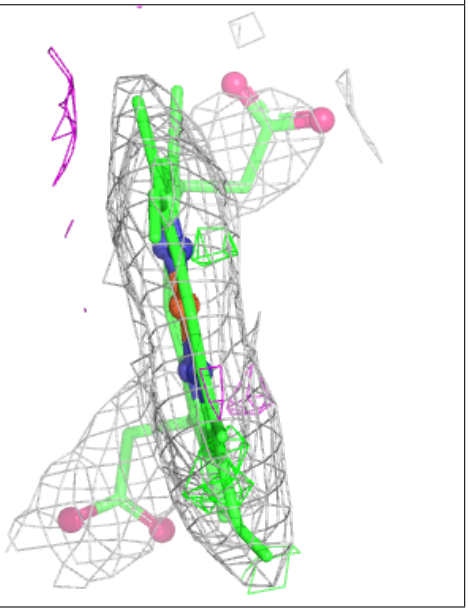


Electron density around HEM A 501:

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

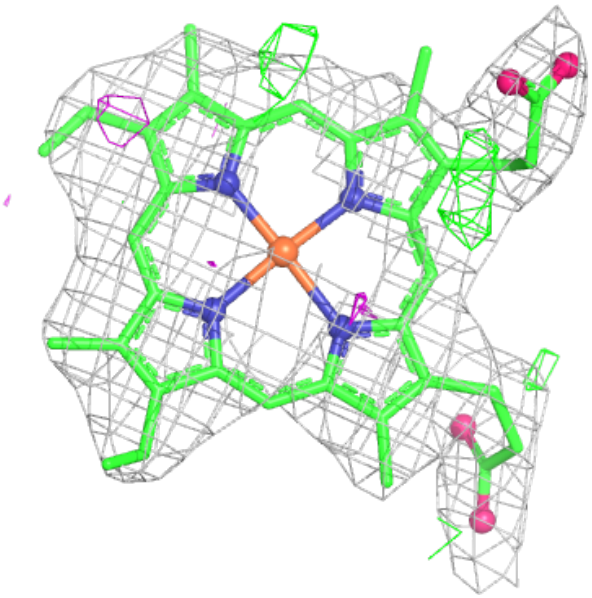


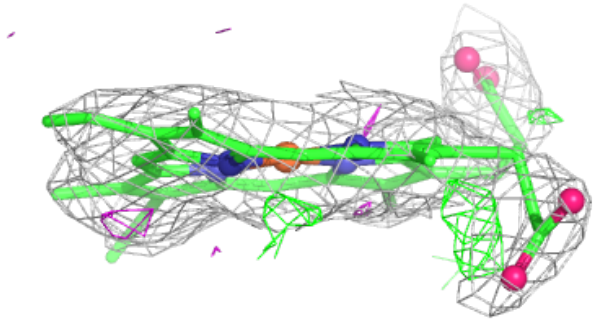


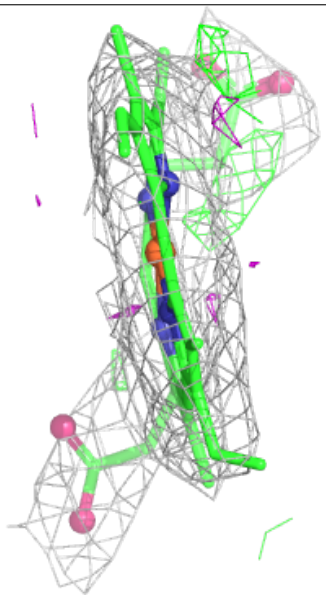


Electron density around HEM B 501:

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

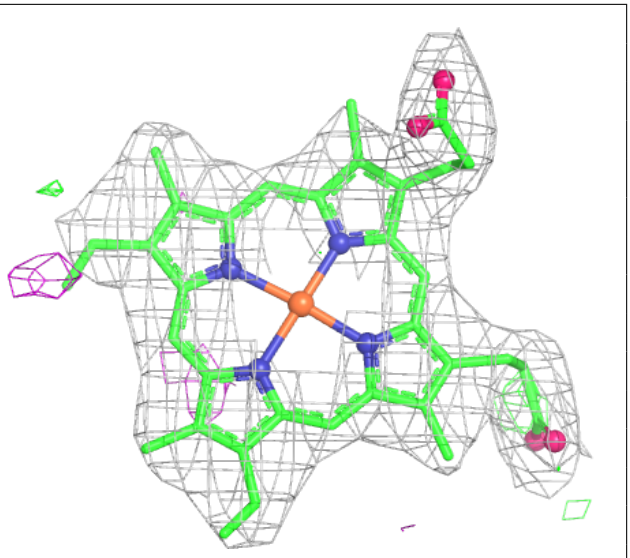


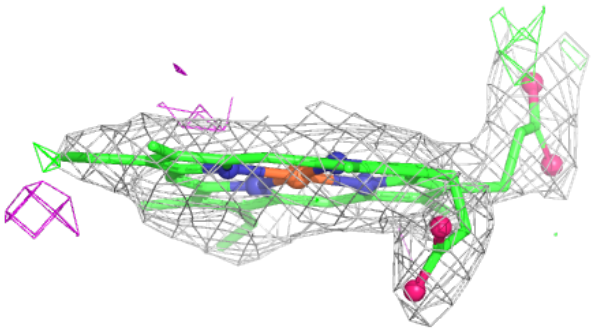




Electron density around HEM C 501:

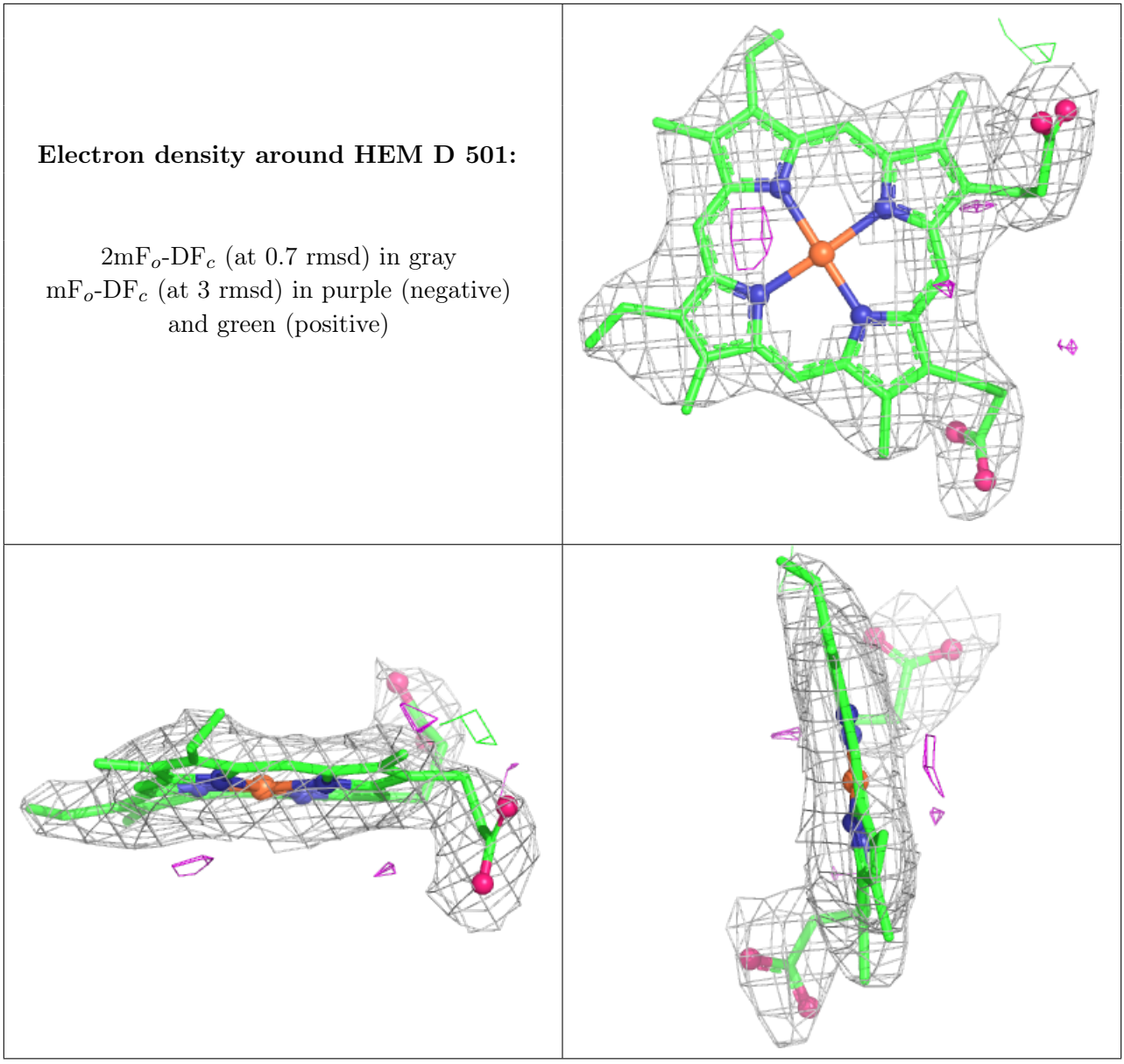
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEM D 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

There are no such residues in this entry.