Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2023 – 12:42 pm GMT

PDB ID	:	7Z2L
Title	:	Crystal structure of L-Kynurenine in the active site of human Indoleamine-2, 3-dioxygenase 1 (hIDO1)
Authors	:	Mirgaux, M.; Wouters, J.
Deposited on	:	2022-02-28
Resolution	:	2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

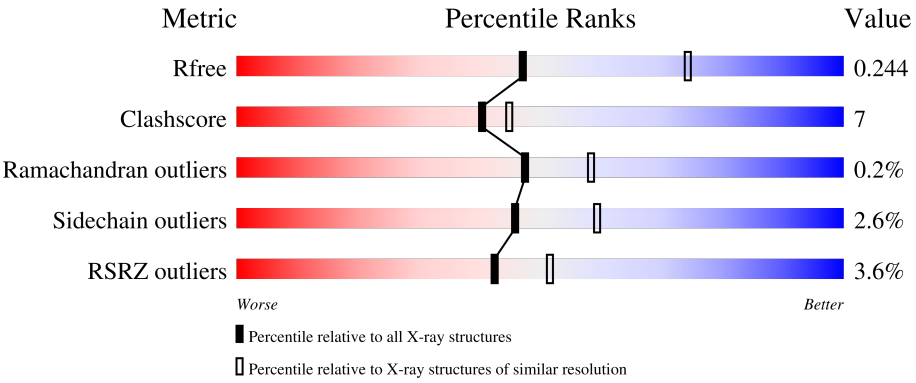
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	% 76% 15% 9%
1	B	405	6% 76% 17% 6%
1	C	405	3% 77% 14% 8%
1	D	405	3% 80% 12% 8%

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	A	505	-	-	-	X
3	GOL	C	505	-	-	-	X
4	KYN	B	502[A]	-	-	-	X
4	KYN	B	502[B]	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13073 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	370	Total	C	N	O	S	0	1	0
			2937	1888	500	531	18			
1	B	381	Total	C	N	O	S	0	3	0
			3012	1932	514	549	17			
1	C	372	Total	C	N	O	S	0	0	0
			2941	1891	501	532	17			
1	D	373	Total	C	N	O	S	0	0	0
			2946	1893	502	534	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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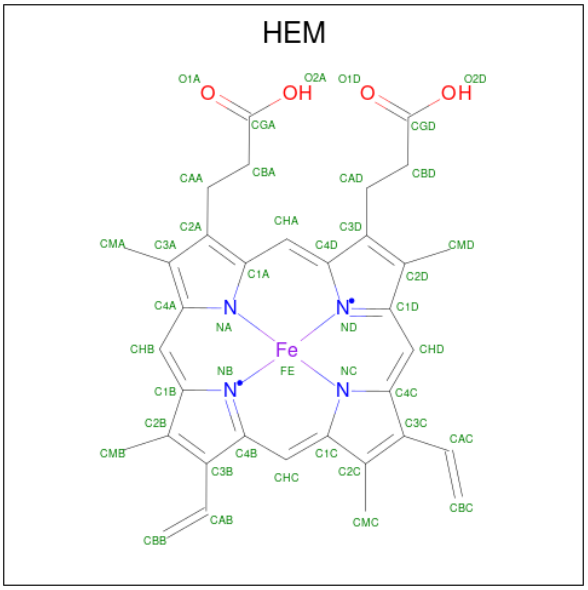
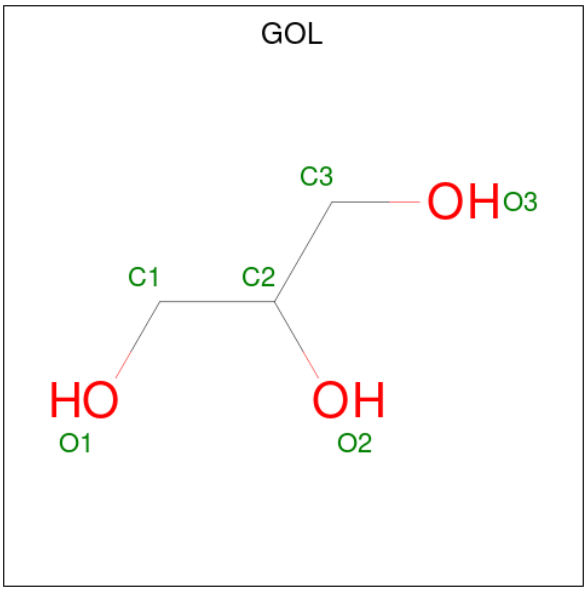
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
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	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	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		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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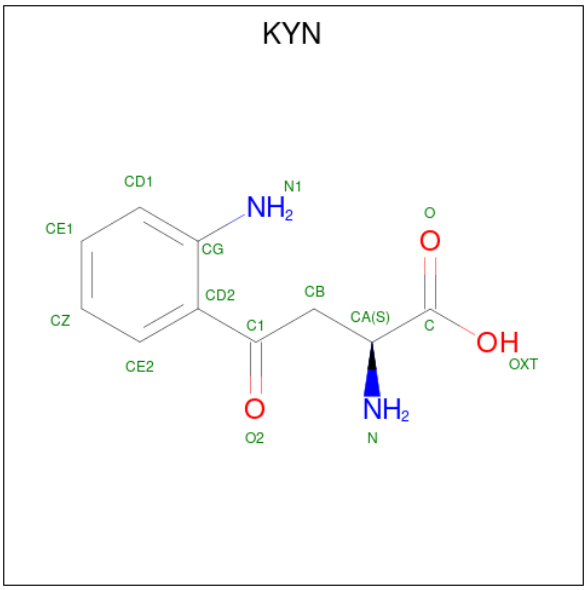
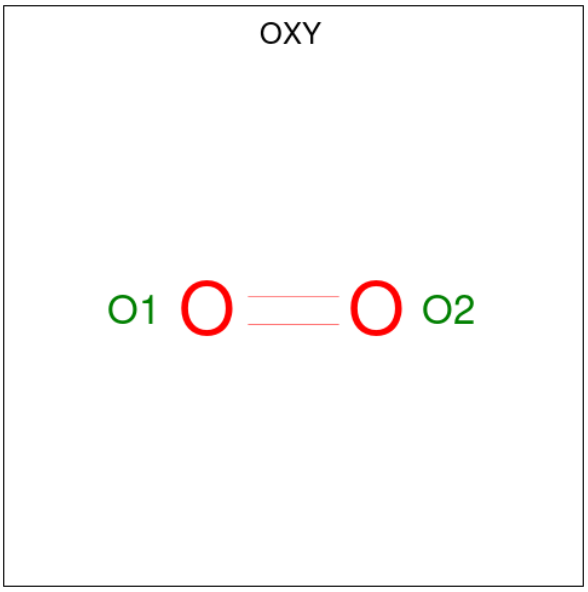
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is (2S)-2-amino-4-(2-aminophenyl)-4-oxobutanoic acid (three-letter code: KYN) (formula: $C_{10}H_{12}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 10 2 3	0	0
4	B	1	Total C N O 22 16 3 3	0	1
4	B	1	Total C N O 15 10 2 3	0	0
4	B	1	Total C N O 15 10 2 3	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



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

- Molecule 6 is water.

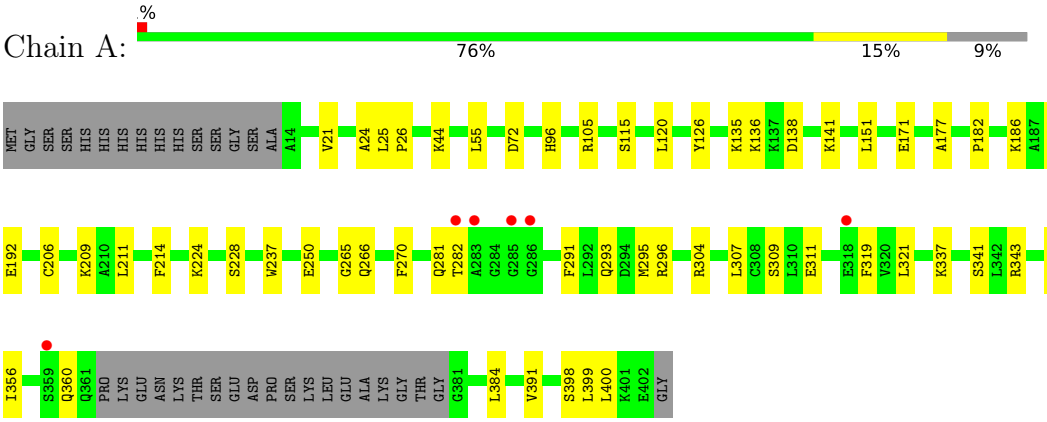
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	219	Total O 219 219	0	0
6	B	214	Total O 214 214	0	0
6	C	225	Total O 225 225	0	0
6	D	246	Total O 246 246	0	0

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.

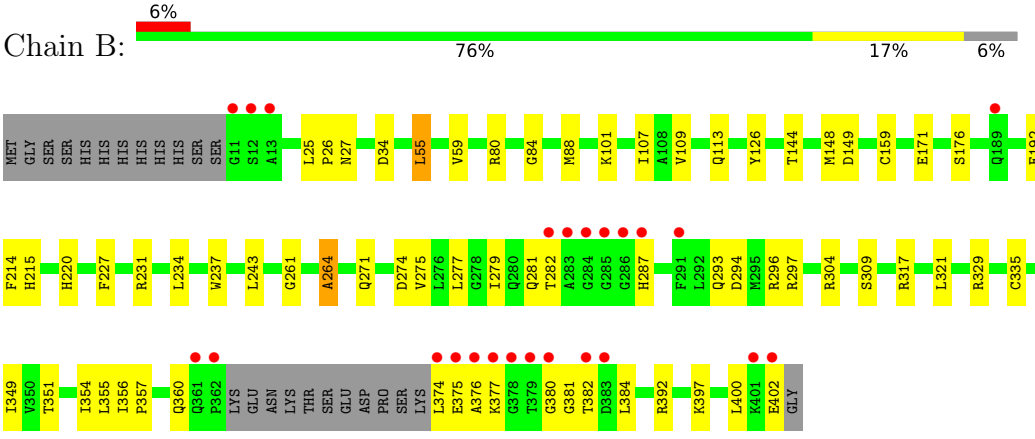
• Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain A:



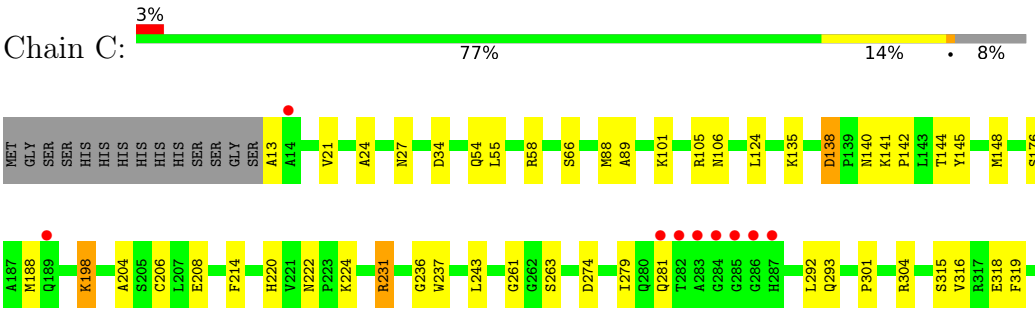
• Molecule 1: Indoleamine 2,3-dioxygenase 1

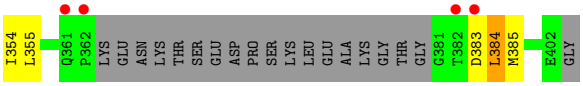
Chain B:



• 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	81.00Å 116.28Å 217.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 2.56 49.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.23-2.56) 99.2 (49.00-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.244 0.181 , 0.244	Depositor DCC
R_{free} test set	3316 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13073	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 46.95 % 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 1.0640e-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

5.1 Standard geometry

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

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	0.42	0/3005	0.61	2/4067 (0.0%)
1	B	0.41	0/3081	0.60	1/4170 (0.0%)
1	C	0.43	0/3010	0.59	0/4076
1	D	0.45	0/3015	0.59	1/4081 (0.0%)
All	All	0.43	0/12111	0.60	4/16394 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	LEU	CA-CB-CG	-5.89	101.75	115.30
1	B	55	LEU	CA-CB-CG	-5.49	102.67	115.30
1	A	138	ASP	CB-CG-OD1	5.32	123.08	118.30
1	D	265	GLY	N-CA-C	-5.26	99.94	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2937	0	2943	38	0
1	B	3012	0	3015	47	0
1	C	2941	0	2947	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2946	0	2950	30	0
2	A	43	0	30	7	0
2	B	43	0	30	7	0
2	C	43	0	30	4	0
2	D	43	0	30	7	0
3	A	30	0	40	1	0
3	B	12	0	16	1	0
3	C	24	0	32	7	0
3	D	24	0	32	0	0
4	A	15	0	11	3	0
4	B	52	0	34	8	0
5	B	2	0	0	1	0
5	C	2	0	0	0	0
6	A	219	0	0	2	0
6	B	214	0	0	6	0
6	C	225	0	0	11	0
6	D	246	0	0	6	0
All	All	13073	0	12140	175	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 7.

All (175) 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	1.54	0.89
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.55	0.86
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.56	0.86
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.58	0.85
1:D:354:ILE:HG13	2:D:501:HEM:HBC1	1.65	0.78
2:B:501:HEM:HBC2	2:B:501:HEM:HHD	1.67	0.75
1:C:354:ILE:HG13	2:C:501:HEM:HBC1	1.70	0.74
1:D:212:GLN:HA	1:D:215:HIS:HD2	1.51	0.74
1:D:57:GLU:HG2	1:D:61:LYS:HE3	1.72	0.72
4:B:505:KYN:N	6:B:603:HOH:O	2.24	0.69
1:B:355:LEU:HD13	1:B:374:LEU:HB2	1.73	0.69
2:D:501:HEM:HBC2	2:D:501:HEM:HHD	1.75	0.68
1:C:315:SER:HB3	1:C:318:GLU:HB2	1.76	0.67
1:B:227:PHE:O	1:B:231:ARG:NH1	2.27	0.67
1:A:182:PRO:HG3	3:A:504:GOL:H32	1.79	0.65
1:B:126:TYR:CD1	1:B:264[B]:ALA:HA	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLY:HA2	2:D:501:HEM:C2A	2.31	0.64
1:D:293:GLN:OE1	6:D:601:HOH:O	2.15	0.64
1:A:224:LYS:HE2	1:A:224:LYS:H	1.63	0.63
1:A:296:ARG:O	1:A:304:ARG:HD2	1.98	0.63
1:C:236:GLY:N	1:C:261:GLY:HA3	2.14	0.63
1:C:355:LEU:HD11	1:C:385:MET:SD	2.39	0.62
1:B:271:GLN:HA	1:B:274:ASP:HB2	1.81	0.62
1:B:171:GLU:HG3	6:B:713:HOH:O	2.00	0.62
1:C:88:MET:HE3	1:C:124:LEU:H	1.64	0.62
2:C:501:HEM:HBC2	2:C:501:HEM:HHD	1.82	0.61
4:B:503:KYN:O2	6:B:601:HOH:O	2.16	0.61
1:C:138:ASP:HB3	1:C:141:LYS:HD3	1.82	0.61
1:B:27:ASN:ND2	6:B:604:HOH:O	2.27	0.61
1:D:351:THR:HA	1:D:355:LEU:HB2	1.81	0.61
1:C:198:LYS:NZ	6:C:602:HOH:O	2.29	0.60
1:A:356:ILE:O	1:A:360:GLN:HG3	2.02	0.60
1:C:34:ASP:OD1	3:C:506:GOL:H11	2.02	0.59
1:A:96:HIS:ND1	6:A:605:HOH:O	2.31	0.58
1:B:261:GLY:H	3:B:504:GOL:H11	1.69	0.57
1:D:119:GLU:O	1:D:304:ARG:NH2	2.37	0.57
1:B:282:THR:OG1	1:B:293:GLN:HG2	2.04	0.57
1:A:171:GLU:HG3	6:A:691:HOH:O	2.05	0.57
1:A:282:THR:HG23	1:A:293:GLN:HE21	1.70	0.57
1:D:171:GLU:HG3	6:D:677:HOH:O	2.03	0.56
1:D:275:VAL:HG13	1:D:311:GLU:HG3	1.86	0.56
1:C:301:PRO:HB3	1:C:304:ARG:NH2	2.22	0.55
1:C:204:ALA:O	1:C:208:GLU:HG3	2.06	0.55
1:D:72:ASP:O	1:D:76:GLN:HG3	2.06	0.55
1:D:101:LYS:HD3	6:D:783:HOH:O	2.06	0.54
1:C:182:PRO:HG3	3:C:505:GOL:H31	1.89	0.54
1:A:190:MET:HB3	1:A:192:GLU:HG2	1.90	0.54
1:C:138:ASP:OD1	1:C:140:ASN:N	2.29	0.54
1:C:220:HIS:HD1	3:C:502:GOL:HO1	1.55	0.53
4:B:505:KYN:HN1A	4:B:505:KYN:HB	1.72	0.53
1:A:321:LEU:HD21	1:A:400:LEU:HD22	1.90	0.53
1:C:385:MET:HE2	6:C:730:HOH:O	2.08	0.53
1:D:350:VAL:HG11	1:D:384:LEU:HD21	1.90	0.53
1:B:357:PRO:HA	1:B:360:GLN:HG3	1.91	0.53
1:A:337:LYS:HG3	1:A:399:LEU:HD21	1.90	0.53
1:D:389:LYS:NZ	6:D:606:HOH:O	2.39	0.52
1:D:399:LEU:O	1:D:401:LYS:NZ	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:THR:O	1:B:356:ILE:HG12	2.10	0.52
1:B:376:ALA:HB3	1:B:380:GLY:HA3	1.90	0.52
1:C:274:ASP:OD2	1:C:281:GLN:HG3	2.10	0.51
1:C:141:LYS:HB3	1:C:142:PRO:HD2	1.92	0.51
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	1.93	0.51
1:D:84:GLY:O	1:D:88:MET:HG2	2.11	0.50
1:A:188:MET:HG2	1:A:319:PHE:CD2	2.46	0.50
2:B:501:HEM:HMA1	2:B:501:HEM:O1A	2.12	0.50
1:D:138:ASP:HB3	1:D:141:LYS:HG3	1.93	0.50
1:B:25:LEU:HD12	1:B:26:PRO:HD2	1.93	0.50
1:A:44:LYS:HA	4:A:506:KYN:HZ	1.93	0.50
1:A:211:LEU:HD22	1:A:341:SER:HB3	1.94	0.50
1:B:264[B]:ALA:HB3	5:B:506[B]:OXY:O2	2.11	0.50
1:C:145:TYR:OH	3:C:502:GOL:H2	2.12	0.49
1:B:317:ARG:O	1:B:321:LEU:HB2	2.13	0.48
1:D:262:GLY:HA2	1:D:266:GLN:NE2	2.28	0.48
1:A:21:VAL:HB	1:A:24:ALA:HB3	1.94	0.48
1:B:296:ARG:O	1:B:304:ARG:HD3	2.13	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:CHD	2.41	0.48
1:C:186:LYS:NZ	6:C:601:HOH:O	2.22	0.47
1:B:329:ARG:NE	1:B:402:GLU:HB3	2.29	0.47
1:C:105:ARG:HD2	6:C:790:HOH:O	2.13	0.47
1:A:354:ILE:HG12	2:A:501:HEM:HBC1	1.97	0.46
1:C:293:GLN:HG3	6:C:711:HOH:O	2.16	0.46
1:B:234:LEU:HB2	4:B:502[B]:KYN:HD1	1.95	0.46
1:A:351:THR:HA	1:A:355:LEU:HB2	1.96	0.46
1:C:13:ALA:HB2	3:C:505:GOL:O1	2.16	0.46
1:D:262:GLY:HA2	1:D:266:GLN:HE22	1.81	0.46
1:C:21:VAL:HB	1:C:24:ALA:HB3	1.98	0.45
1:D:64:MET:HB2	1:D:106:ASN:OD1	2.17	0.45
1:C:325:ASP:HB3	1:C:328:LEU:HB2	1.98	0.45
1:D:76:GLN:HB3	1:D:114:LEU:HD11	1.97	0.45
1:A:25:LEU:HD12	1:A:26:PRO:HD2	1.98	0.45
1:D:25:LEU:HD12	1:D:26:PRO:HD2	1.99	0.45
1:B:321:LEU:HD12	1:B:321:LEU:HA	1.78	0.45
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.77	0.45
1:C:279:ILE:HG22	1:C:281:GLN:HG2	1.99	0.45
1:A:295[B]:MET:HE2	1:A:295[B]:MET:HB2	1.88	0.44
1:C:188:MET:SD	1:C:316:VAL:HG22	2.57	0.44
1:C:138:ASP:OD1	1:C:138:ASP:C	2.54	0.44
1:B:215:HIS:HD2	6:B:625:HOH:O	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LYS:HE2	1:A:141:LYS:O	2.18	0.44
1:B:397:LYS:HB2	1:B:397:LYS:HE2	1.81	0.44
2:C:501:HEM:HBC2	2:C:501:HEM:CHD	2.47	0.44
1:D:274:ASP:OD2	1:D:281:GLN:HG3	2.18	0.44
1:C:144:THR:O	1:C:148:MET:HG3	2.18	0.44
1:C:188:MET:HE3	1:C:319:PHE:HB2	1.98	0.44
1:C:292:LEU:HD23	6:C:780:HOH:O	2.17	0.44
1:A:151:LEU:O	4:A:506:KYN:HE2	2.17	0.44
2:D:501:HEM:HBB2	2:D:501:HEM:CHC	2.36	0.44
1:B:192:GLU:OE2	6:B:602:HOH:O	2.21	0.44
1:D:271:GLN:HA	1:D:274:ASP:HB2	1.98	0.44
2:D:501:HEM:HBC2	2:D:501:HEM:CHD	2.41	0.44
1:B:274:ASP:OD2	1:B:281:GLN:HG3	2.18	0.44
1:A:135:LYS:HD3	4:A:506:KYN:O	2.17	0.44
1:D:356:ILE:HB	1:D:357:PRO:HD3	2.00	0.44
1:D:339:LEU:HD12	1:D:339:LEU:HA	1.77	0.43
1:C:222:ASN:ND2	6:C:605:HOH:O	2.41	0.43
1:A:265:GLY:HA2	2:A:501:HEM:C1A	2.54	0.43
1:A:384:LEU:HD11	2:A:501:HEM:HAD1	2.00	0.43
1:B:384:LEU:HD11	2:B:501:HEM:HAD1	2.00	0.43
1:C:176:SER:HB3	1:C:206:CYS:SG	2.58	0.43
1:C:27:ASN:ND2	6:C:614:HOH:O	2.51	0.43
1:B:34:ASP:N	1:B:34:ASP:OD1	2.52	0.43
1:C:54:GLN:O	1:C:58:ARG:HG2	2.19	0.43
1:C:101:LYS:HB2	1:C:101:LYS:HE2	1.46	0.43
1:B:392:ARG:HE	1:B:392:ARG:HB3	1.71	0.43
1:C:231:ARG:HD2	6:C:771:HOH:O	2.17	0.43
1:D:279:ILE:HD13	1:D:395:THR:HG23	2.01	0.43
1:B:321:LEU:HD13	1:B:400:LEU:HD22	2.01	0.42
1:B:109:VAL:O	1:B:113:GLN:HG3	2.20	0.42
1:C:55:LEU:HD22	1:C:89:ALA:HB1	2.01	0.42
1:A:115:SER:HB3	1:A:120:LEU:O	2.20	0.42
1:B:345:TYR:CE2	1:B:349:ILE:HD11	2.54	0.42
3:C:506:GOL:H32	6:C:766:HOH:O	2.19	0.42
1:A:270:PHE:HB3	1:A:343:ARG:NH2	2.34	0.42
1:B:59:VAL:HG13	1:B:107:ILE:HG13	2.01	0.42
1:B:101:LYS:HG2	1:B:243:LEU:CD2	2.50	0.42
1:A:190:MET:HA	1:A:190:MET:HE2	2.00	0.42
1:B:294:ASP:O	1:B:297:ARG:HB2	2.19	0.42
1:C:301:PRO:HB3	1:C:304:ARG:HH21	1.85	0.42
4:B:505:KYN:HD1	1:D:117:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:501:HEM:HHC	2:D:501:HEM:CBB	2.40	0.42
1:A:224:LYS:O	1:A:228:SER:HB2	2.20	0.42
1:A:281:GLN:NE2	1:A:391:VAL:HG13	2.35	0.42
1:A:291:PHE:CZ	2:A:501:HEM:HBD1	2.55	0.42
1:A:384:LEU:HD21	2:A:501:HEM:HMD2	2.01	0.41
1:B:271:GLN:O	1:B:275:VAL:HG23	2.20	0.41
1:B:354:ILE:HG12	2:B:501:HEM:CBC	2.50	0.41
1:A:72:ASP:N	1:A:72:ASP:OD1	2.54	0.41
1:A:209:LYS:HB3	1:A:209:LYS:HE2	1.84	0.41
1:B:356:ILE:HG12	1:B:356:ILE:H	1.74	0.41
1:B:400:LEU:O	1:B:402:GLU:HB2	2.20	0.41
1:B:144:THR:O	1:B:148:MET:HG3	2.20	0.41
1:B:159:CYS:SG	4:B:503:KYN:HB	2.60	0.41
1:B:374:LEU:HB3	1:B:375:GLU:H	1.64	0.41
1:A:188:MET:HG2	1:A:319:PHE:CG	2.56	0.41
1:B:176:SER:HB3	1:B:206:CYS:SG	2.61	0.41
1:B:220:HIS:HA	4:B:503:KYN:HE2	2.02	0.41
1:D:401:LYS:NZ	6:D:602:HOH:O	2.33	0.41
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.83	0.41
2:B:501:HEM:HBB2	2:B:501:HEM:CHC	2.35	0.41
1:A:126:TYR:HB2	1:A:266:GLN:HB2	2.02	0.41
1:B:84:GLY:O	1:B:88:MET:HG2	2.20	0.41
1:C:106:ASN:HB2	6:C:663:HOH:O	2.21	0.41
1:C:188:MET:HE3	1:C:319:PHE:CB	2.50	0.41
1:A:105:ARG:N	1:A:250:GLU:OE2	2.44	0.41
1:A:291:PHE:CE1	1:A:295[B]:MET:SD	3.14	0.41
1:A:307:LEU:O	1:A:311:GLU:HG3	2.21	0.41
1:B:55:LEU:O	1:B:55:LEU:HG	2.14	0.41
1:B:277:LEU:HD11	1:B:335:CYS:HB3	2.03	0.40
1:D:58:ARG:HD2	6:D:604:HOH:O	2.20	0.40
1:C:384:LEU:HD23	1:C:385:MET:N	2.36	0.40
1:C:182:PRO:CG	3:C:505:GOL:H31	2.51	0.40
1:A:177:ALA:HB2	1:A:206:CYS:HB2	2.03	0.40
1:B:277:LEU:HB2	1:B:279:ILE:HD12	2.03	0.40
4:B:505:KYN:HD1	1:D:76:GLN:HE22	1.86	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	367/405 (91%)	352 (96%)	15 (4%)	0	100	100
1	B	380/405 (94%)	360 (95%)	17 (4%)	3 (1%)	19	27
1	C	368/405 (91%)	350 (95%)	17 (5%)	1 (0%)	41	50
1	D	369/405 (91%)	354 (96%)	15 (4%)	0	100	100
All	All	1484/1620 (92%)	1416 (95%)	64 (4%)	4 (0%)	47	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	263	SER
1	B	264[A]	ALA
1	B	264[B]	ALA
1	B	381	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	319/346 (92%)	313 (98%)	6 (2%)	57	71
1	B	325/346 (94%)	316 (97%)	9 (3%)	43	56
1	C	319/346 (92%)	308 (97%)	11 (3%)	37	49
1	D	319/346 (92%)	312 (98%)	7 (2%)	52	66
All	All	1282/1384 (93%)	1249 (97%)	33 (3%)	46	59

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	LYS
1	A	189	GLN
1	A	214	PHE
1	A	237	TRP
1	A	309	SER
1	A	398	SER
1	B	80	ARG
1	B	149	ASP
1	B	205	SER
1	B	214	PHE
1	B	237	TRP
1	B	287	HIS
1	B	309	SER
1	B	377	LYS
1	B	382	THR
1	C	66	SER
1	C	135	LYS
1	C	138	ASP
1	C	198	LYS
1	C	214	PHE
1	C	224	LYS
1	C	231	ARG
1	C	237	TRP
1	C	243	LEU
1	C	383	ASP
1	C	384	LEU
1	D	80	ARG
1	D	149	ASP
1	D	214	PHE
1	D	237	TRP
1	D	295	MET
1	D	309	SER
1	D	315	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	D	348	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)

26 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	GOL	D	502	-	5,5,5	1.36	1 (20%)	5,5,5	0.89	0
3	GOL	C	505	-	5,5,5	1.14	0	5,5,5	0.79	0
5	OXY	C	504	-	1,1,1	0.32	0	-		
3	GOL	D	505	-	5,5,5	0.93	0	5,5,5	1.04	0
3	GOL	C	502	-	5,5,5	1.00	0	5,5,5	0.79	0
3	GOL	A	502	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	C	503	-	5,5,5	1.12	0	5,5,5	0.81	0
2	HEM	C	501	1	41,50,50	1.47	5 (12%)	45,82,82	1.95	15 (33%)
4	KYN	B	505	-	13,15,15	1.44	3 (23%)	17,20,20	1.69	4 (23%)
2	HEM	B	501	5,1	41,50,50	1.63	6 (14%)	45,82,82	1.92	13 (28%)
4	KYN	B	503	-	13,15,15	1.60	4 (30%)	17,20,20	1.45	3 (17%)
3	GOL	A	507	-	5,5,5	0.90	0	5,5,5	1.01	0
2	HEM	D	501	1	41,50,50	1.50	7 (17%)	45,82,82	2.04	14 (31%)
3	GOL	C	506	-	5,5,5	1.01	0	5,5,5	1.23	1 (20%)
3	GOL	B	507	-	5,5,5	0.90	0	5,5,5	1.03	0
3	GOL	A	505	-	5,5,5	0.92	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	D	504	-	5,5,5	1.16	0	5,5,5	0.79	0
4	KYN	B	502[B]	-	13,15,15	1.43	3 (23%)	17,20,20	1.15	1 (5%)
4	KYN	A	506	-	13,15,15	1.39	2 (15%)	17,20,20	1.42	3 (17%)
3	GOL	A	503	-	5,5,5	0.92	0	5,5,5	1.01	0
2	HEM	A	501	1	41,50,50	1.56	5 (12%)	45,82,82	1.92	12 (26%)
3	GOL	D	503	-	5,5,5	0.95	0	5,5,5	1.07	0
5	OXY	B	506[B]	2	1,1,1	0.34	0	-		
3	GOL	B	504	-	5,5,5	1.16	0	5,5,5	0.69	0
3	GOL	A	504	-	5,5,5	1.03	1 (20%)	5,5,5	1.10	0
4	KYN	B	502[A]	-	13,15,15	1.47	3 (23%)	17,20,20	1.12	1 (5%)

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	D	502	-	-	1/4/4/4	-
3	GOL	C	505	-	-	2/4/4/4	-
3	GOL	D	505	-	-	2/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	C	503	-	-	3/4/4/4	-
2	HEM	C	501	1	-	3/12/54/54	-
4	KYN	B	505	-	-	7/12/12/12	0/1/1/1
2	HEM	B	501	5,1	-	3/12/54/54	-
4	KYN	B	503	-	-	4/12/12/12	0/1/1/1
3	GOL	A	507	-	-	2/4/4/4	-
2	HEM	D	501	1	-	3/12/54/54	-
3	GOL	C	506	-	-	4/4/4/4	-
3	GOL	B	507	-	-	2/4/4/4	-
3	GOL	A	505	-	-	4/4/4/4	-
3	GOL	D	504	-	-	4/4/4/4	-
4	KYN	B	502[B]	-	-	7/12/12/12	0/1/1/1
4	KYN	A	506	-	-	4/12/12/12	0/1/1/1
3	GOL	A	503	-	-	4/4/4/4	-
2	HEM	A	501	1	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	B	504	-	-	1/4/4/4	-
3	GOL	A	504	-	-	4/4/4/4	-
4	KYN	B	502[A]	-	-	8/12/12/12	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-5.17	1.33	1.40
2	C	501	HEM	C3C-C2C	-4.96	1.33	1.40
2	D	501	HEM	C3C-C2C	-4.53	1.34	1.40
2	A	501	HEM	C3C-C2C	-4.52	1.34	1.40
2	B	501	HEM	FE-NB	4.24	2.17	1.96
2	A	501	HEM	FE-NB	3.58	2.14	1.96
2	A	501	HEM	C3C-CAC	3.43	1.54	1.47
4	B	505	KYN	CD2-C1	3.01	1.54	1.48
2	B	501	HEM	C3C-CAC	2.99	1.53	1.47
2	D	501	HEM	FE-NB	2.90	2.11	1.96
4	B	503	KYN	CD2-C1	2.85	1.54	1.48
4	B	502[A]	KYN	CD2-C1	2.77	1.54	1.48
2	D	501	HEM	C3C-CAC	2.74	1.53	1.47
2	A	501	HEM	CAB-C3B	2.73	1.54	1.47
4	B	502[B]	KYN	CD2-C1	2.71	1.53	1.48
2	B	501	HEM	CAB-C3B	2.67	1.54	1.47
2	C	501	HEM	C3C-CAC	2.67	1.53	1.47
4	B	505	KYN	CG-N1	2.65	1.46	1.37
4	B	503	KYN	CG-N1	2.56	1.46	1.37
4	A	506	KYN	CG-N1	2.54	1.46	1.37
2	D	501	HEM	CAA-C2A	2.46	1.55	1.52
4	B	503	KYN	CD2-CG	-2.46	1.38	1.41
4	B	503	KYN	CB-C1	2.40	1.54	1.51
2	B	501	HEM	CAA-C2A	2.38	1.55	1.52
4	B	502[B]	KYN	CG-N1	2.37	1.45	1.37
4	B	505	KYN	O2-C1	-2.30	1.18	1.22
3	D	502	GOL	C1-C2	2.24	1.60	1.51
2	C	501	HEM	CMB-C2B	2.24	1.55	1.50
4	B	502[A]	KYN	CG-N1	2.23	1.45	1.37
2	C	501	HEM	FE-NB	2.23	2.07	1.96
2	B	501	HEM	CMB-C2B	2.21	1.55	1.50
2	D	501	HEM	CMB-C2B	2.19	1.55	1.50
2	D	501	HEM	CAB-C3B	2.14	1.53	1.47
4	B	502[A]	KYN	CB-C1	2.13	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502[B]	KYN	CB-C1	2.13	1.54	1.51
2	C	501	HEM	CAB-C3B	2.12	1.53	1.47
2	D	501	HEM	C3B-C2B	-2.08	1.33	1.37
2	A	501	HEM	CAA-C2A	2.03	1.55	1.52
4	A	506	KYN	CD2-C1	2.03	1.52	1.48
3	A	504	GOL	C1-C2	2.00	1.60	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C4B-CHC-C1C	4.57	128.59	122.56
2	A	501	HEM	C4D-ND-C1D	4.43	109.64	105.07
2	B	501	HEM	C4D-ND-C1D	4.41	109.62	105.07
2	D	501	HEM	C4C-CHD-C1D	4.31	128.25	122.56
2	D	501	HEM	C2C-C3C-C4C	4.16	109.81	106.90
4	B	505	KYN	O2-C1-CB	-4.13	115.97	120.76
2	C	501	HEM	C2C-C3C-C4C	4.09	109.75	106.90
2	A	501	HEM	CAD-CBD-CGD	-3.95	105.10	113.60
2	C	501	HEM	C4C-CHD-C1D	3.89	127.69	122.56
2	D	501	HEM	C4D-ND-C1D	3.87	109.07	105.07
2	B	501	HEM	C2C-C3C-C4C	3.87	109.60	106.90
2	A	501	HEM	C4B-CHC-C1C	3.84	127.62	122.56
2	D	501	HEM	C4B-C3B-C2B	3.76	110.10	107.11
4	B	505	KYN	CB-C1-CD2	3.65	124.94	119.86
2	D	501	HEM	C1B-NB-C4B	3.59	108.78	105.07
2	C	501	HEM	CAD-CBD-CGD	-3.45	106.17	113.60
2	B	501	HEM	C3D-C4D-ND	-3.33	106.46	110.17
2	C	501	HEM	C1B-NB-C4B	3.30	108.48	105.07
2	C	501	HEM	C4B-C3B-C2B	3.28	109.72	107.11
2	A	501	HEM	CHA-C4D-ND	3.28	128.43	124.38
2	C	501	HEM	C4D-ND-C1D	3.18	108.36	105.07
2	C	501	HEM	CBA-CAA-C2A	-3.17	107.21	112.62
2	A	501	HEM	CBA-CAA-C2A	-3.16	107.22	112.62
2	D	501	HEM	C3D-C4D-ND	-3.00	106.82	110.17
2	B	501	HEM	CMA-C3A-C4A	-2.95	123.92	128.46
4	B	503	KYN	OXT-C-CA	2.94	123.39	113.38
2	D	501	HEM	CBA-CAA-C2A	-2.93	107.61	112.62
2	B	501	HEM	C1B-NB-C4B	2.93	108.10	105.07
2	D	501	HEM	C4B-CHC-C1C	2.91	126.40	122.56
2	A	501	HEM	C3D-C4D-ND	-2.90	106.94	110.17
2	C	501	HEM	C4B-CHC-C1C	2.86	126.33	122.56
2	A	501	HEM	C1B-NB-C4B	2.85	108.01	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C2D-C1D-ND	-2.84	106.48	109.88
4	B	503	KYN	CD2-CG-N1	-2.84	118.92	122.67
2	A	501	HEM	C2C-C3C-C4C	2.78	108.84	106.90
4	A	506	KYN	OXT-C-O	-2.67	118.02	124.09
2	B	501	HEM	C3C-C4C-NC	-2.57	106.09	110.94
2	D	501	HEM	C3C-C4C-NC	-2.55	106.12	110.94
2	B	501	HEM	C4B-C3B-C2B	2.53	109.12	107.11
2	B	501	HEM	CBA-CAA-C2A	-2.51	108.33	112.62
2	D	501	HEM	C2D-C1D-ND	-2.49	106.90	109.88
4	A	506	KYN	OXT-C-CA	2.48	121.81	113.38
2	D	501	HEM	CHD-C1D-ND	2.46	127.11	124.43
2	C	501	HEM	C3C-C4C-NC	-2.45	106.32	110.94
4	B	502[A]	KYN	CA-CB-C1	-2.41	110.63	113.70
4	B	502[B]	KYN	CA-CB-C1	-2.41	110.63	113.70
2	A	501	HEM	C3C-C4C-NC	-2.39	106.44	110.94
2	B	501	HEM	C4C-CHD-C1D	2.37	125.68	122.56
2	B	501	HEM	C2D-C1D-ND	-2.32	107.10	109.88
2	D	501	HEM	CMB-C2B-C1B	2.31	128.56	125.04
2	A	501	HEM	C4C-CHD-C1D	2.31	125.60	122.56
2	C	501	HEM	CHA-C4D-ND	2.28	127.20	124.38
2	C	501	HEM	CHD-C1D-ND	2.24	126.87	124.43
2	D	501	HEM	C1D-C2D-C3D	2.22	109.29	106.96
2	B	501	HEM	CHA-C4D-ND	2.22	127.12	124.38
2	A	501	HEM	CHD-C1D-ND	2.21	126.83	124.43
4	B	505	KYN	OXT-C-CA	2.18	120.82	113.38
2	C	501	HEM	CMB-C2B-C1B	2.14	128.30	125.04
2	C	501	HEM	C3D-C4D-ND	-2.14	107.79	110.17
4	B	503	KYN	OXT-C-O	-2.14	119.23	124.09
2	C	501	HEM	C2D-C1D-ND	-2.12	107.34	109.88
2	D	501	HEM	CAD-CBD-CGD	-2.06	109.18	113.60
2	B	501	HEM	CAA-CBA-CGA	-2.05	108.02	113.76
3	C	506	GOL	O3-C3-C2	-2.05	100.39	110.20
4	A	506	KYN	CE2-CD2-CG	2.02	121.07	118.93
2	C	501	HEM	CAB-C3B-C2B	-2.01	122.00	128.60
4	B	505	KYN	OXT-C-O	-2.00	119.54	124.09

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	503	GOL	C1-C2-C3-O3
3	A	504	GOL	O1-C1-C2-C3
3	A	504	GOL	C1-C2-C3-O3
3	A	505	GOL	O1-C1-C2-C3
3	A	507	GOL	O1-C1-C2-O2
3	A	507	GOL	O1-C1-C2-C3
3	B	507	GOL	O1-C1-C2-C3
3	C	502	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-C3
3	C	505	GOL	O1-C1-C2-C3
3	C	506	GOL	O1-C1-C2-C3
3	C	506	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	D	505	GOL	C1-C2-C3-O3
4	A	506	KYN	C-CA-CB-C1
4	B	502[A]	KYN	O2-C1-CB-CA
4	B	502[A]	KYN	CD2-C1-CB-CA
4	B	502[A]	KYN	C-CA-CB-C1
4	B	502[B]	KYN	O2-C1-CB-CA
4	B	502[B]	KYN	CD2-C1-CB-CA
4	B	502[B]	KYN	C-CA-CB-C1
4	B	503	KYN	O-C-CA-N
4	B	505	KYN	O2-C1-CD2-CG
4	B	505	KYN	CB-C1-CD2-CG
4	B	505	KYN	C-CA-CB-C1
4	B	505	KYN	N-CA-CB-C1
4	B	503	KYN	OXT-C-CA-N
3	D	503	GOL	O1-C1-C2-O2
4	B	502[A]	KYN	CB-C1-CD2-CE2
3	A	505	GOL	C1-C2-C3-O3
3	B	504	GOL	O1-C1-C2-C3
3	D	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O2-C2-C3-O3
3	A	505	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	B	507	GOL	O1-C1-C2-O2
3	C	502	GOL	O1-C1-C2-O2
3	C	503	GOL	O1-C1-C2-O2
3	C	506	GOL	O1-C1-C2-O2
4	B	502[A]	KYN	O2-C1-CD2-CE2

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Mol	Chain	Res	Type	Atoms
4	A	506	KYN	N-CA-CB-C1
4	B	502[A]	KYN	N-CA-CB-C1
4	B	502[B]	KYN	N-CA-CB-C1
4	A	506	KYN	OXT-C-CA-CB
4	B	505	KYN	O2-C1-CB-CA
4	B	505	KYN	CD2-C1-CB-CA
3	A	504	GOL	O1-C1-C2-O2
3	A	504	GOL	O2-C2-C3-O3
3	C	506	GOL	O2-C2-C3-O3
3	D	505	GOL	O2-C2-C3-O3
4	A	506	KYN	O-C-CA-CB
4	B	502[B]	KYN	O2-C1-CD2-CG
3	C	505	GOL	O1-C1-C2-O2
4	B	502[B]	KYN	O2-C1-CD2-CE2
4	B	503	KYN	OXT-C-CA-CB
4	B	503	KYN	O-C-CA-CB
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
3	D	504	GOL	O1-C1-C2-O2
3	D	504	GOL	O2-C2-C3-O3
4	B	502[A]	KYN	O2-C1-CD2-CG
2	B	501	HEM	CAD-CBD-CGD-O2D
4	B	502[A]	KYN	CB-C1-CD2-CG
2	B	501	HEM	CAD-CBD-CGD-O1D
4	B	502[B]	KYN	CB-C1-CD2-CE2
2	A	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O1D
4	B	505	KYN	OXT-C-CA-N
3	C	503	GOL	O2-C2-C3-O3
3	D	504	GOL	O1-C1-C2-C3
3	D	504	GOL	C1-C2-C3-O3

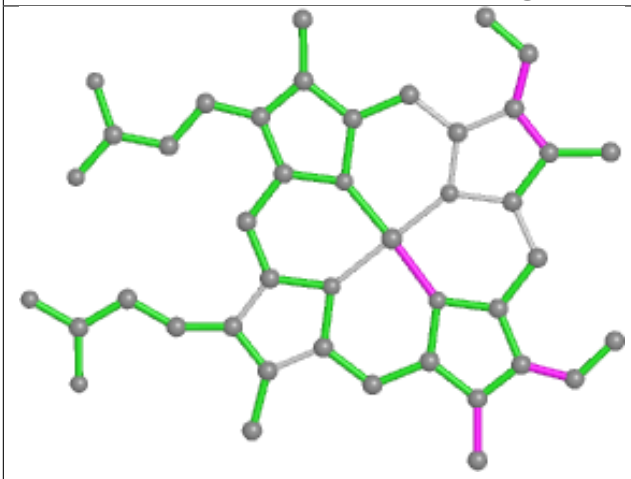
There are no ring outliers.

14 monomers are involved in 46 short contacts:

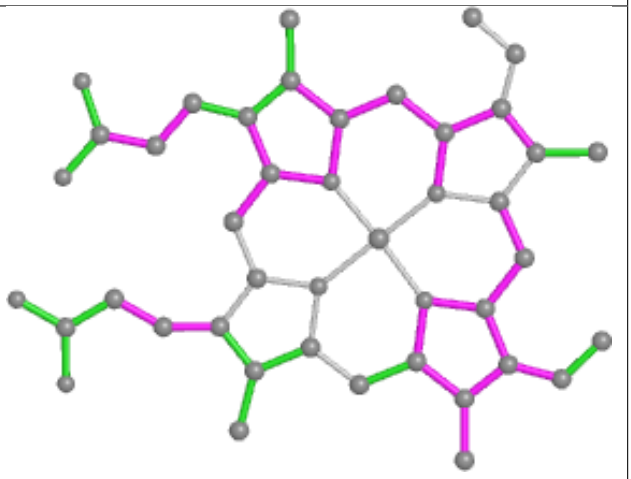
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	505	GOL	3	0
3	C	502	GOL	2	0
2	C	501	HEM	4	0
4	B	505	KYN	4	0
2	B	501	HEM	7	0
4	B	503	KYN	3	0
2	D	501	HEM	7	0
3	C	506	GOL	2	0
4	B	502[B]	KYN	1	0
4	A	506	KYN	3	0
2	A	501	HEM	7	0
5	B	506[B]	OXY	1	0
3	B	504	GOL	1	0
3	A	504	GOL	1	0

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.

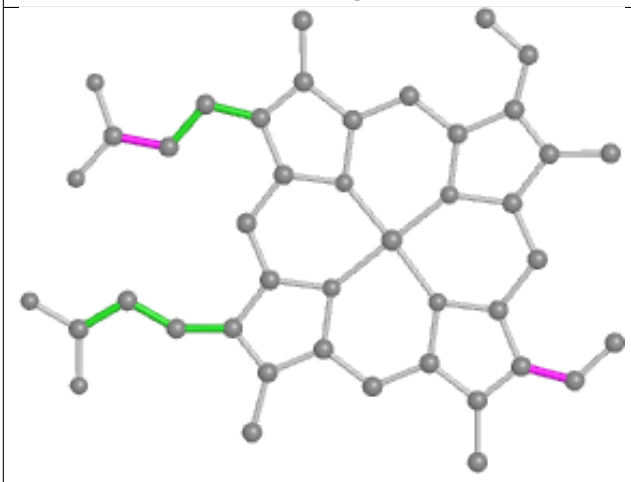
Ligand HEM C 501



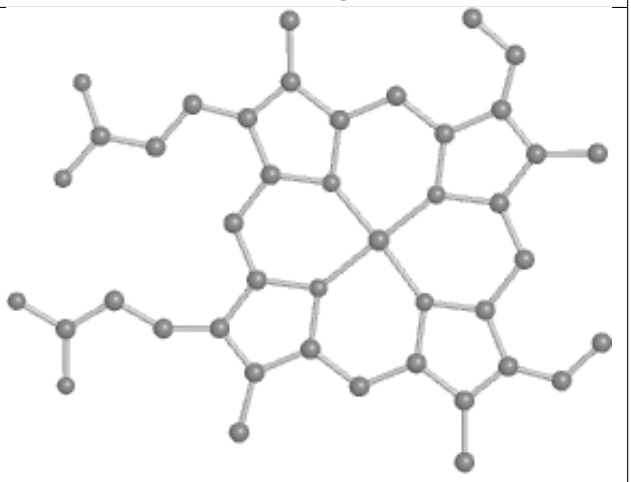
Bond lengths



Bond angles

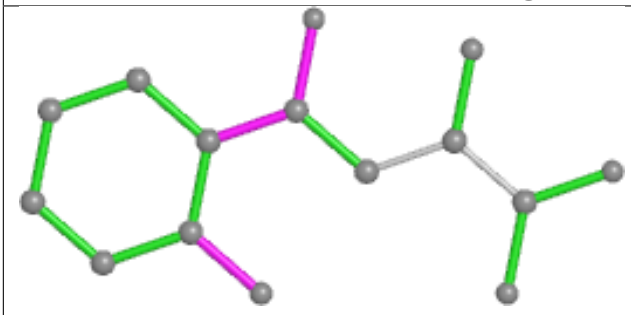


Torsions

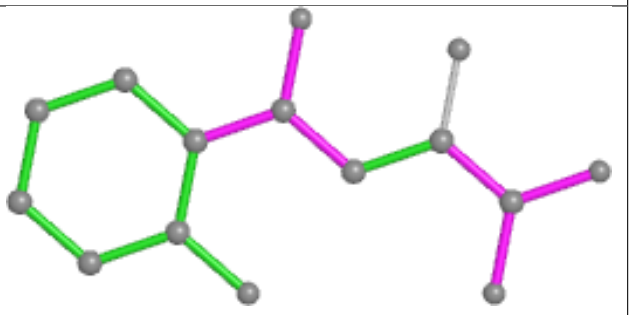


Rings

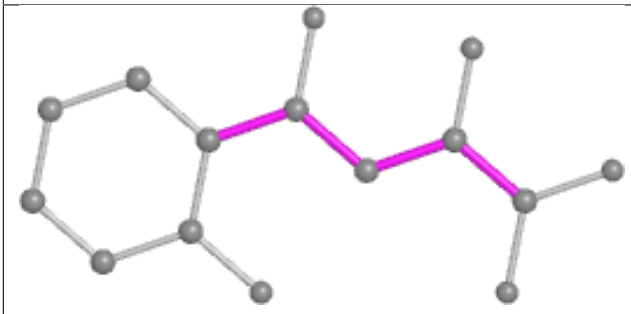
Ligand KYN B 505



Bond lengths



Bond angles



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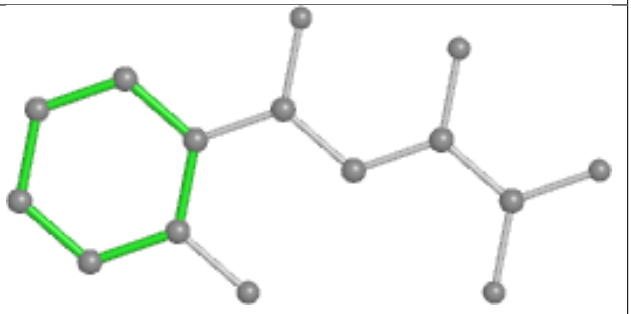
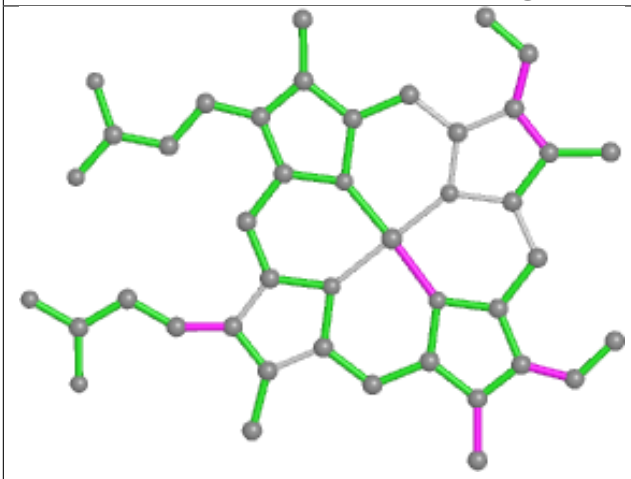
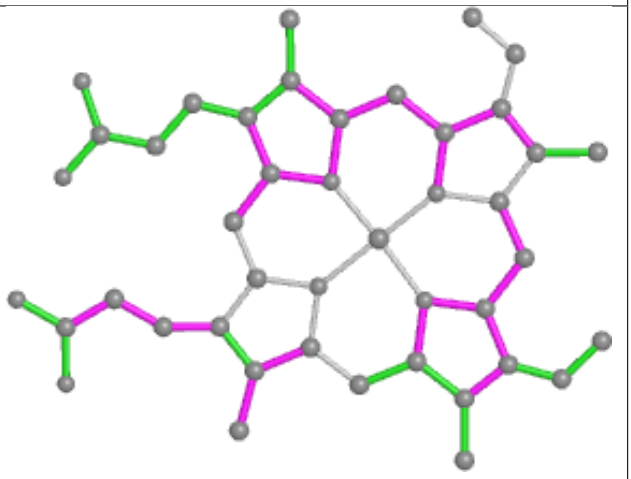


Rings

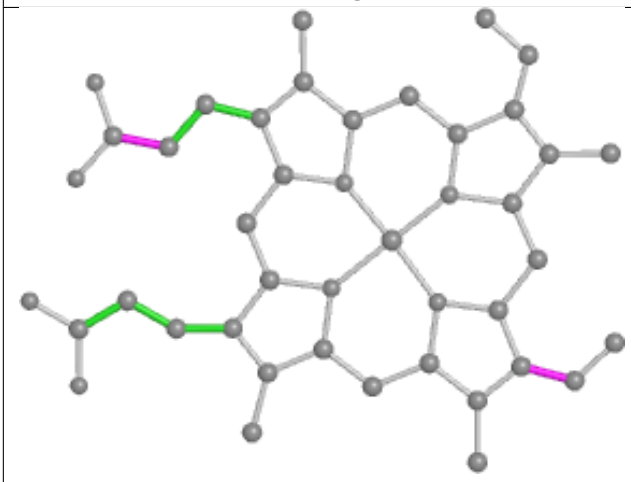
Ligand HEM B 501



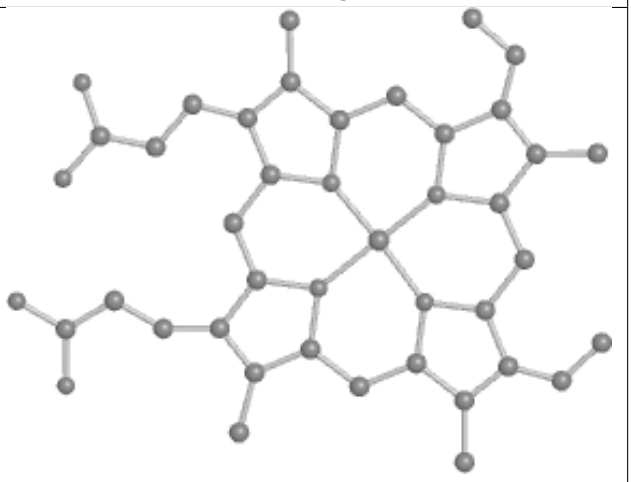
Bond lengths



Bond angles

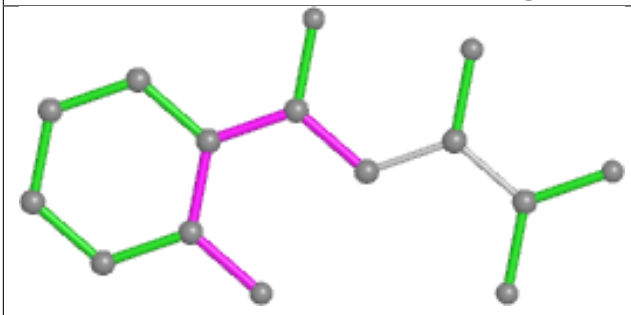


Torsions

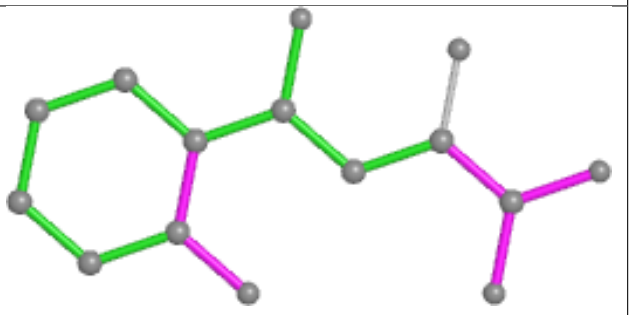


Rings

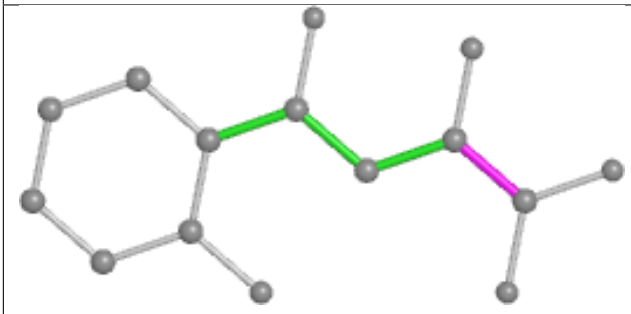
Ligand KYN B 503



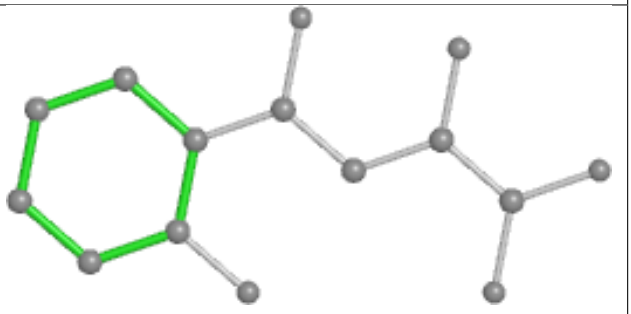
Bond lengths



Bond angles

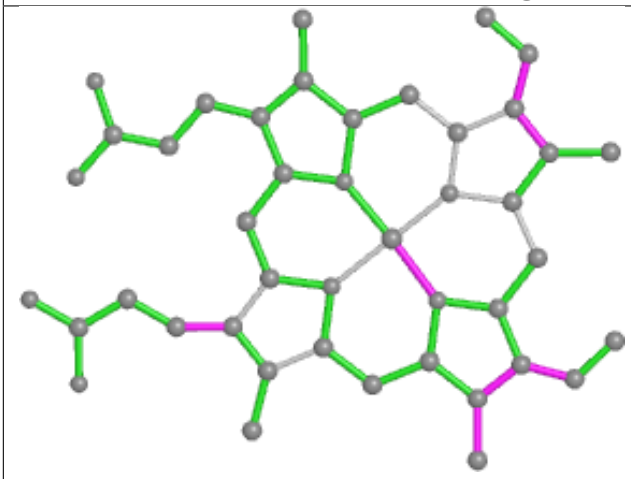


Torsions

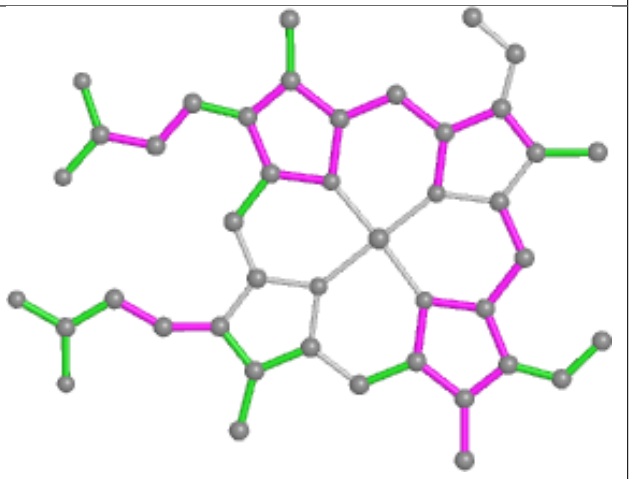


Rings

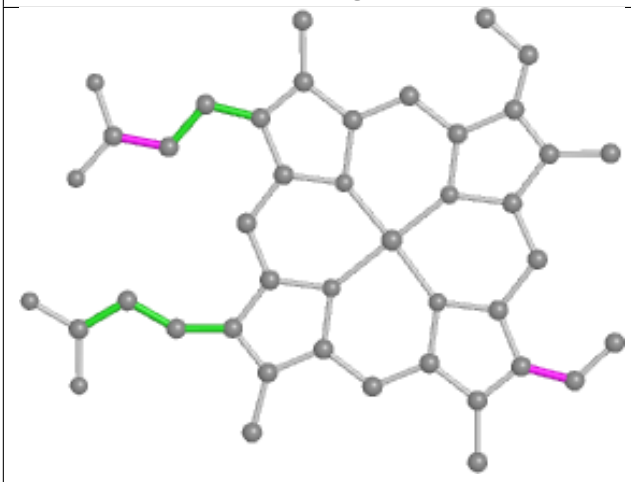
Ligand HEM D 501



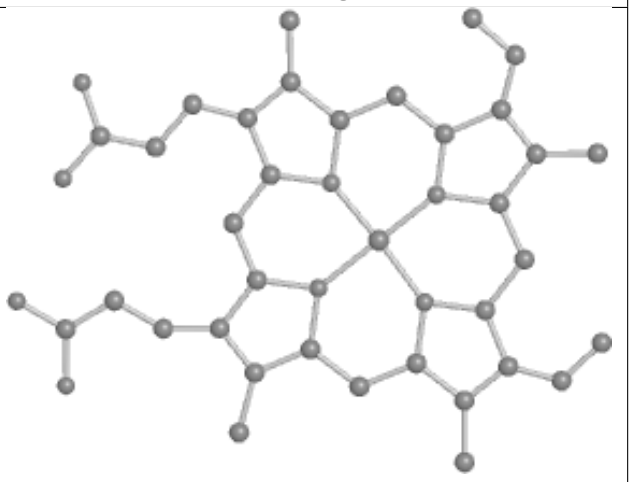
Bond lengths



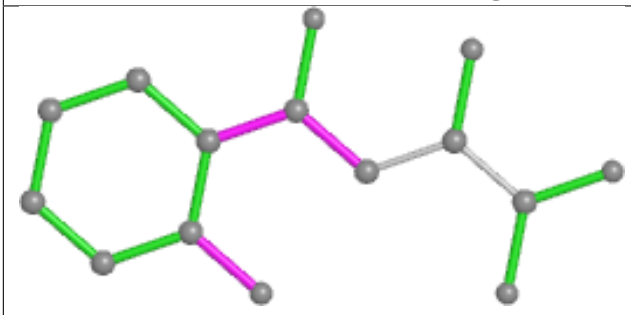
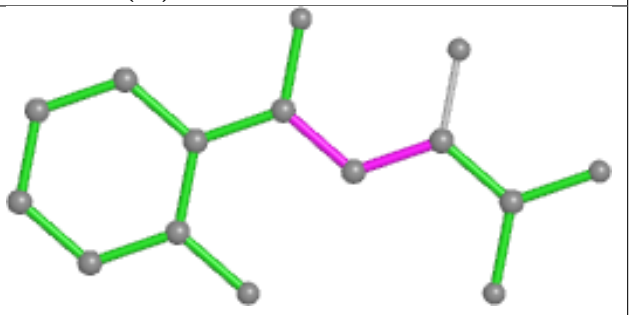
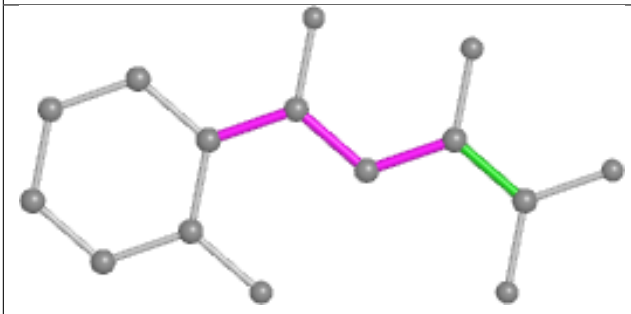
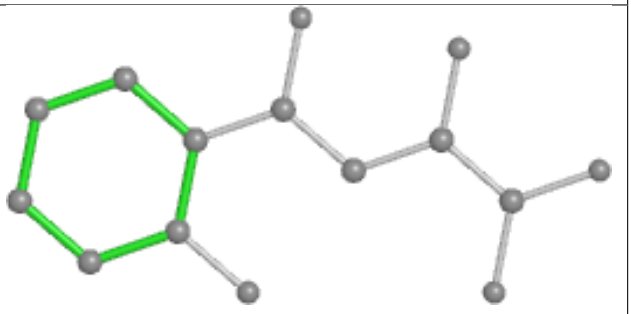
Bond angles

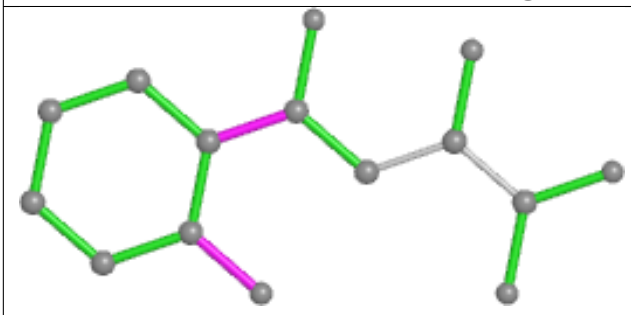
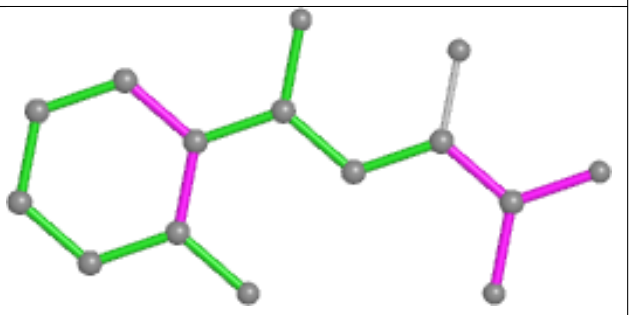
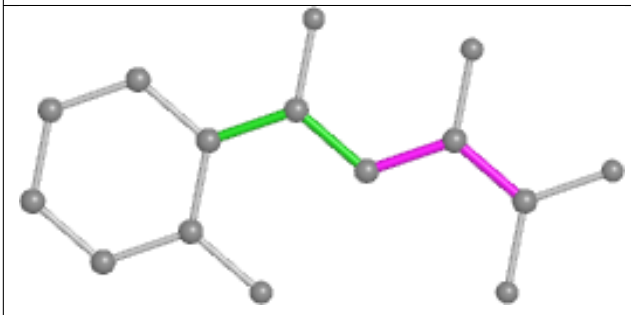
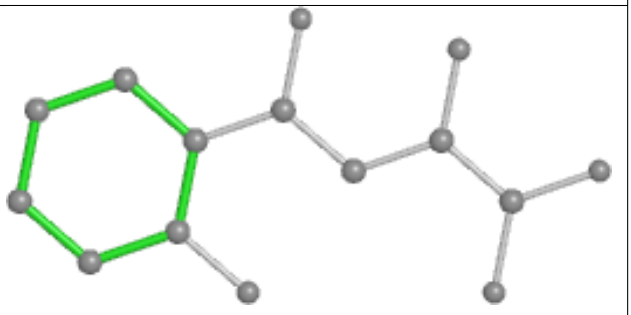


Torsions

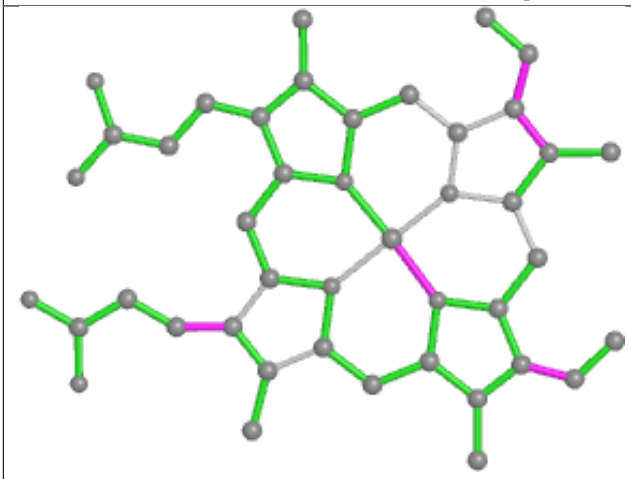


Rings

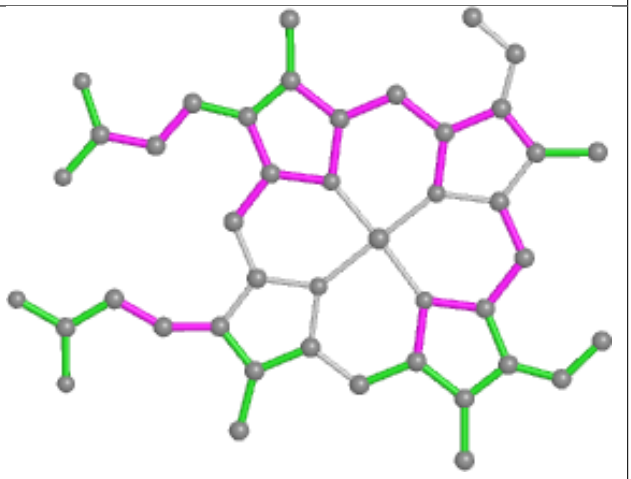
Ligand KYN B 502 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KYN A 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

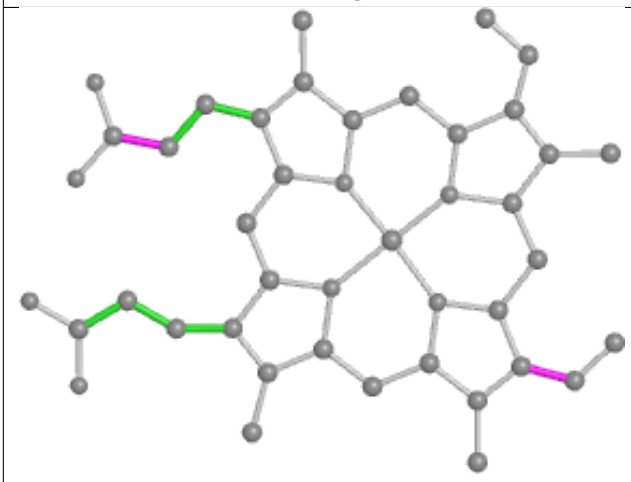
Ligand HEM A 501



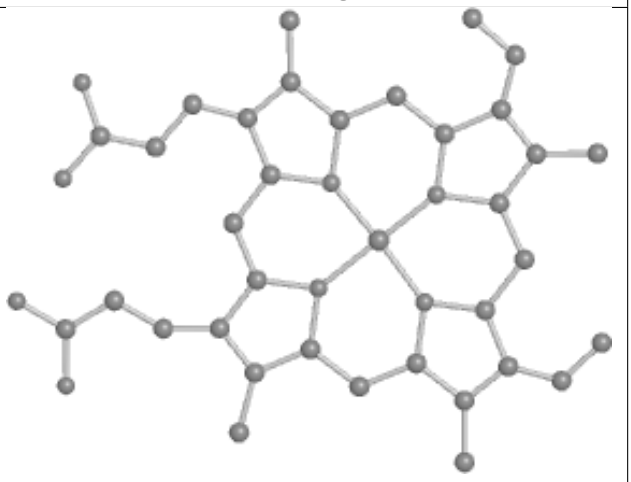
Bond lengths



Bond angles

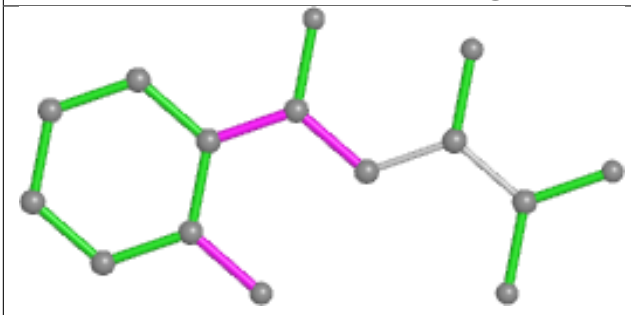


Torsions

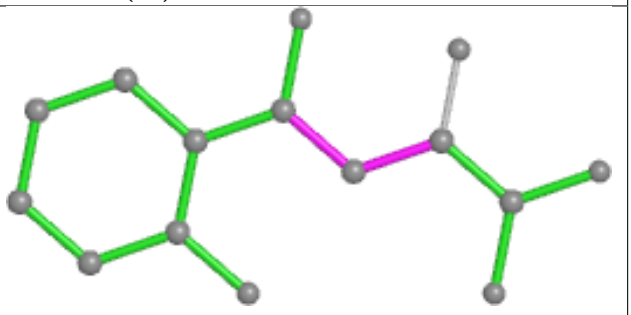


Rings

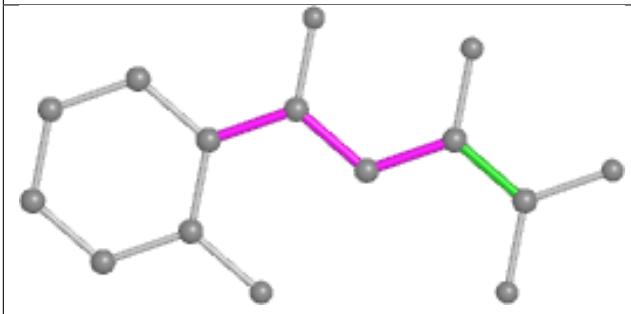
Ligand KYN B 502 (A)



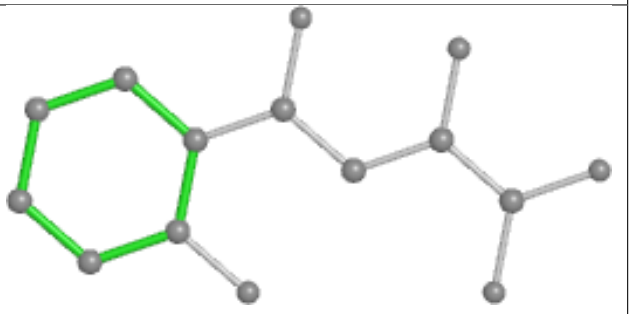
Bond lengths



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	370/405 (91%)	0.02	6 (1%)	72	78	26, 42, 72, 99	0
1	B	381/405 (94%)	0.26	24 (6%)	20	25	28, 46, 80, 109	4 (1%)
1	C	372/405 (91%)	0.06	13 (3%)	44	53	28, 44, 67, 97	1 (0%)
1	D	373/405 (92%)	0.03	11 (2%)	51	61	27, 42, 66, 101	1 (0%)
All	All	1496/1620 (92%)	0.09	54 (3%)	42	51	26, 43, 72, 109	6 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	THR	10.7
1	B	379	THR	7.6
1	A	285	GLY	7.0
1	A	283	ALA	7.0
1	D	403	GLY	6.3
1	B	376	ALA	6.2
1	B	374	LEU	6.2
1	B	377	LYS	6.2
1	B	380	GLY	6.1
1	D	382	THR	6.0
1	B	362	PRO	5.7
1	C	362	PRO	5.1
1	D	362	PRO	5.0
1	C	361	GLN	4.8
1	B	13	ALA	4.7
1	C	283	ALA	4.7
1	C	382	THR	4.6
1	B	12	SER	4.6
1	B	382	THR	4.2
1	B	282	THR	4.1
1	B	378	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	284	GLY	3.9
1	C	282	THR	3.8
1	C	383	ASP	3.7
1	B	11	GLY	3.6
1	D	14	ALA	3.6
1	B	401	LYS	3.5
1	B	375	GLU	3.5
1	B	283	ALA	3.4
1	C	286	GLY	3.3
1	B	287	HIS	3.2
1	B	402	GLU	3.1
1	D	284	GLY	3.1
1	B	284	GLY	3.0
1	C	189	GLN	2.9
1	D	283	ALA	2.9
1	C	281	GLN	2.8
1	D	381	GLY	2.8
1	A	286	GLY	2.8
1	D	360	GLN	2.7
1	A	318	GLU	2.6
1	C	14	ALA	2.6
1	D	402	GLU	2.6
1	B	189	GLN	2.5
1	A	359	SER	2.4
1	D	189	GLN	2.4
1	B	291	PHE	2.4
1	C	285	GLY	2.3
1	B	361	GLN	2.2
1	D	13	ALA	2.2
1	B	383	ASP	2.2
1	B	285	GLY	2.2
1	B	286	GLY	2.1
1	C	287	HIS	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)

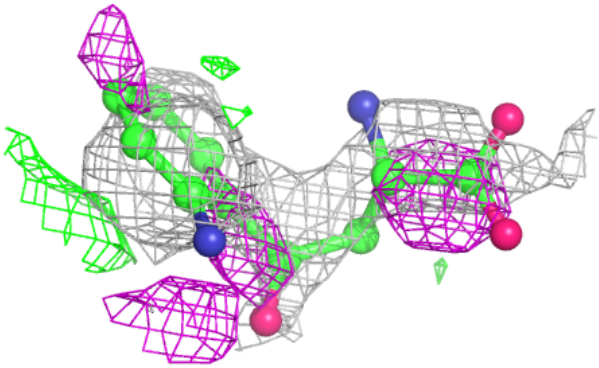
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

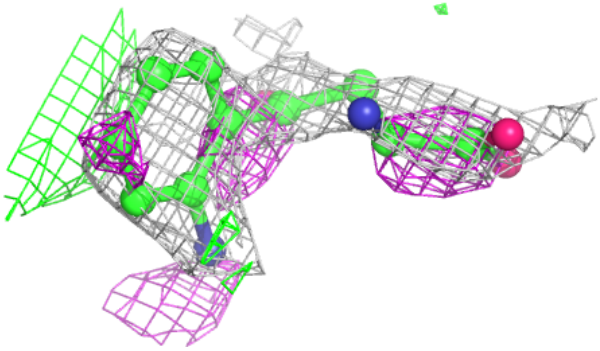
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	505	6/6	0.65	0.41	59,66,69,69	0
5	OXY	C	504	2/2	0.75	0.24	67,67,67,68	0
4	KYN	B	502[B]	15/15	0.77	0.50	59,68,83,87	7
5	OXY	B	506[B]	2/2	0.77	0.33	54,54,54,55	2
4	KYN	B	502[A]	15/15	0.77	0.50	59,67,83,87	7
3	GOL	A	505	6/6	0.78	0.41	50,59,65,66	0
4	KYN	A	506	15/15	0.78	0.36	40,46,53,54	15
4	KYN	B	503	15/15	0.80	0.34	42,52,59,63	15
4	KYN	B	505	15/15	0.81	0.32	40,48,54,56	15
3	GOL	C	503	6/6	0.82	0.24	57,59,66,69	0
3	GOL	B	507	6/6	0.84	0.39	80,84,92,94	0
3	GOL	C	502	6/6	0.85	0.20	49,53,58,60	0
3	GOL	D	504	6/6	0.87	0.23	61,64,67,69	0
3	GOL	A	504	6/6	0.88	0.34	53,63,66,71	0
3	GOL	B	504	6/6	0.89	0.43	51,57,61,67	0
3	GOL	A	507	6/6	0.91	0.36	73,79,79,82	0
3	GOL	D	503	6/6	0.91	0.40	56,58,66,70	0
3	GOL	D	502	6/6	0.92	0.13	42,51,54,58	0
3	GOL	A	502	6/6	0.93	0.17	48,53,54,56	0
3	GOL	C	506	6/6	0.93	0.19	42,46,48,54	0
3	GOL	A	503	6/6	0.93	0.15	46,52,54,55	0
2	HEM	B	501	43/43	0.93	0.16	35,52,66,69	0
2	HEM	D	501	43/43	0.94	0.16	34,43,58,65	0
2	HEM	A	501	43/43	0.94	0.15	37,51,66,67	0
2	HEM	C	501	43/43	0.95	0.14	37,45,57,64	0
3	GOL	D	505	6/6	0.97	0.19	40,42,43,45	0

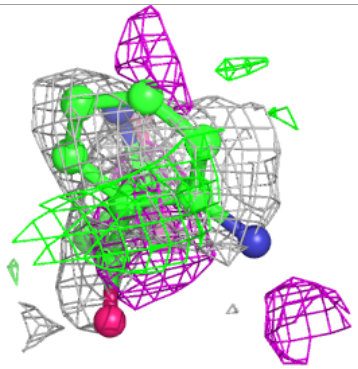
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KYN B 502 (B):

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

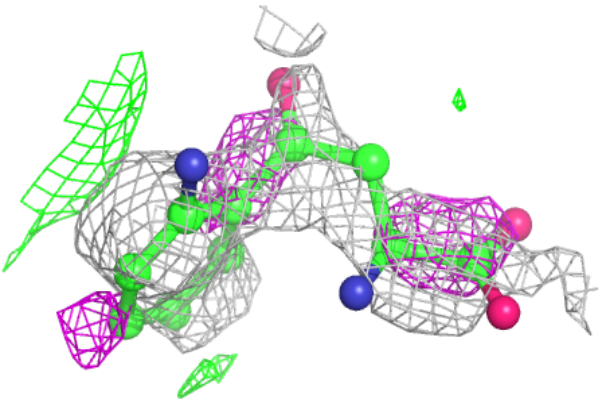


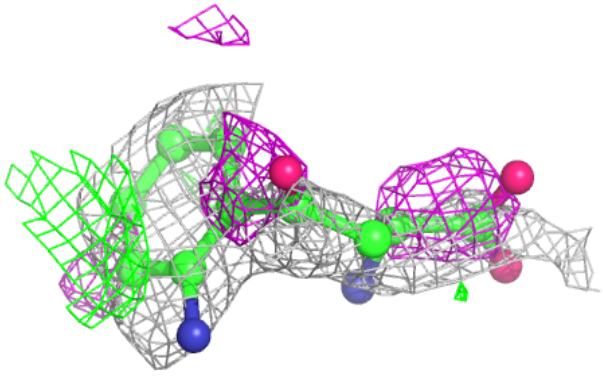


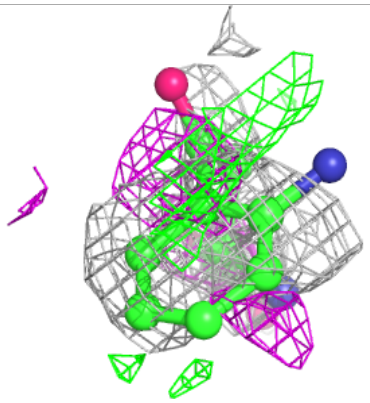


Electron density around KYN B 502 (A):

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

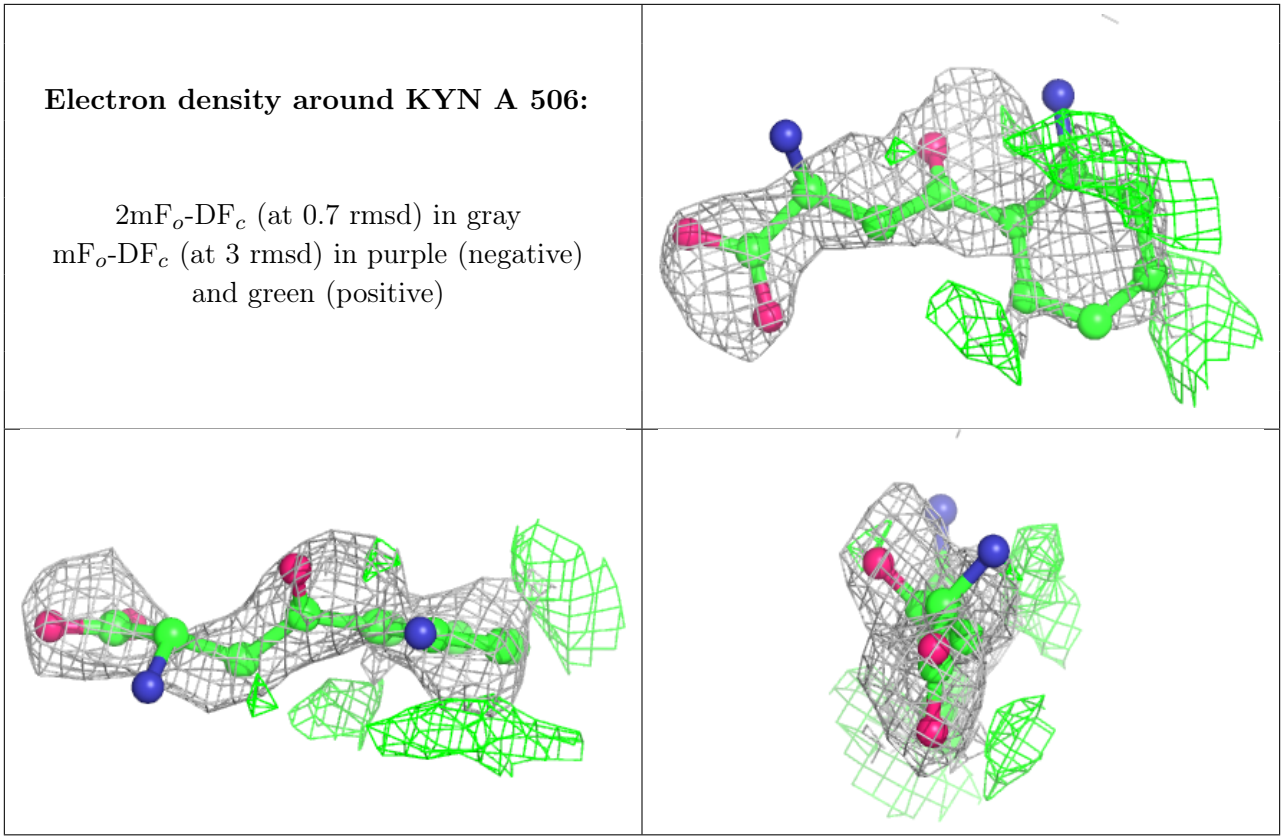






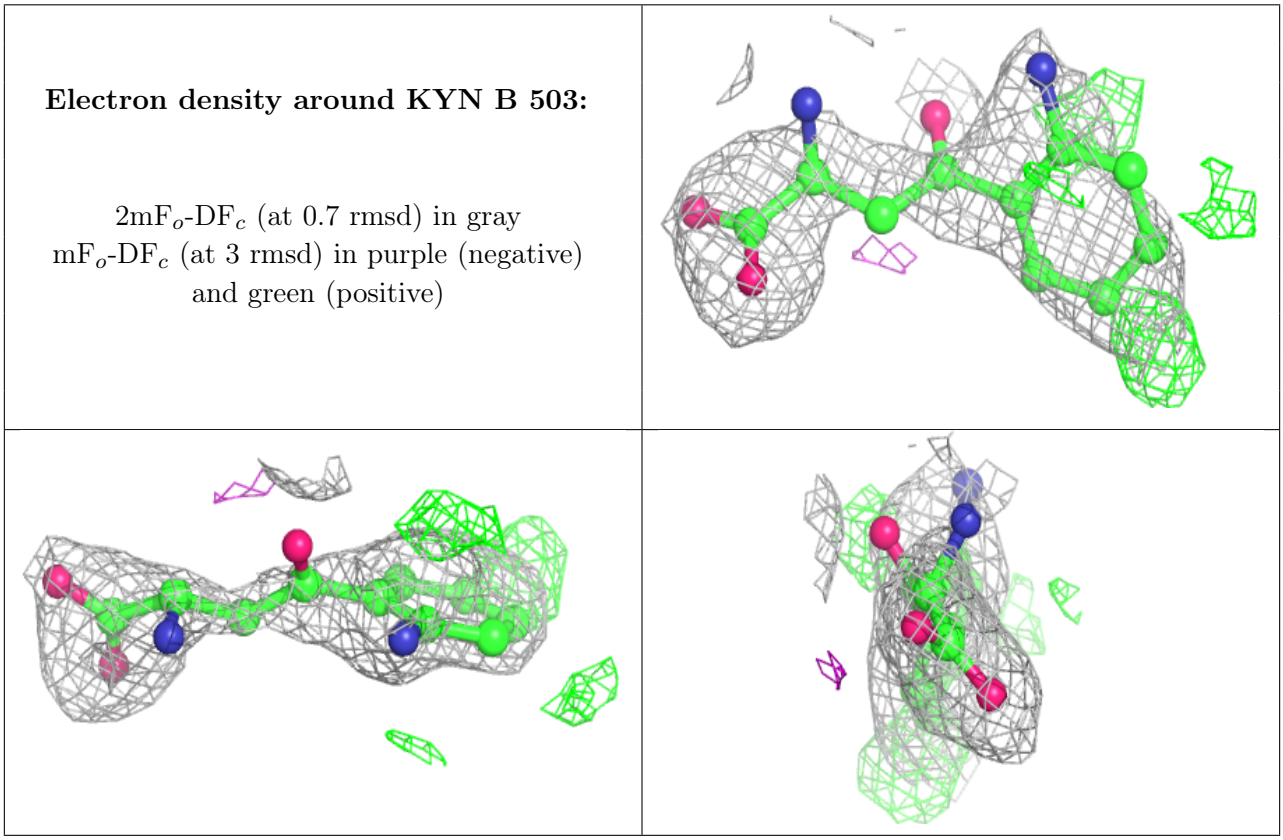
Electron density around KYN A 506:

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



Electron density around KYN 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 KYN B 505:

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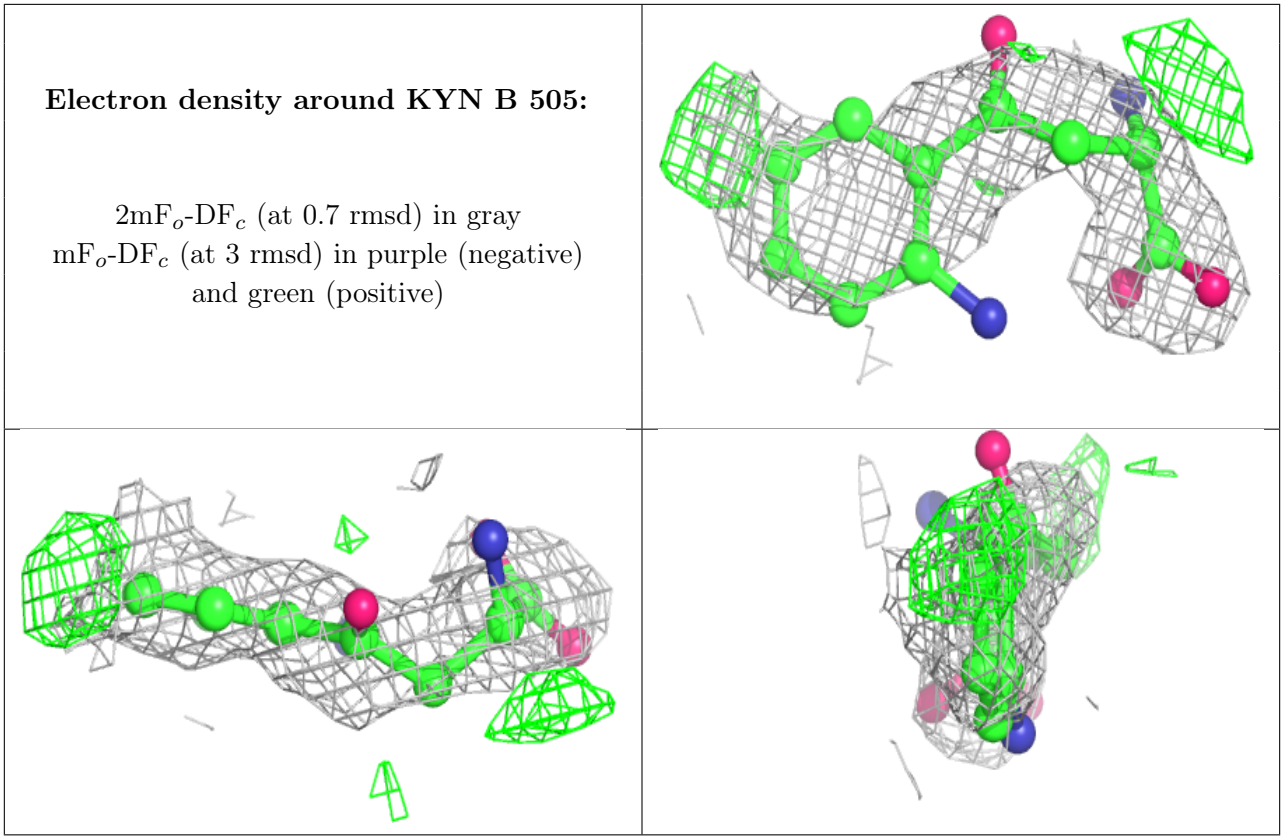
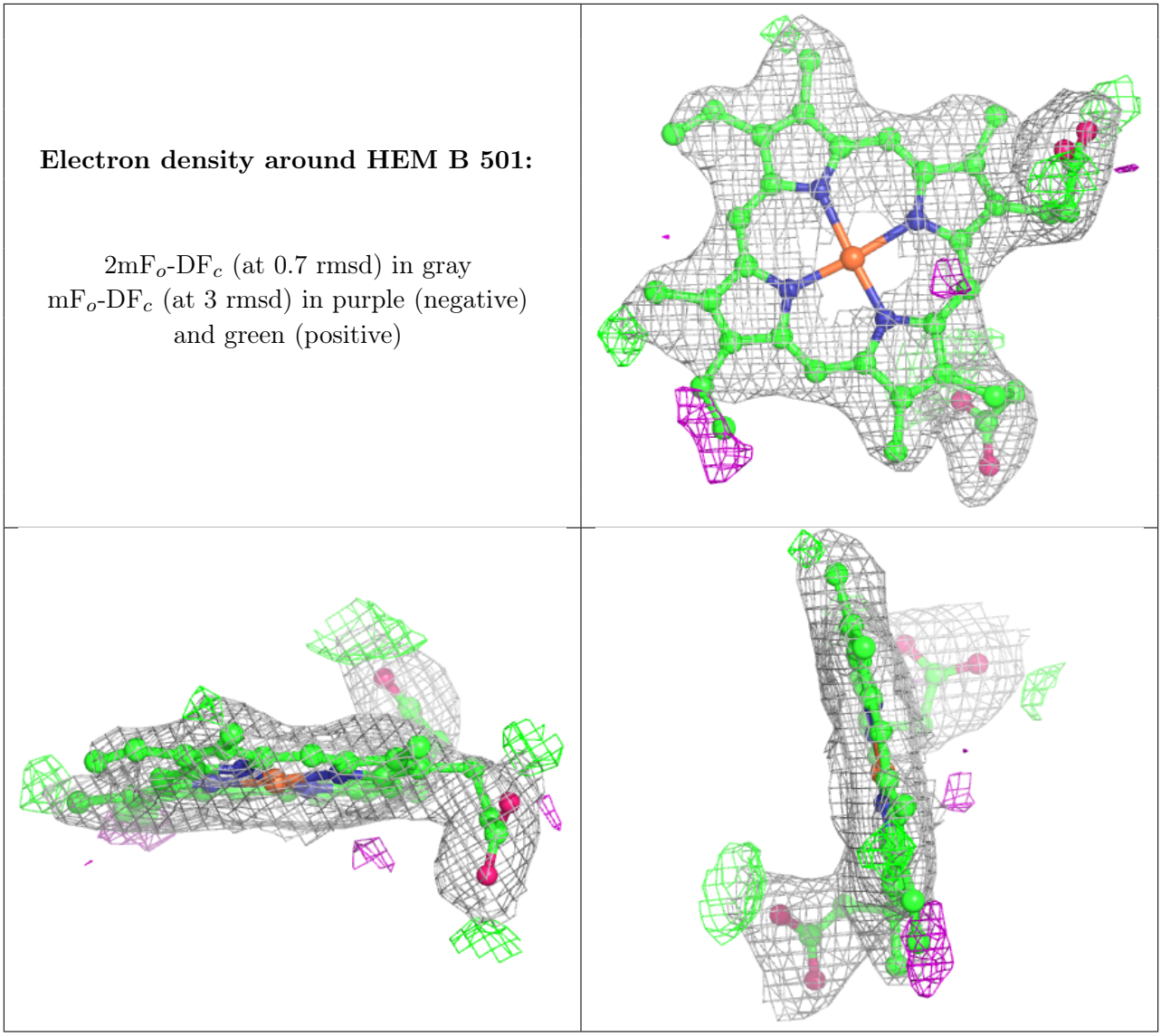
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



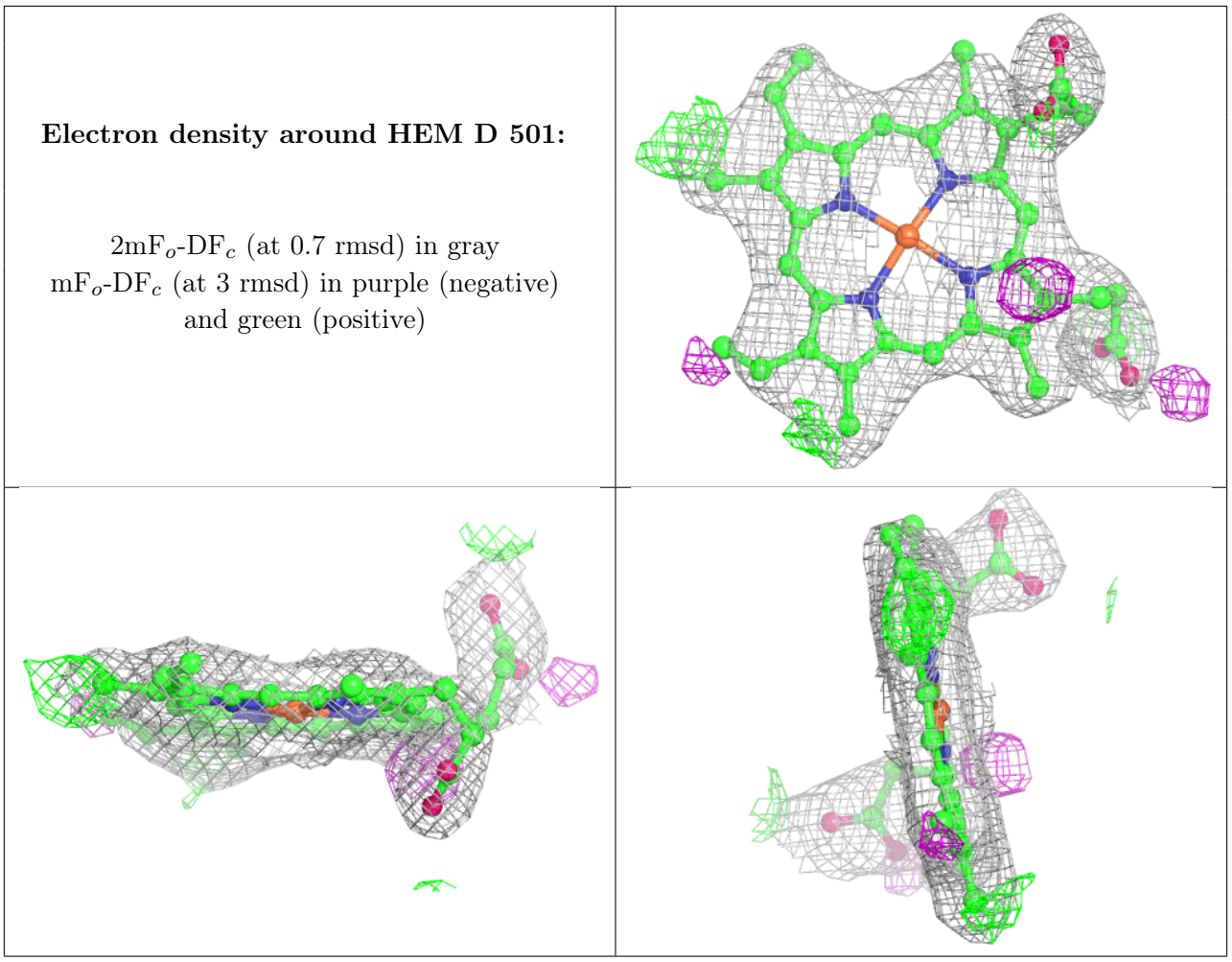
Electron density around HEM B 501:

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



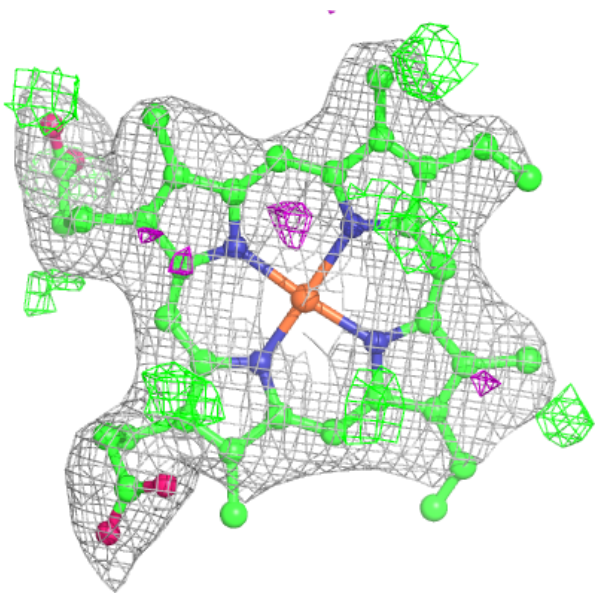
Electron density around HEM D 501:

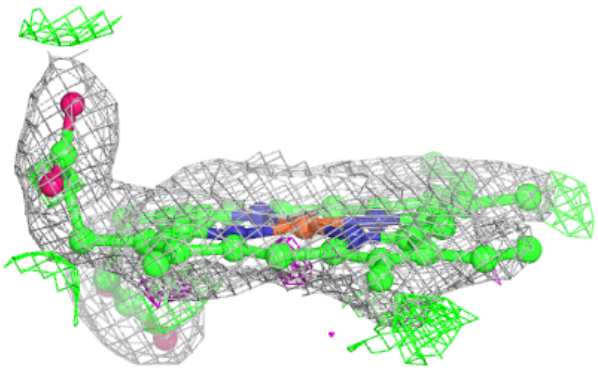
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

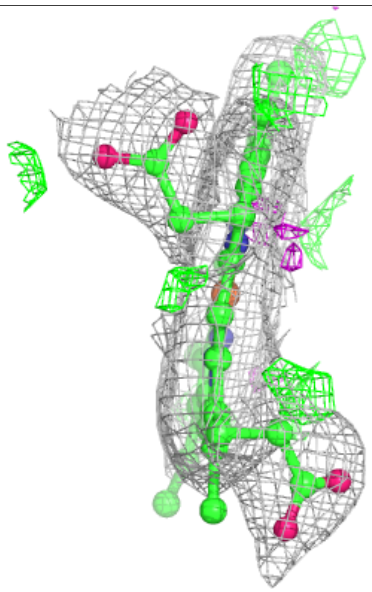


Electron density around HEM A 501:

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

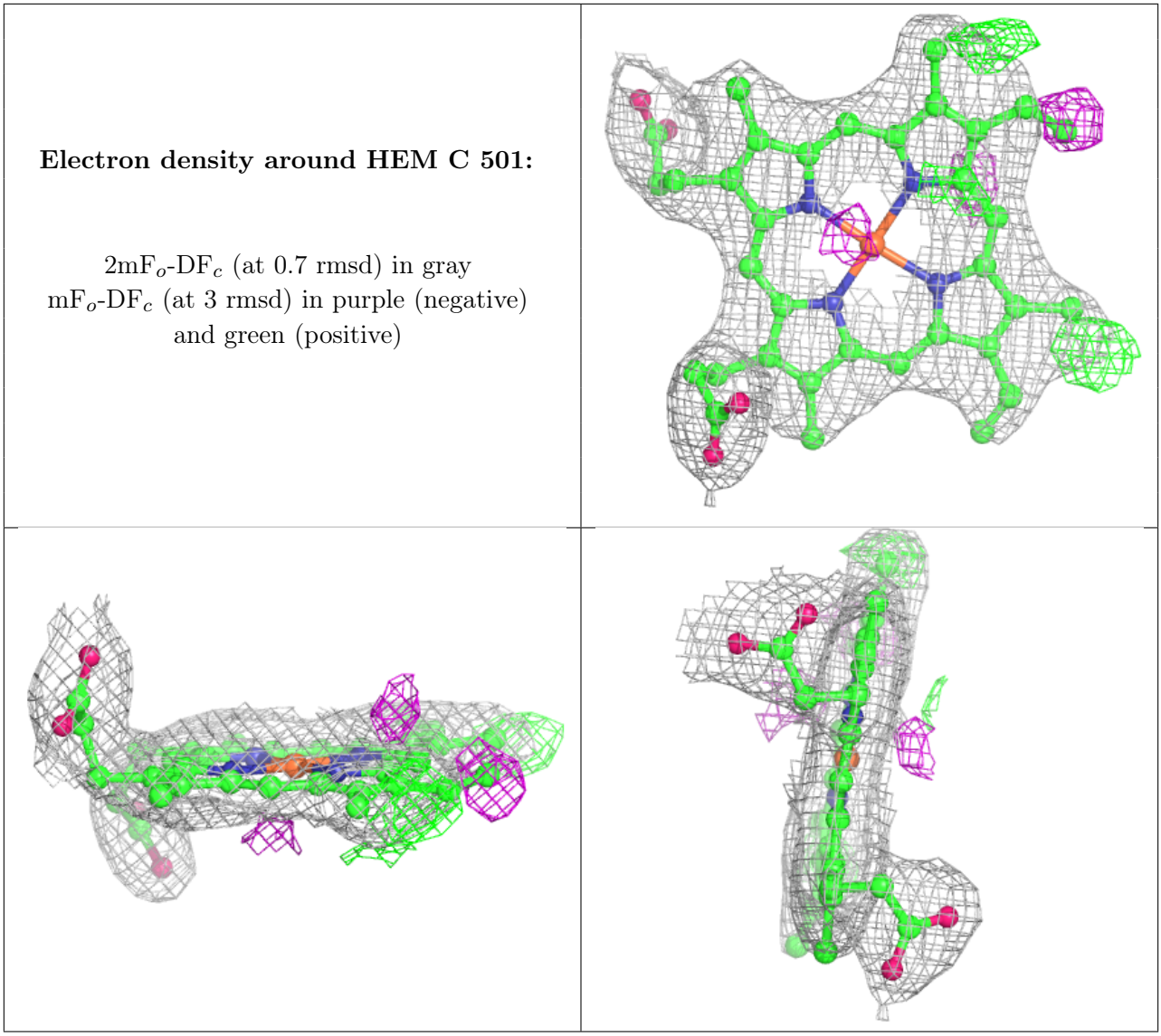






Electron density around HEM C 501:

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



6.5 Other polymers

There are no such residues in this entry.