Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2024 – 04:22 PM EDT

PDB ID	:	8VZV
Title	:	Human TDO (hTDO) in complex with LM10
Authors	:	Ishigami, I.; Yeh, S.-R.; Lewis-Ballester, A.
Deposited on	:	2024-02-12
Resolution	:	2.29 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:

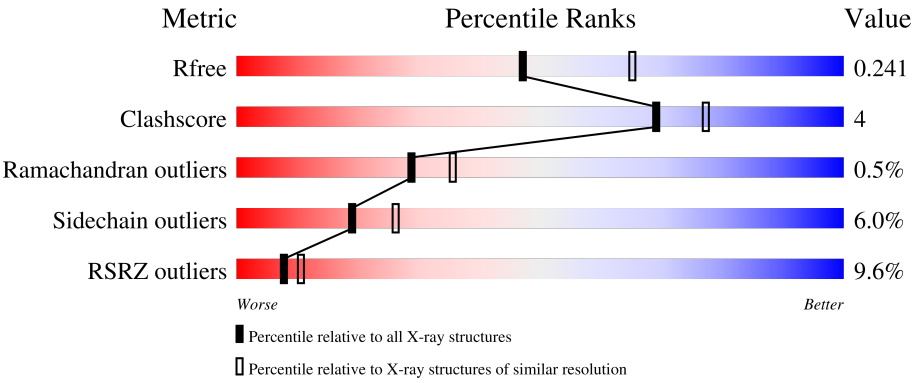
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	AAA	380	8% 80% 9% • 9%
1	BBB	380	7% 81% 9% • 9%
1	CCC	380	12% 73% 10% • 14%
1	DDD	380	7% 80% 8% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11959 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	344	Total	C	N	O	S	0	0	0
			2915	1876	507	521	11			
1	BBB	344	Total	C	N	O	S	0	0	0
			2899	1866	503	519	11			
1	CCC	326	Total	C	N	O	S	0	0	0
			2761	1780	482	488	11			
1	DDD	343	Total	C	N	O	S	0	0	0
			2908	1869	509	519	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	17	MET	-	initiating methionine	UNP P48775
AAA	390	GLU	-	expression tag	UNP P48775
AAA	391	HIS	-	expression tag	UNP P48775
AAA	392	HIS	-	expression tag	UNP P48775
AAA	393	HIS	-	expression tag	UNP P48775
AAA	394	HIS	-	expression tag	UNP P48775
AAA	395	HIS	-	expression tag	UNP P48775
AAA	396	HIS	-	expression tag	UNP P48775
BBB	17	MET	-	initiating methionine	UNP P48775
BBB	390	GLU	-	expression tag	UNP P48775
BBB	391	HIS	-	expression tag	UNP P48775
BBB	392	HIS	-	expression tag	UNP P48775
BBB	393	HIS	-	expression tag	UNP P48775
BBB	394	HIS	-	expression tag	UNP P48775
BBB	395	HIS	-	expression tag	UNP P48775
BBB	396	HIS	-	expression tag	UNP P48775
CCC	17	MET	-	initiating methionine	UNP P48775
CCC	390	GLU	-	expression tag	UNP P48775
CCC	391	HIS	-	expression tag	UNP P48775
CCC	392	HIS	-	expression tag	UNP P48775
CCC	393	HIS	-	expression tag	UNP P48775

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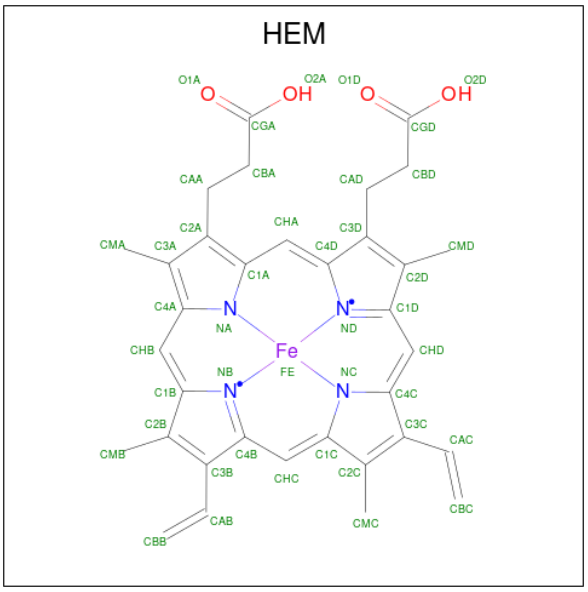
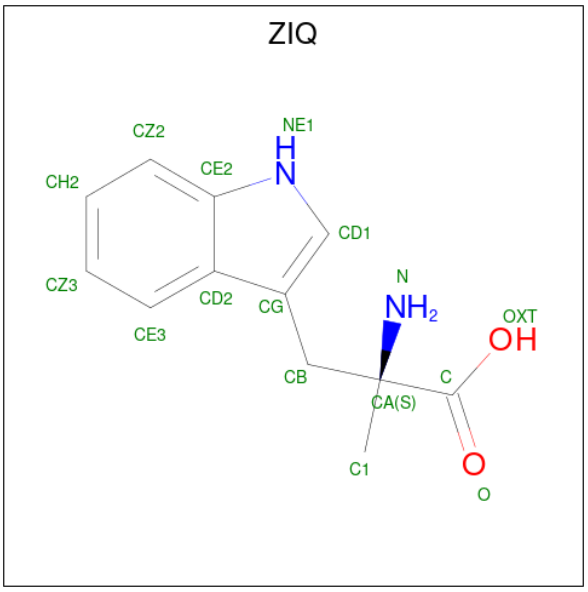
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	394	HIS	-	expression tag	UNP P48775
CCC	395	HIS	-	expression tag	UNP P48775
CCC	396	HIS	-	expression tag	UNP P48775
DDD	17	MET	-	initiating methionine	UNP P48775
DDD	390	GLU	-	expression tag	UNP P48775
DDD	391	HIS	-	expression tag	UNP P48775
DDD	392	HIS	-	expression tag	UNP P48775
DDD	393	HIS	-	expression tag	UNP P48775
DDD	394	HIS	-	expression tag	UNP P48775
DDD	395	HIS	-	expression tag	UNP P48775
DDD	396	HIS	-	expression tag	UNP P48775

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



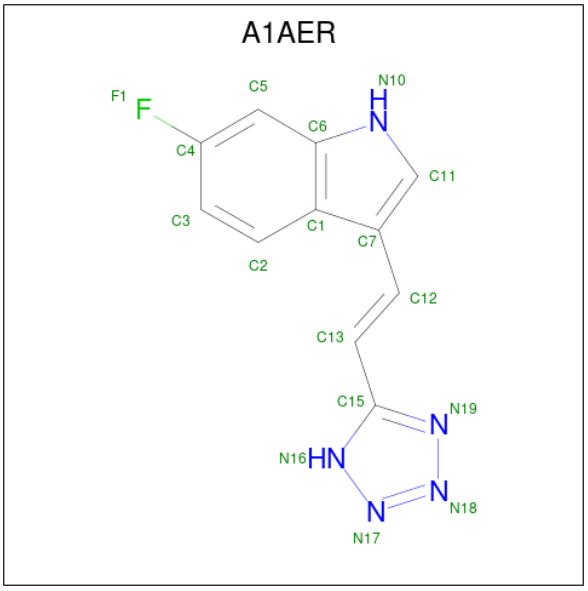
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	BBB	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	DDD	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is alpha-methyl-L-tryptophan (three-letter code: ZIQ) (formula: $C_{12}H_{14}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C N O 16 12 2 2	0	0
3	BBB	1	Total C N O 16 12 2 2	0	0
3	CCC	1	Total C N O 16 12 2 2	0	0
3	DDD	1	Total C N O 16 12 2 2	0	0

- Molecule 4 is 6-fluoro-3-[(E)-2-(1H-tetrazol-5-yl)ethenyl]-1H-indole (three-letter code: A1AER) (formula: $C_{11}H_8FN_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	F	N	0	0
			17	11	1	5		
4	BBB	1	Total	C	F	N	0	0
			17	11	1	5		
4	DDD	1	Total	C	F	N	0	0
			17	11	1	5		

- Molecule 5 is water.

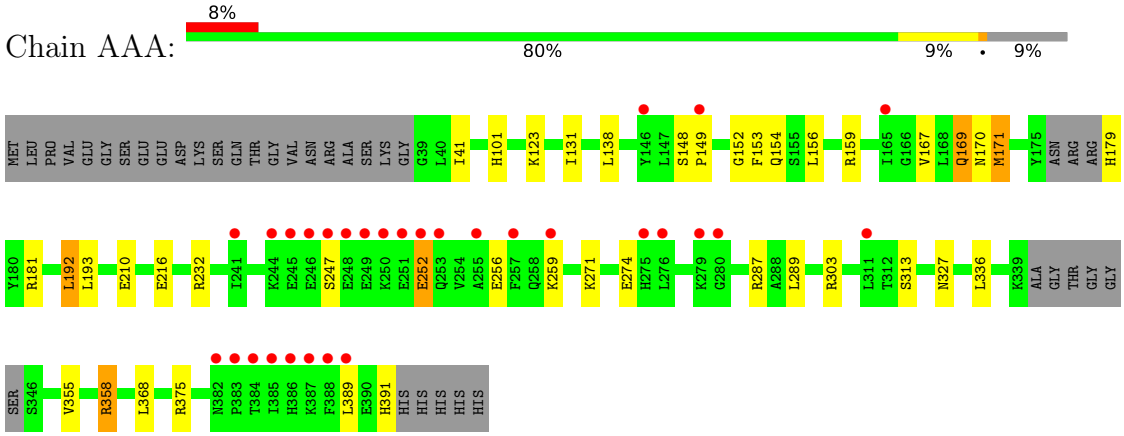
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	43	Total	O	0	0
			43	43		
5	BBB	60	Total	O	0	0
			60	60		
5	CCC	39	Total	O	0	0
			39	39		
5	DDD	47	Total	O	0	0
			47	47		

3 Residue-property plots (i)

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

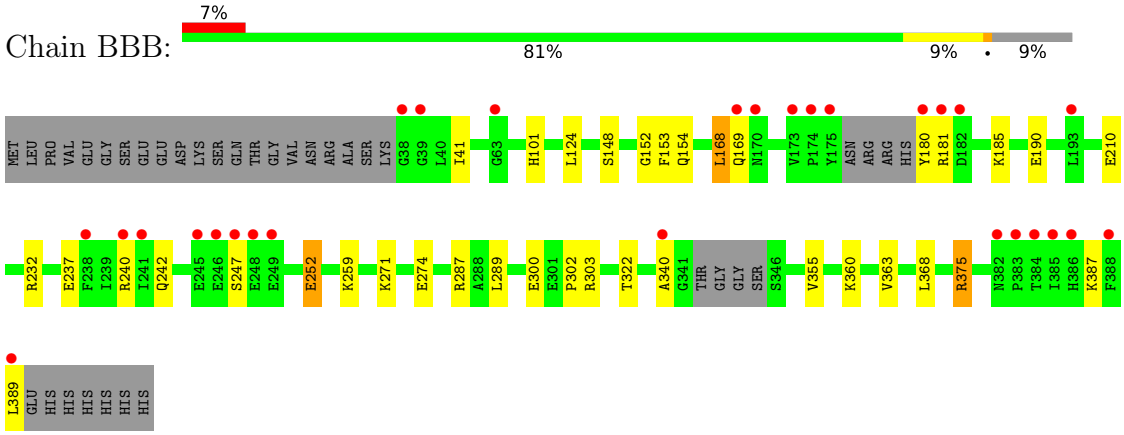
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain AAA:



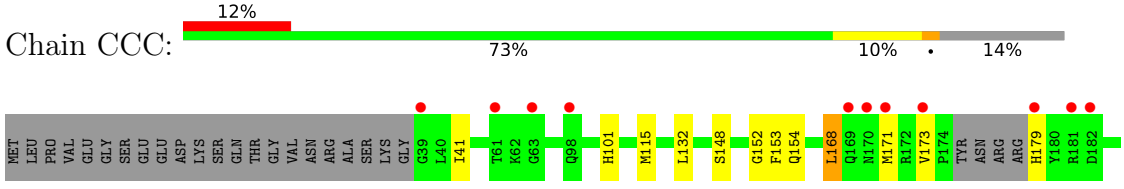
• Molecule 1: Tryptophan 2,3-dioxygenase

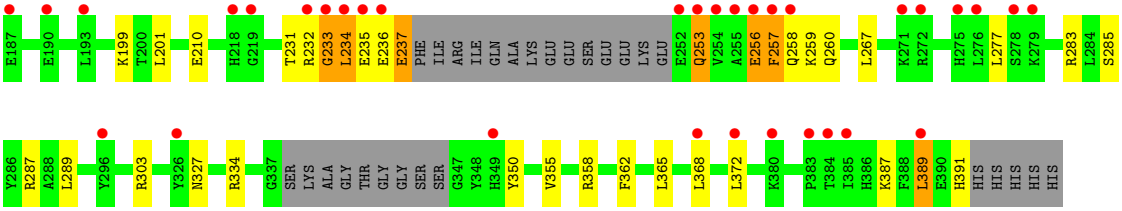
Chain BBB:



• Molecule 1: Tryptophan 2,3-dioxygenase

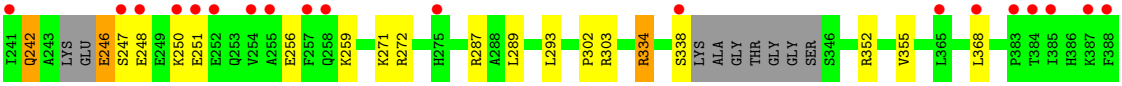
Chain CCC:





• Molecule 1: Tryptophan 2,3-dioxygenase

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.43Å 152.92Å 87.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.29 29.91 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.29) 97.3 (29.91-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.238 0.207 , 0.241	Depositor DCC
R_{free} test set	4274 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11959	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, A1AER, ZIQ

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	AAA	0.71	0/2983	0.81	1/4013 (0.0%)
1	BBB	0.71	1/2965 (0.0%)	0.83	2/3988 (0.1%)
1	CCC	0.71	0/2826	0.80	0/3804
1	DDD	0.72	0/2975	0.81	1/4003 (0.0%)
All	All	0.71	1/11749 (0.0%)	0.81	4/15808 (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	DDD	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	300	GLU	CD-OE2	5.48	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	252	GLU	CB-CA-C	5.70	121.80	110.40
1	BBB	232	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	AAA	252	GLU	CB-CA-C	5.16	120.71	110.40
1	DDD	390	GLU	CA-C-O	5.10	130.81	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	242	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2915	0	2897	20	0
1	BBB	2899	0	2888	16	0
1	CCC	2761	0	2746	29	0
1	DDD	2908	0	2890	21	0
2	AAA	43	0	30	5	0
2	BBB	43	0	30	4	0
2	CCC	43	0	30	3	0
2	DDD	43	0	30	3	0
3	AAA	16	0	0	0	0
3	BBB	16	0	0	0	0
3	CCC	16	0	0	0	0
3	DDD	16	0	0	0	0
4	AAA	17	0	0	3	0
4	BBB	17	0	0	1	0
4	DDD	17	0	0	1	0
5	AAA	43	0	0	2	0
5	BBB	60	0	0	2	0
5	CCC	39	0	0	2	0
5	DDD	47	0	0	2	0
All	All	11959	0	11541	87	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 4.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:391:HIS:C	1:DDD:390:GLU:C	2.14	1.05
1:DDD:334:ARG:NH1	5:DDD:501:HOH:O	2.15	0.79
4:BBB:403:A1AER:N10	5:BBB:501:HOH:O	2.20	0.73
1:DDD:246:GLU:HB3	1:DDD:250:LYS:HD3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:169:GLN:HG3	1:DDD:179:HIS:NE2	2.05	0.72
4:DDD:403:A1AER:N10	5:DDD:502:HOH:O	2.23	0.71
4:AAA:403:A1AER:N10	5:AAA:501:HOH:O	2.24	0.69
1:CCC:232:ARG:C	1:CCC:233:GLY:O	2.33	0.66
1:DDD:169:GLN:CG	1:DDD:179:HIS:NE2	2.61	0.64
2:AAA:401:HEM:HBC2	2:AAA:401:HEM:HHD	1.78	0.63
2:DDD:401:HEM:HBC2	2:DDD:401:HEM:HHD	1.80	0.63
1:AAA:41:ILE:HA	1:BBB:154:GLN:HE22	1.62	0.63
1:CCC:277:LEU:CD2	5:CCC:539:HOH:O	2.49	0.60
2:CCC:401:HEM:HMB1	2:CCC:401:HEM:HBB2	1.82	0.59
1:AAA:169:GLN:HG2	1:AAA:170:ASN:N	2.16	0.59
2:BBB:401:HEM:HBC2	2:BBB:401:HEM:HHD	1.87	0.56
1:CCC:173:VAL:HG23	1:CCC:350:TYR:CE1	2.43	0.54
1:AAA:154:GLN:HE22	1:BBB:41:ILE:HA	1.72	0.54
4:AAA:403:A1AER:C11	5:AAA:501:HOH:O	2.55	0.53
1:CCC:235:GLU:C	1:CCC:237:GLU:H	2.11	0.53
1:AAA:156:LEU:HD12	1:AAA:192:LEU:CD1	2.38	0.53
1:CCC:154:GLN:HE22	1:DDD:41:ILE:HA	1.74	0.53
1:DDD:248:GLU:HA	1:DDD:248:GLU:OE1	2.08	0.53
1:CCC:231:THR:O	1:CCC:233:GLY:O	2.27	0.52
1:CCC:334:ARG:HD2	5:CCC:530:HOH:O	2.09	0.52
2:CCC:401:HEM:HBB2	2:CCC:401:HEM:CMB	2.40	0.51
1:DDD:115:MET:HA	1:DDD:115:MET:CE	2.40	0.51
1:CCC:253:GLN:HA	1:CCC:253:GLN:OE1	2.11	0.51
1:DDD:303:ARG:HD3	1:DDD:389:LEU:HA	1.93	0.50
1:CCC:210:GLU:HG2	1:CCC:287:ARG:HB3	1.94	0.50
1:DDD:152:GLY:HA3	2:DDD:401:HEM:C1D	2.46	0.50
1:AAA:156:LEU:CD1	1:AAA:192:LEU:CD1	2.89	0.50
1:CCC:168:LEU:HD22	1:CCC:283:ARG:NH2	2.26	0.50
1:CCC:256:GLU:HG3	1:CCC:257:PHE:N	2.27	0.50
1:CCC:303:ARG:HD3	1:CCC:389:LEU:HA	1.93	0.49
1:AAA:167:VAL:HG13	1:AAA:171:MET:HE2	1.95	0.49
1:CCC:234:LEU:O	1:CCC:237:GLU:N	2.45	0.49
1:BBB:302:PRO:HB3	1:CCC:391:HIS:CD2	2.47	0.49
1:BBB:210:GLU:HG2	1:BBB:287:ARG:HB3	1.94	0.49
1:BBB:303:ARG:HD3	1:BBB:389:LEU:HA	1.96	0.48
1:DDD:210:GLU:HG2	1:DDD:287:ARG:HB3	1.94	0.48
1:AAA:210:GLU:HG2	1:AAA:287:ARG:HB3	1.94	0.48
1:AAA:391:HIS:ND1	1:DDD:302:PRO:HB3	2.28	0.47
1:CCC:152:GLY:HA3	2:CCC:401:HEM:C1D	2.49	0.47
1:CCC:256:GLU:O	1:CCC:259:LYS:N	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:391:HIS:C	1:DDD:390:GLU:CA	2.83	0.47
1:BBB:303:ARG:HG3	1:CCC:391:HIS:HB2	1.96	0.47
1:AAA:303:ARG:HD3	1:AAA:389:LEU:HA	1.97	0.46
1:AAA:152:GLY:HA3	2:AAA:401:HEM:C1D	2.50	0.46
1:BBB:168:LEU:HD22	1:BBB:168:LEU:HA	1.88	0.46
2:DDD:401:HEM:HMB1	2:DDD:401:HEM:HBB2	1.97	0.45
2:AAA:401:HEM:HBC2	2:AAA:401:HEM:CHD	2.45	0.45
1:AAA:131:ILE:CD1	1:BBB:124:LEU:HD22	2.47	0.45
1:AAA:138:LEU:CD1	1:CCC:372:LEU:HD22	2.46	0.44
1:CCC:168:LEU:HD12	1:CCC:168:LEU:HA	1.78	0.44
1:BBB:237:GLU:HG3	1:BBB:240:ARG:NH2	2.33	0.44
1:AAA:171:MET:HE3	1:AAA:358:ARG:O	2.17	0.44
1:AAA:336:LEU:HD11	4:AAA:403:A1AER:N16	2.33	0.44
1:BBB:355:VAL:HG12	1:BBB:355:VAL:O	2.18	0.44
1:CCC:41:ILE:HA	1:DDD:154:GLN:HE22	1.83	0.43
1:CCC:173:VAL:HG23	1:CCC:350:TYR:HE1	1.80	0.43
1:BBB:152:GLY:HA3	2:BBB:401:HEM:C1D	2.53	0.43
1:DDD:289:LEU:HD11	1:DDD:368:LEU:HD21	2.00	0.43
1:CCC:115:MET:HE2	1:CCC:201:LEU:HD21	1.99	0.43
1:CCC:256:GLU:O	1:CCC:258:GLN:N	2.51	0.43
1:CCC:289:LEU:HD11	1:CCC:368:LEU:HD21	1.99	0.43
1:BBB:180:TYR:N	5:BBB:504:HOH:O	2.52	0.43
1:AAA:159:ARG:NH2	2:AAA:401:HEM:O1D	2.47	0.43
2:AAA:401:HEM:HBB2	2:AAA:401:HEM:HMB1	2.01	0.43
1:DDD:238:PHE:C	1:DDD:238:PHE:CD2	2.92	0.43
1:AAA:131:ILE:HD12	1:BBB:124:LEU:HD22	2.02	0.42
1:AAA:355:VAL:HG12	1:AAA:355:VAL:O	2.20	0.42
1:CCC:355:VAL:HG12	1:CCC:355:VAL:O	2.19	0.42
1:DDD:355:VAL:O	1:DDD:355:VAL:HG12	2.19	0.42
1:CCC:233:GLY:O	1:CCC:235:GLU:N	2.53	0.42
1:AAA:289:LEU:HD11	1:AAA:368:LEU:HD21	2.02	0.42
1:BBB:289:LEU:HD11	1:BBB:368:LEU:HD21	2.01	0.42
1:BBB:322:THR:HG21	1:BBB:360:LYS:HE2	2.02	0.42
1:CCC:362:PHE:HB3	1:CCC:365:LEU:HD12	2.03	0.41
1:DDD:289:LEU:CD1	1:DDD:368:LEU:HD21	2.50	0.41
1:BBB:375:ARG:NH2	1:DDD:142:ASP:OD2	2.54	0.41
2:BBB:401:HEM:HMB1	2:BBB:401:HEM:HBB2	2.03	0.41
2:BBB:401:HEM:HHD	2:BBB:401:HEM:CBC	2.52	0.40
1:CCC:132:LEU:HD12	1:CCC:132:LEU:HA	1.87	0.40
1:DDD:191:LEU:HD12	1:DDD:191:LEU:HA	1.83	0.40
1:CCC:232:ARG:O	1:CCC:233:GLY:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:293:LEU:HD12	1:DDD:293:LEU:HA	1.96	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	AAA	338/380 (89%)	329 (97%)	9 (3%)	0	100 100
1	BBB	338/380 (89%)	325 (96%)	12 (4%)	1 (0%)	41 50
1	CCC	318/380 (84%)	306 (96%)	7 (2%)	5 (2%)	9 9
1	DDD	337/380 (89%)	328 (97%)	9 (3%)	0	100 100
All	All	1331/1520 (88%)	1288 (97%)	37 (3%)	6 (0%)	29 35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	340	ALA
1	CCC	257	PHE
1	CCC	233	GLY
1	CCC	234	LEU
1	CCC	236	GLU
1	CCC	285	SER

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	AAA	320/348 (92%)	297 (93%)	23 (7%)	14 18
1	BBB	317/348 (91%)	300 (95%)	17 (5%)	22 30
1	CCC	303/348 (87%)	287 (95%)	16 (5%)	22 31
1	DDD	319/348 (92%)	299 (94%)	20 (6%)	18 24
All	All	1259/1392 (90%)	1183 (94%)	76 (6%)	19 26

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	101	HIS
1	AAA	123	LYS
1	AAA	148	SER
1	AAA	149	PRO
1	AAA	153	PHE
1	AAA	169	GLN
1	AAA	171	MET
1	AAA	179	HIS
1	AAA	181	ARG
1	AAA	192	LEU
1	AAA	193	LEU
1	AAA	216	GLU
1	AAA	232	ARG
1	AAA	247	SER
1	AAA	252	GLU
1	AAA	256	GLU
1	AAA	259	LYS
1	AAA	271	LYS
1	AAA	274	GLU
1	AAA	313	SER
1	AAA	327	ASN
1	AAA	358	ARG
1	AAA	375	ARG
1	BBB	101	HIS
1	BBB	148	SER
1	BBB	153	PHE
1	BBB	168	LEU
1	BBB	169	GLN
1	BBB	181	ARG
1	BBB	185	LYS
1	BBB	190	GLU

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Mol	Chain	Res	Type
1	BBB	242	GLN
1	BBB	247	SER
1	BBB	252	GLU
1	BBB	259	LYS
1	BBB	271	LYS
1	BBB	274	GLU
1	BBB	363	VAL
1	BBB	375	ARG
1	BBB	387	LYS
1	CCC	101	HIS
1	CCC	148	SER
1	CCC	153	PHE
1	CCC	168	LEU
1	CCC	171	MET
1	CCC	179	HIS
1	CCC	199	LYS
1	CCC	237	GLU
1	CCC	253	GLN
1	CCC	256	GLU
1	CCC	260	GLN
1	CCC	267	LEU
1	CCC	327	ASN
1	CCC	358	ARG
1	CCC	387	LYS
1	CCC	389	LEU
1	DDD	101	HIS
1	DDD	148	SER
1	DDD	149	PRO
1	DDD	153	PHE
1	DDD	169	GLN
1	DDD	185	LYS
1	DDD	191	LEU
1	DDD	193	LEU
1	DDD	238	PHE
1	DDD	242	GLN
1	DDD	246	GLU
1	DDD	247	SER
1	DDD	251	GLU
1	DDD	256	GLU
1	DDD	259	LYS
1	DDD	271	LYS
1	DDD	272	ARG

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Mol	Chain	Res	Type
1	DDD	334	ARG
1	DDD	338	SER
1	DDD	352	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

11 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	$\#\|Z\| > 2$
2	HEM	AAA	401	5,1	41,50,50	1.50	7 (17%)	45,82,82	2.00	16 (35%)
4	A1AER	BBB	403	-	18,19,19	2.35	8 (44%)	19,26,26	3.07	8 (42%)
3	ZIQ	BBB	402	-	13,17,17	2.78	6 (46%)	14,25,25	5.36	7 (50%)
2	HEM	CCC	401	5,1	41,50,50	1.46	7 (17%)	45,82,82	1.85	11 (24%)
3	ZIQ	DDD	402	-	13,17,17	2.89	5 (38%)	14,25,25	5.82	8 (57%)
4	A1AER	DDD	403	-	18,19,19	2.08	6 (33%)	19,26,26	3.19	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ZIQ	AAA	402	-	13,17,17	3.11	2 (15%)	14,25,25	5.85	8 (57%)
2	HEM	DDD	401	5,1	41,50,50	1.35	7 (17%)	45,82,82	1.88	15 (33%)
3	ZIQ	CCC	402	-	13,17,17	2.99	4 (30%)	14,25,25	5.60	6 (42%)
4	A1AER	AAA	403	-	18,19,19	2.41	5 (27%)	19,26,26	3.34	7 (36%)
2	HEM	BBB	401	5,1	41,50,50	1.50	8 (19%)	45,82,82	2.08	17 (37%)

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
2	HEM	AAA	401	5,1	-	3/12/54/54	-
4	A1AER	BBB	403	-	-	0/3/5/5	0/3/3/3
3	ZIQ	BBB	402	-	-	2/9/11/11	0/2/2/2
2	HEM	CCC	401	5,1	-	2/12/54/54	-
3	ZIQ	DDD	402	-	-	4/9/11/11	0/2/2/2
4	A1AER	DDD	403	-	-	0/3/5/5	0/3/3/3
3	ZIQ	AAA	402	-	-	4/9/11/11	0/2/2/2
2	HEM	DDD	401	5,1	-	2/12/54/54	-
3	ZIQ	CCC	402	-	-	0/9/11/11	0/2/2/2
4	A1AER	AAA	403	-	-	0/3/5/5	0/3/3/3
2	HEM	BBB	401	5,1	-	2/12/54/54	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	402	ZIQ	CE3-CD2	-9.05	1.23	1.42
3	CCC	402	ZIQ	CE3-CD2	-8.15	1.25	1.42
3	DDD	402	ZIQ	CE3-CD2	-7.39	1.27	1.42
3	BBB	402	ZIQ	CE3-CD2	-7.30	1.27	1.42
4	AAA	403	A1AER	N18-N17	5.49	1.42	1.32
4	BBB	403	A1AER	N18-N17	5.27	1.41	1.32
4	DDD	403	A1AER	N18-N17	5.22	1.41	1.32
3	AAA	402	ZIQ	CZ3-CE3	-4.84	1.25	1.36
3	DDD	402	ZIQ	CZ3-CE3	-4.69	1.26	1.36
3	CCC	402	ZIQ	CZ3-CE3	-4.51	1.26	1.36
4	BBB	403	A1AER	N19-N18	4.42	1.41	1.34
4	AAA	403	A1AER	C15-N16	-4.33	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	401	HEM	C4D-ND	-4.00	1.33	1.40
4	AAA	403	A1AER	N19-N18	3.90	1.40	1.34
4	AAA	403	A1AER	N16-N17	3.63	1.40	1.34
2	CCC	401	HEM	C1B-NB	-3.50	1.34	1.40
4	BBB	403	A1AER	C15-N16	-3.48	1.30	1.33
4	DDD	403	A1AER	C15-N16	-3.41	1.30	1.33
4	BBB	403	A1AER	N16-N17	3.32	1.39	1.34
2	CCC	401	HEM	C4B-NB	-3.26	1.32	1.38
2	AAA	401	HEM	C2C-C1C	-3.24	1.35	1.42
2	DDD	401	HEM	C1B-NB	-3.16	1.34	1.40
4	DDD	403	A1AER	N19-N18	3.14	1.39	1.34
2	CCC	401	HEM	C4D-ND	-3.02	1.35	1.40
4	AAA	403	A1AER	C5-C4	2.99	1.41	1.36
2	BBB	401	HEM	CBD-CGD	2.97	1.57	1.50
2	AAA	401	HEM	C4D-ND	-2.96	1.35	1.40
3	BBB	402	ZIQ	CZ3-CE3	-2.95	1.30	1.36
3	CCC	402	ZIQ	CH2-CZ2	2.92	1.43	1.36
2	DDD	401	HEM	C3B-C4B	2.91	1.50	1.44
3	DDD	402	ZIQ	CB-CA	-2.87	1.51	1.55
3	BBB	402	ZIQ	CH2-CZ3	2.84	1.45	1.38
3	BBB	402	ZIQ	CD2-CE2	2.81	1.50	1.42
4	DDD	403	A1AER	C5-C6	-2.79	1.37	1.41
2	AAA	401	HEM	C1B-NB	-2.78	1.35	1.40
3	DDD	402	ZIQ	CH2-CZ2	2.78	1.43	1.36
2	AAA	401	HEM	C4B-NB	-2.74	1.33	1.38
2	AAA	401	HEM	CHB-C1B	2.74	1.42	1.35
2	AAA	401	HEM	C3C-C2C	-2.74	1.36	1.40
3	BBB	402	ZIQ	CH2-CZ2	2.60	1.42	1.36
4	BBB	403	A1AER	C1-C6	2.55	1.49	1.42
2	CCC	401	HEM	FE-NB	2.55	2.09	1.96
4	DDD	403	A1AER	C2-C1	-2.54	1.37	1.42
2	AAA	401	HEM	FE-NB	2.54	2.09	1.96
2	BBB	401	HEM	C4B-NB	-2.48	1.33	1.38
2	DDD	401	HEM	C4D-ND	-2.45	1.36	1.40
2	BBB	401	HEM	FE-NB	2.44	2.08	1.96
2	BBB	401	HEM	C3B-C4B	2.42	1.49	1.44
2	DDD	401	HEM	C4B-NB	-2.35	1.34	1.38
2	BBB	401	HEM	CHB-C1B	2.32	1.40	1.35
2	BBB	401	HEM	CBA-CGA	2.28	1.55	1.50
2	CCC	401	HEM	C4D-C3D	2.21	1.48	1.45
2	BBB	401	HEM	CBD-CAD	2.21	1.59	1.52
4	DDD	403	A1AER	N16-N17	2.14	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	403	A1AER	C5-C4	2.14	1.39	1.36
2	CCC	401	HEM	C3B-C4B	2.13	1.49	1.44
4	BBB	403	A1AER	C7-C1	2.13	1.46	1.41
3	DDD	402	ZIQ	O-C	2.12	1.29	1.22
2	CCC	401	HEM	CHB-C1B	2.12	1.40	1.35
2	DDD	401	HEM	C1D-C2D	2.10	1.48	1.44
3	BBB	402	ZIQ	CD1-NE1	2.09	1.40	1.36
4	BBB	403	A1AER	F1-C4	-2.08	1.31	1.36
2	DDD	401	HEM	FE-NB	2.04	2.06	1.96
3	CCC	402	ZIQ	CB-CA	-2.03	1.52	1.55
2	DDD	401	HEM	FE-ND	-2.02	1.86	1.96

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	402	ZIQ	CZ3-CE3-CD2	17.51	145.18	120.89
3	DDD	402	ZIQ	CZ3-CE3-CD2	17.34	144.94	120.89
3	CCC	402	ZIQ	CZ3-CE3-CD2	17.02	144.50	120.89
3	BBB	402	ZIQ	CZ3-CE3-CD2	16.07	143.18	120.89
3	AAA	402	ZIQ	CH2-CZ3-CE3	-9.19	107.55	120.44
3	DDD	402	ZIQ	CH2-CZ3-CE3	-9.08	107.71	120.44
3	BBB	402	ZIQ	CH2-CZ3-CE3	-8.25	108.87	120.44
3	CCC	402	ZIQ	CH2-CZ3-CE3	-7.90	109.37	120.44
4	BBB	403	A1AER	N16-N17-N18	-7.55	104.60	109.53
3	CCC	402	ZIQ	CE3-CD2-CE2	-6.87	109.05	118.17
4	AAA	403	A1AER	C15-C13-C12	-6.48	109.85	123.69
3	BBB	402	ZIQ	CE3-CD2-CE2	-6.45	109.61	118.17
4	AAA	403	A1AER	C2-C1-C6	6.36	126.61	118.17
3	DDD	402	ZIQ	CE3-CD2-CE2	-6.27	109.86	118.17
4	DDD	403	A1AER	C15-C13-C12	-6.26	110.31	123.69
4	DDD	403	A1AER	N16-N17-N18	-6.11	105.54	109.53
4	AAA	403	A1AER	C5-C6-C1	-6.07	113.34	121.16
4	AAA	403	A1AER	N16-N17-N18	-5.87	105.70	109.53
4	DDD	403	A1AER	C2-C1-C6	5.72	125.75	118.17
3	AAA	402	ZIQ	CE3-CD2-CE2	-5.62	110.71	118.17
4	DDD	403	A1AER	N16-C15-N19	5.18	117.16	111.45
4	DDD	403	A1AER	C5-C6-C1	-5.06	114.64	121.16
4	BBB	403	A1AER	C15-C13-C12	-4.98	113.03	123.69
4	BBB	403	A1AER	C2-C1-C6	4.98	124.77	118.17
4	BBB	403	A1AER	C5-C6-C1	-4.91	114.84	121.16
3	AAA	402	ZIQ	CB-CG-CD1	4.58	133.62	127.97
4	AAA	403	A1AER	N16-C15-N19	4.51	116.41	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	401	HEM	CHC-C4B-NB	4.44	129.26	124.43
2	AAA	401	HEM	CHC-C4B-NB	4.44	129.26	124.43
2	AAA	401	HEM	C1B-NB-C4B	4.31	109.53	105.07
2	CCC	401	HEM	CHD-C1D-ND	4.26	129.06	124.43
2	AAA	401	HEM	CBD-CAD-C3D	-4.13	101.15	112.63
4	BBB	403	A1AER	N16-C15-N19	4.08	115.94	111.45
2	DDD	401	HEM	CBD-CAD-C3D	-3.95	101.66	112.63
2	DDD	401	HEM	CHD-C1D-ND	3.89	128.66	124.43
2	BBB	401	HEM	C4A-C3A-C2A	3.86	109.68	107.00
2	BBB	401	HEM	CHD-C1D-ND	3.83	128.60	124.43
2	DDD	401	HEM	CHC-C4B-NB	3.82	128.58	124.43
2	CCC	401	HEM	CBD-CAD-C3D	-3.82	102.02	112.63
2	BBB	401	HEM	CHD-C1D-C2D	-3.81	119.03	124.98
2	CCC	401	HEM	CHC-C4B-NB	3.78	128.54	124.43
2	BBB	401	HEM	C1B-NB-C4B	3.72	108.92	105.07
3	DDD	402	ZIQ	CB-CG-CD1	3.62	132.43	127.97
2	BBB	401	HEM	CBD-CAD-C3D	-3.61	102.59	112.63
2	CCC	401	HEM	CBA-CAA-C2A	-3.56	106.55	112.62
2	AAA	401	HEM	CHA-C4D-ND	3.55	128.76	124.38
4	DDD	403	A1AER	C3-C2-C1	-3.53	116.22	121.13
2	DDD	401	HEM	CBA-CAA-C2A	-3.48	106.68	112.62
3	CCC	402	ZIQ	CE3-CD2-CG	3.48	140.80	134.42
2	AAA	401	HEM	CHD-C1D-ND	3.48	128.21	124.43
2	AAA	401	HEM	C4B-C3B-C2B	-3.44	104.39	107.11
2	CCC	401	HEM	CHD-C1D-C2D	-3.41	119.65	124.98
4	AAA	403	A1AER	C3-C2-C1	-3.28	116.57	121.13
2	DDD	401	HEM	CHA-C4D-ND	3.24	128.38	124.38
3	DDD	402	ZIQ	CZ2-CE2-NE1	3.23	139.74	130.80
3	DDD	402	ZIQ	CB-CA-C	-3.18	104.53	109.02
2	AAA	401	HEM	CHB-C1B-NB	3.16	128.29	124.38
2	BBB	401	HEM	O2D-CGD-O1D	-3.11	115.54	123.30
3	AAA	402	ZIQ	CZ2-CE2-CD2	-3.11	115.07	120.76
3	BBB	402	ZIQ	CE3-CD2-CG	3.04	139.99	134.42
4	BBB	403	A1AER	C7-C12-C13	-3.01	116.81	125.76
2	DDD	401	HEM	C1B-NB-C4B	2.99	108.16	105.07
3	AAA	402	ZIQ	CB-CA-C	-2.95	104.85	109.02
2	CCC	401	HEM	CAD-C3D-C4D	2.93	129.78	124.66
3	DDD	402	ZIQ	CE3-CD2-CG	2.91	139.75	134.42
4	BBB	403	A1AER	C3-C2-C1	-2.89	117.11	121.13
3	AAA	402	ZIQ	CZ2-CE2-NE1	2.88	138.77	130.80
2	DDD	401	HEM	CHA-C4D-C3D	-2.83	120.01	125.33
2	DDD	401	HEM	CMA-C3A-C4A	-2.78	124.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	401	HEM	O2D-CGD-CBD	2.76	122.90	114.03
2	AAA	401	HEM	CHA-C4D-C3D	-2.75	120.17	125.33
2	BBB	401	HEM	CMA-C3A-C4A	-2.74	124.25	128.46
2	BBB	401	HEM	CAD-CBD-CGD	2.70	119.42	113.60
2	CCC	401	HEM	O2D-CGD-CBD	2.67	122.61	114.03
3	CCC	402	ZIQ	CZ2-CE2-NE1	2.66	138.16	130.80
2	AAA	401	HEM	C3C-C4C-NC	-2.62	106.00	110.94
3	BBB	402	ZIQ	CZ2-CE2-NE1	2.56	137.89	130.80
2	AAA	401	HEM	CHD-C1D-C2D	-2.56	120.98	124.98
2	DDD	401	HEM	C4B-C3B-C2B	-2.56	105.08	107.11
3	CCC	402	ZIQ	C1-CA-CB	-2.53	107.52	110.94
2	AAA	401	HEM	CAD-CBD-CGD	2.51	119.01	113.60
2	DDD	401	HEM	CHD-C1D-C2D	-2.50	121.07	124.98
4	AAA	403	A1AER	C11-C7-C1	2.46	114.08	107.94
2	CCC	401	HEM	CAD-CBD-CGD	2.46	118.89	113.60
3	BBB	402	ZIQ	CB-CG-CD1	2.45	130.99	127.97
2	BBB	401	HEM	O2A-CGA-O1A	-2.44	117.22	123.30
3	DDD	402	ZIQ	CZ2-CE2-CD2	-2.42	116.33	120.76
3	AAA	402	ZIQ	CE3-CD2-CG	2.36	138.76	134.42
2	BBB	401	HEM	CAD-C3D-C4D	2.36	128.78	124.66
3	BBB	402	ZIQ	C1-CA-CB	-2.35	107.75	110.94
2	CCC	401	HEM	CHB-C1B-NB	2.34	127.27	124.38
2	CCC	401	HEM	C1B-NB-C4B	2.31	107.45	105.07
2	CCC	401	HEM	C4B-C3B-C2B	-2.30	105.29	107.11
2	BBB	401	HEM	CHB-C1B-NB	2.29	127.22	124.38
2	BBB	401	HEM	CHA-C4D-ND	2.28	127.20	124.38
2	BBB	401	HEM	O2A-CGA-CBA	2.28	121.36	114.03
2	AAA	401	HEM	O2D-CGD-CBD	2.23	121.19	114.03
2	BBB	401	HEM	CAA-CBA-CGA	2.21	119.96	113.76
2	AAA	401	HEM	CBA-CAA-C2A	-2.19	108.89	112.62
4	BBB	403	A1AER	C3-C4-C5	2.18	125.63	123.23
2	AAA	401	HEM	CMD-C2D-C1D	2.16	128.33	125.04
2	DDD	401	HEM	C4A-C3A-C2A	2.16	108.50	107.00
2	BBB	401	HEM	CHA-C4D-C3D	-2.12	121.34	125.33
2	DDD	401	HEM	CHB-C1B-NB	2.12	127.00	124.38
2	AAA	401	HEM	C3B-C2B-C1B	2.07	108.02	106.49
2	DDD	401	HEM	CAA-CBA-CGA	-2.06	107.97	113.76
2	DDD	401	HEM	CAD-CBD-CGD	2.02	117.96	113.60
2	AAA	401	HEM	O2D-CGD-O1D	-2.01	118.28	123.30
2	DDD	401	HEM	O2D-CGD-CBD	2.01	120.49	114.03

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	402	ZIQ	OXT-C-CA-C1
3	DDD	402	ZIQ	O-C-CA-C1
3	DDD	402	ZIQ	OXT-C-CA-C1
3	AAA	402	ZIQ	O-C-CA-C1
3	DDD	402	ZIQ	O-C-CA-CB
3	DDD	402	ZIQ	OXT-C-CA-CB
2	AAA	401	HEM	CAA-CBA-CGA-O1A
2	CCC	401	HEM	CAA-CBA-CGA-O1A
3	AAA	402	ZIQ	OXT-C-CA-CB
2	DDD	401	HEM	CAA-CBA-CGA-O2A
2	BBB	401	HEM	CAA-CBA-CGA-O1A
2	BBB	401	HEM	CAA-CBA-CGA-O2A
2	AAA	401	HEM	CAA-CBA-CGA-O2A
2	CCC	401	HEM	CAA-CBA-CGA-O2A
2	DDD	401	HEM	CAA-CBA-CGA-O1A
3	BBB	402	ZIQ	O-C-CA-C1
3	BBB	402	ZIQ	OXT-C-CA-C1
3	AAA	402	ZIQ	O-C-CA-CB
2	AAA	401	HEM	C2A-CAA-CBA-CGA

There are no ring outliers.

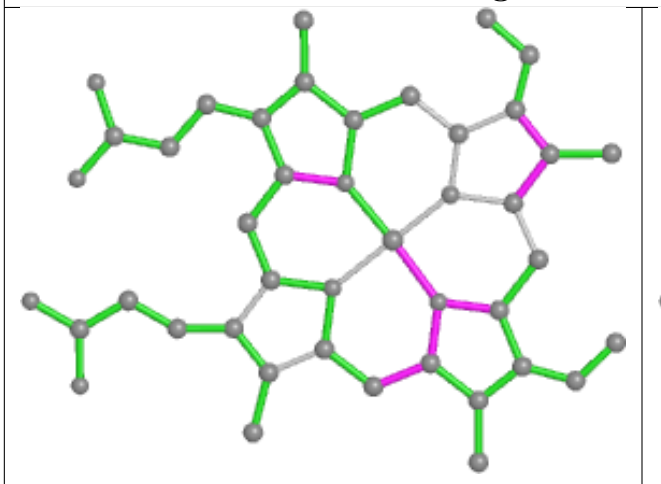
7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	HEM	5	0
4	BBB	403	A1AER	1	0
2	CCC	401	HEM	3	0
4	DDD	403	A1AER	1	0
2	DDD	401	HEM	3	0
4	AAA	403	A1AER	3	0
2	BBB	401	HEM	4	0

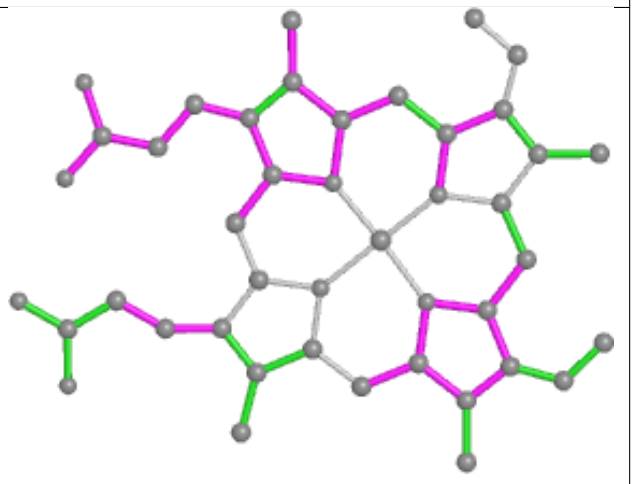
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

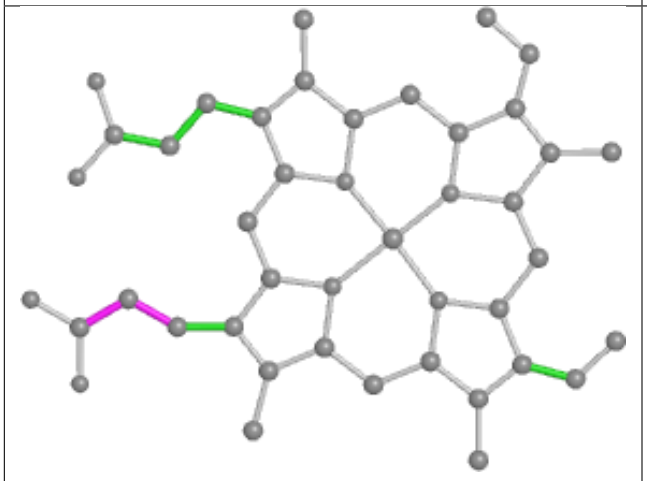
Ligand HEM AAA 401



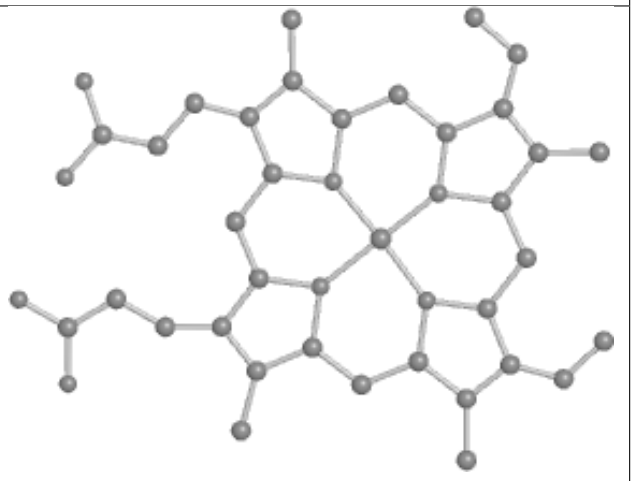
Bond lengths



Bond angles

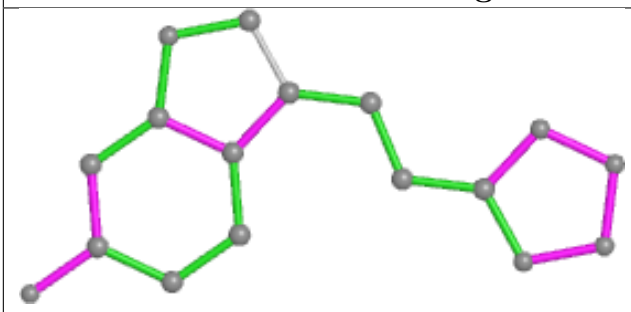


Torsions

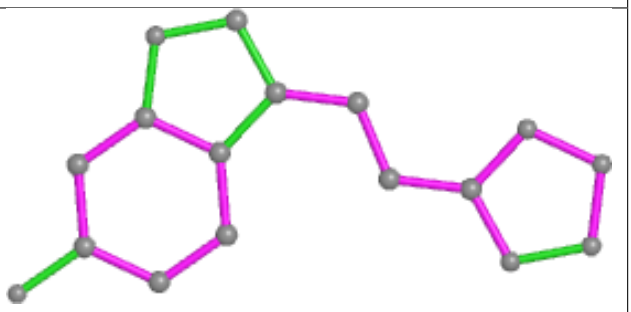


Rings

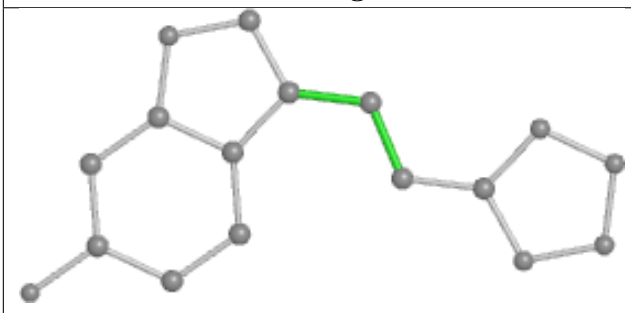
Ligand A1AER BBB 403



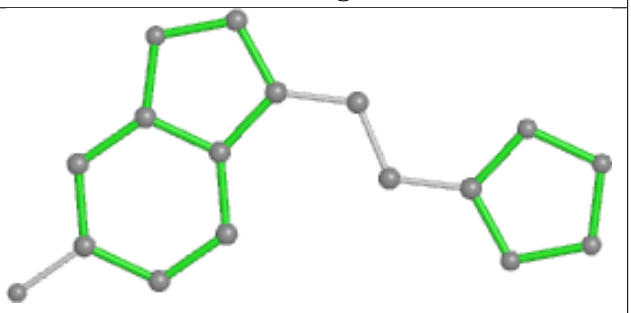
Bond lengths



Bond angles

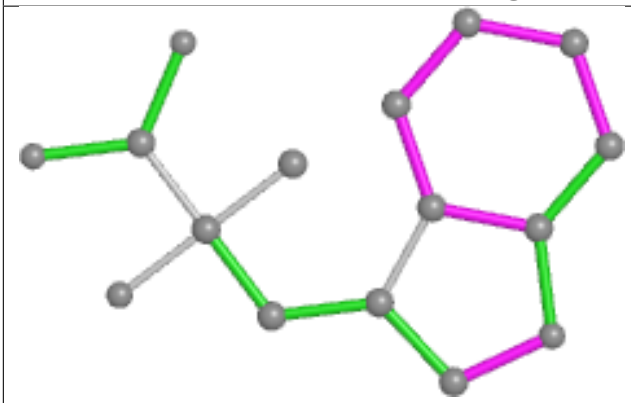


Torsions

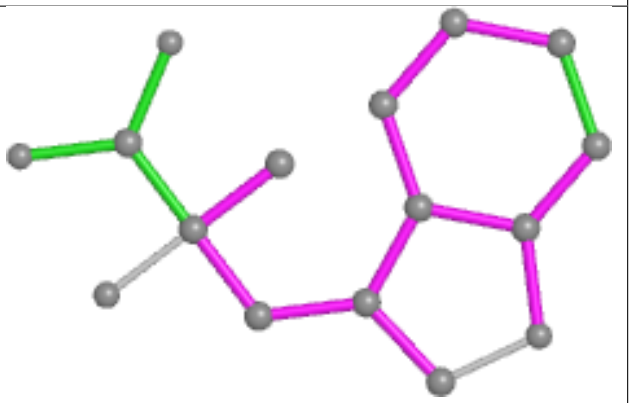


Rings

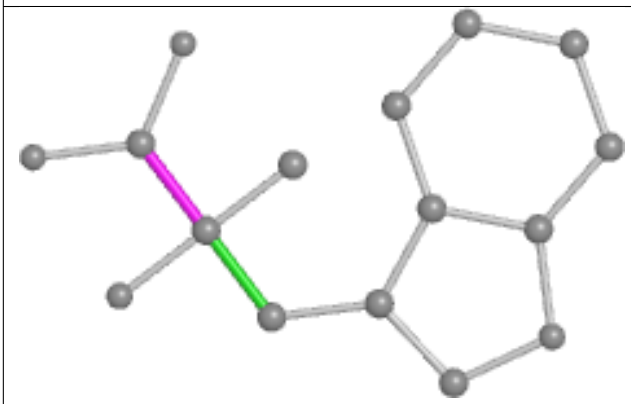
Ligand ZIQ BBB 402



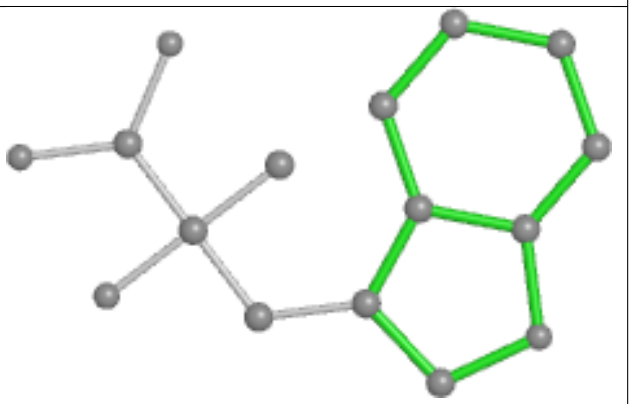
Bond lengths



Bond angles

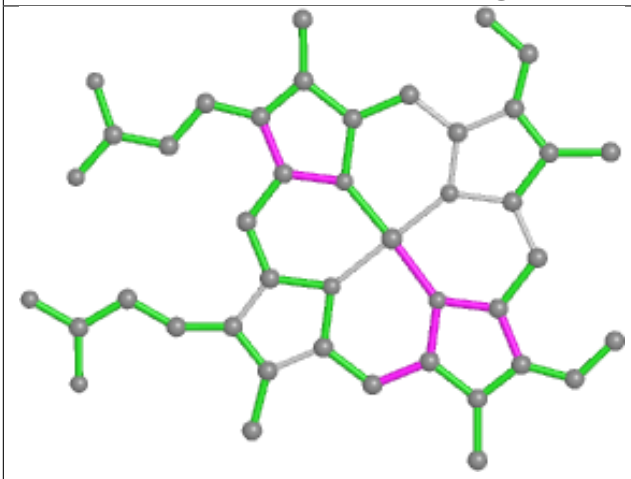


Torsions

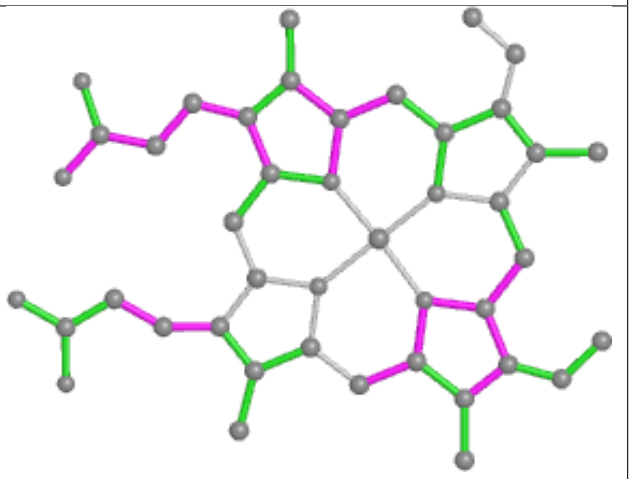


Rings

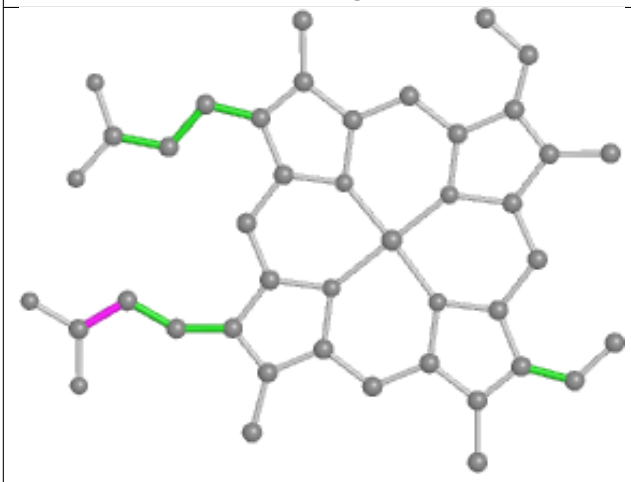
Ligand HEM CCC 401



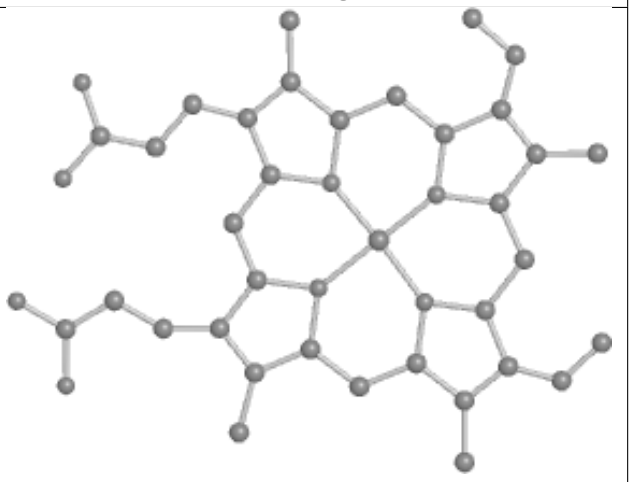
Bond lengths



Bond angles

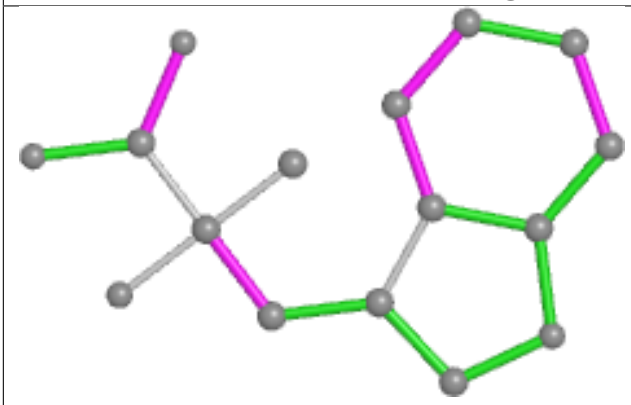


Torsions

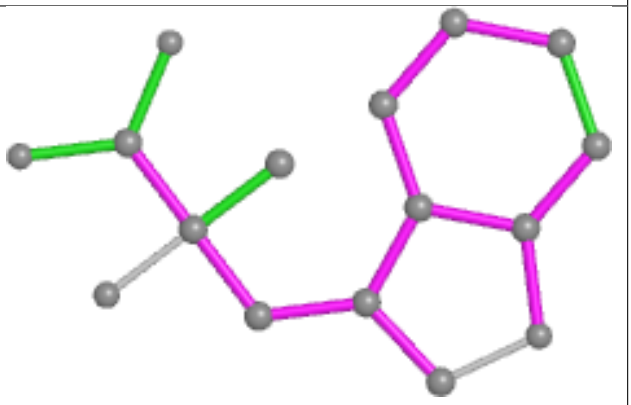


Rings

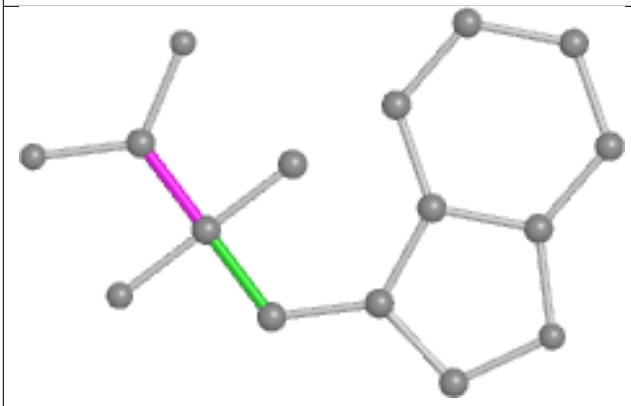
Ligand ZIQ DDD 402



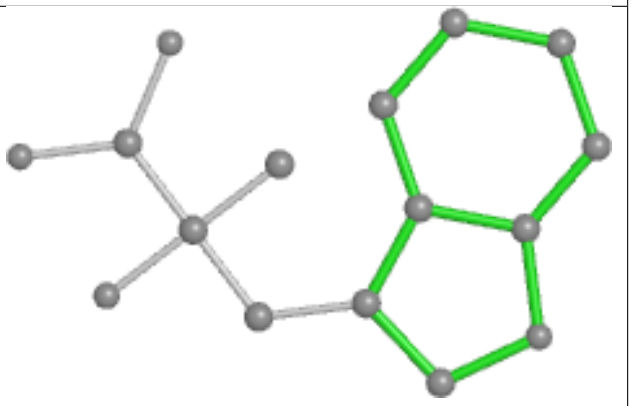
Bond lengths



Bond angles

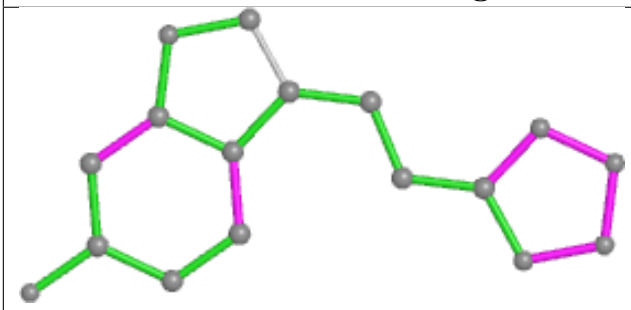


Torsions



Rings

Ligand A1AER DDD 403



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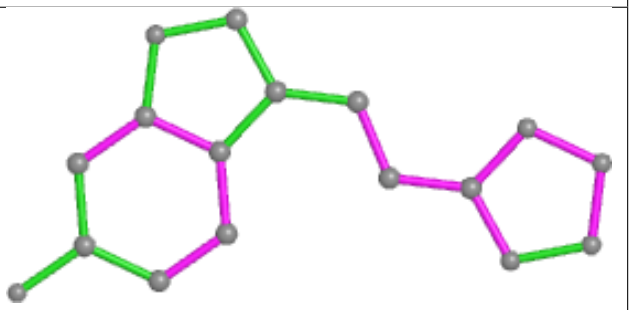
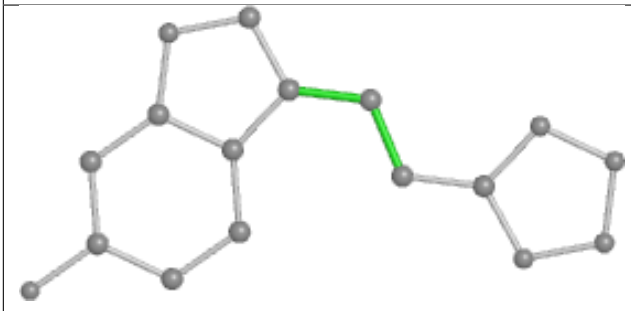
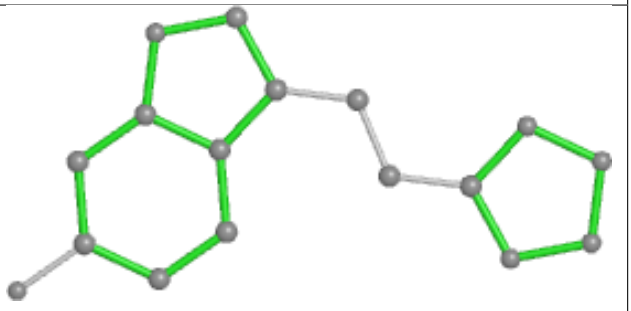


Bond angles

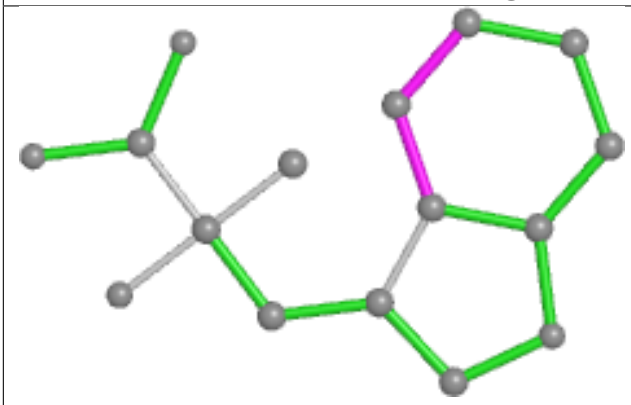


Torsions

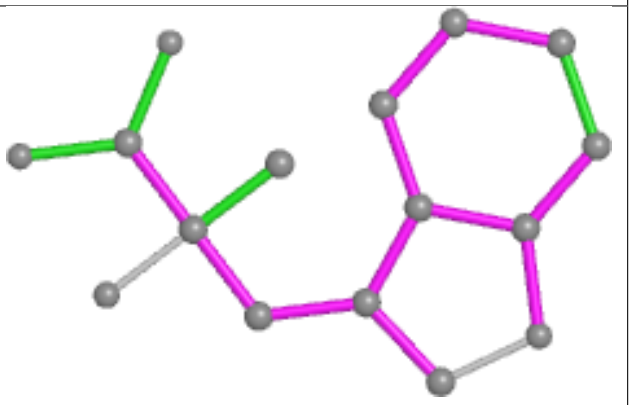


Rings

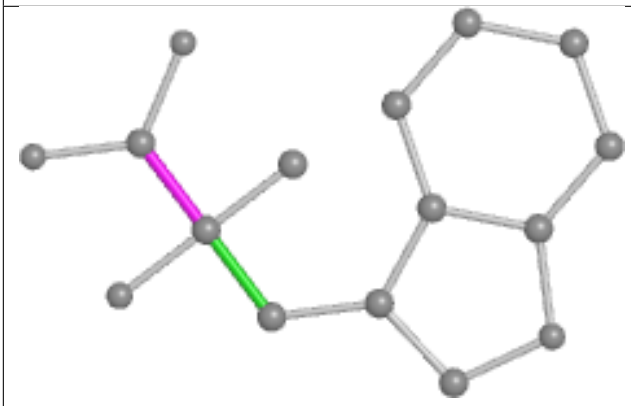
Ligand ZIQ AAA 402



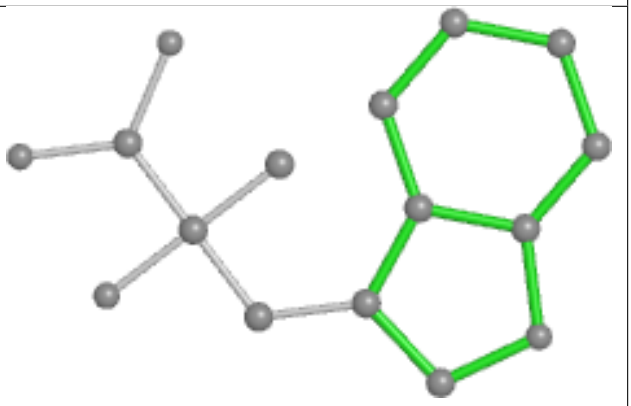
Bond lengths



Bond angles

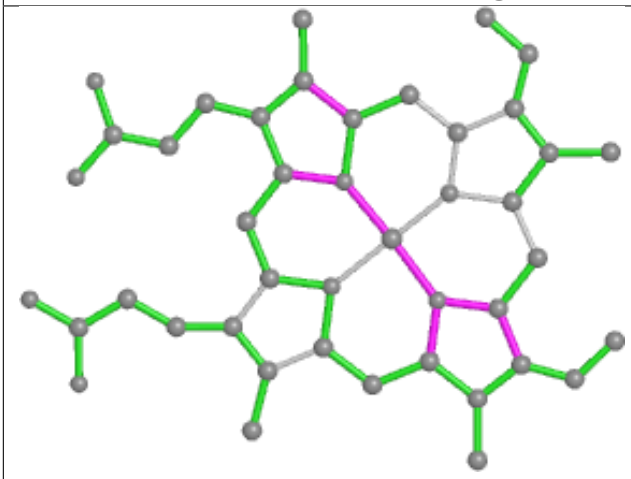


Torsions

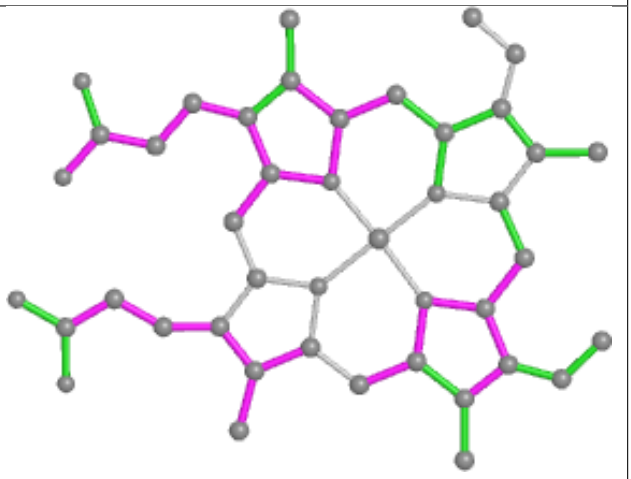


Rings

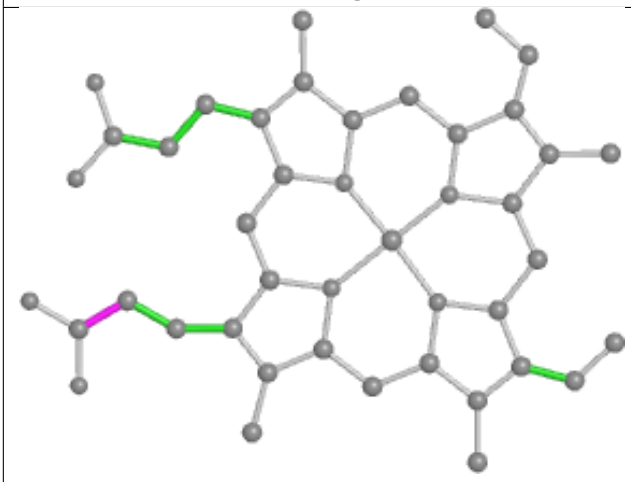
Ligand HEM DDD 401



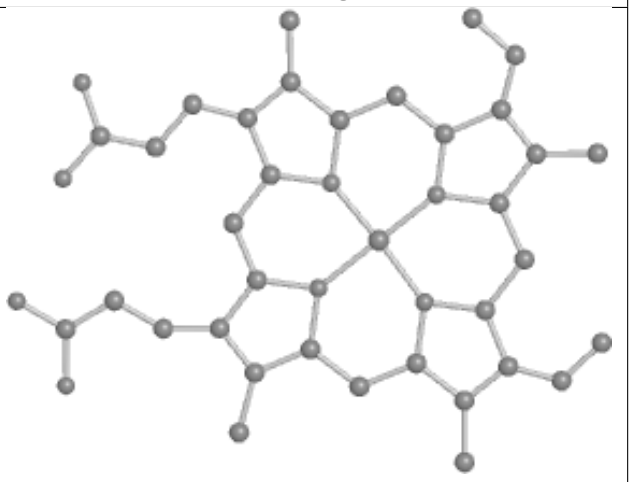
Bond lengths



Bond angles

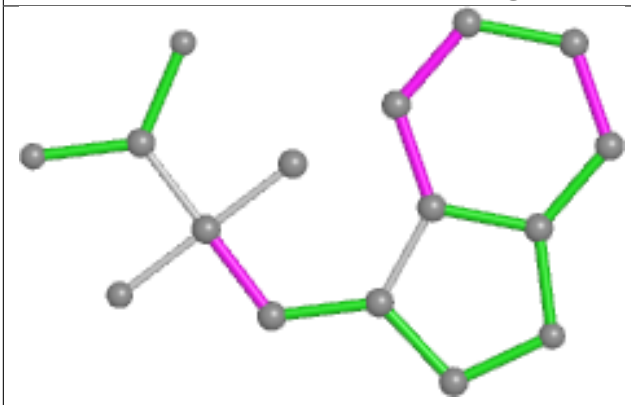


Torsions

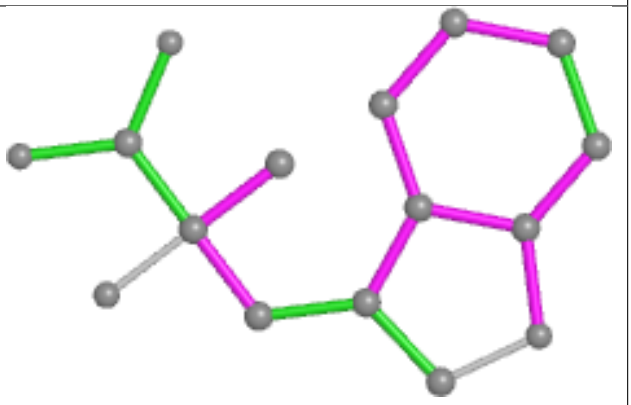


Rings

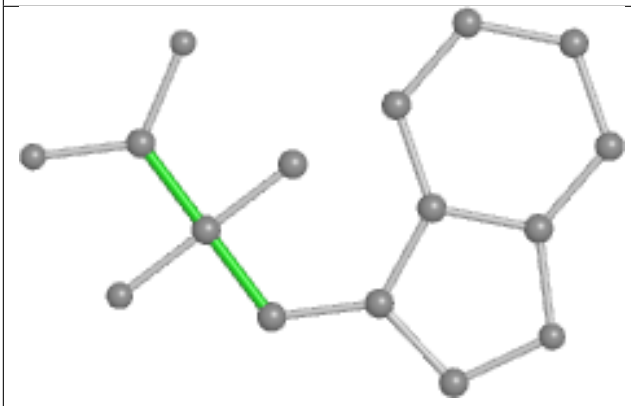
Ligand ZIQ CCC 402



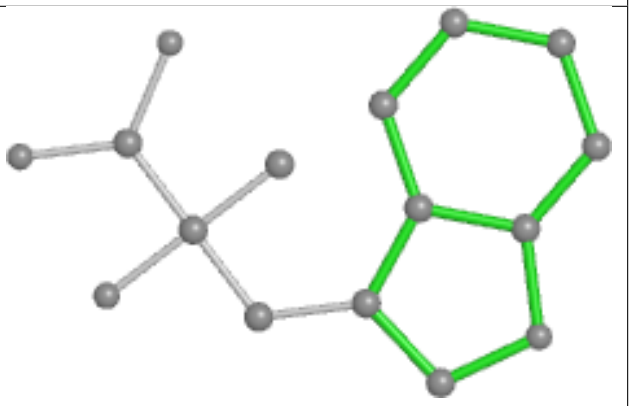
Bond lengths



Bond angles

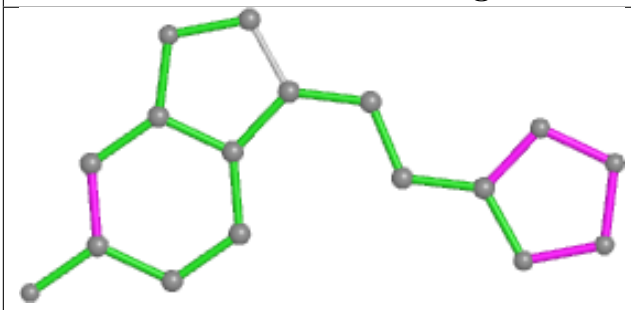


Torsions

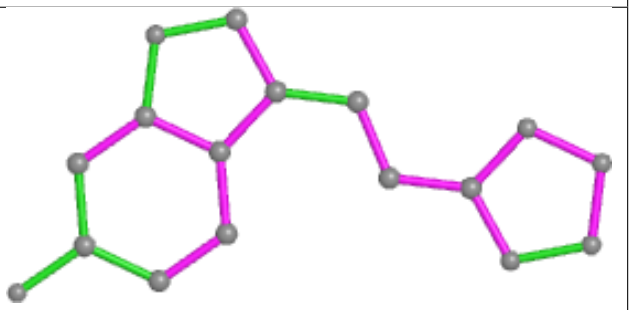


Rings

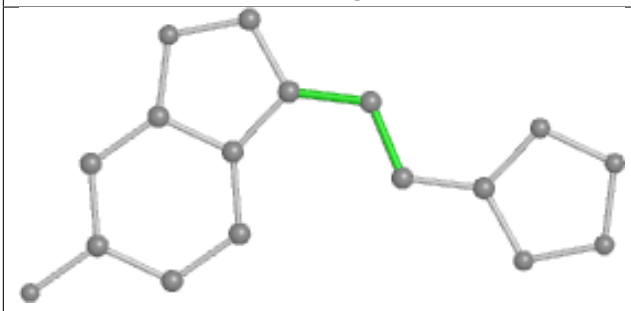
Ligand A1AER AAA 403



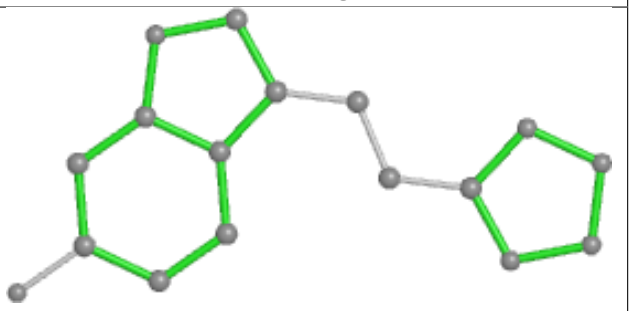
Bond lengths



Bond angles

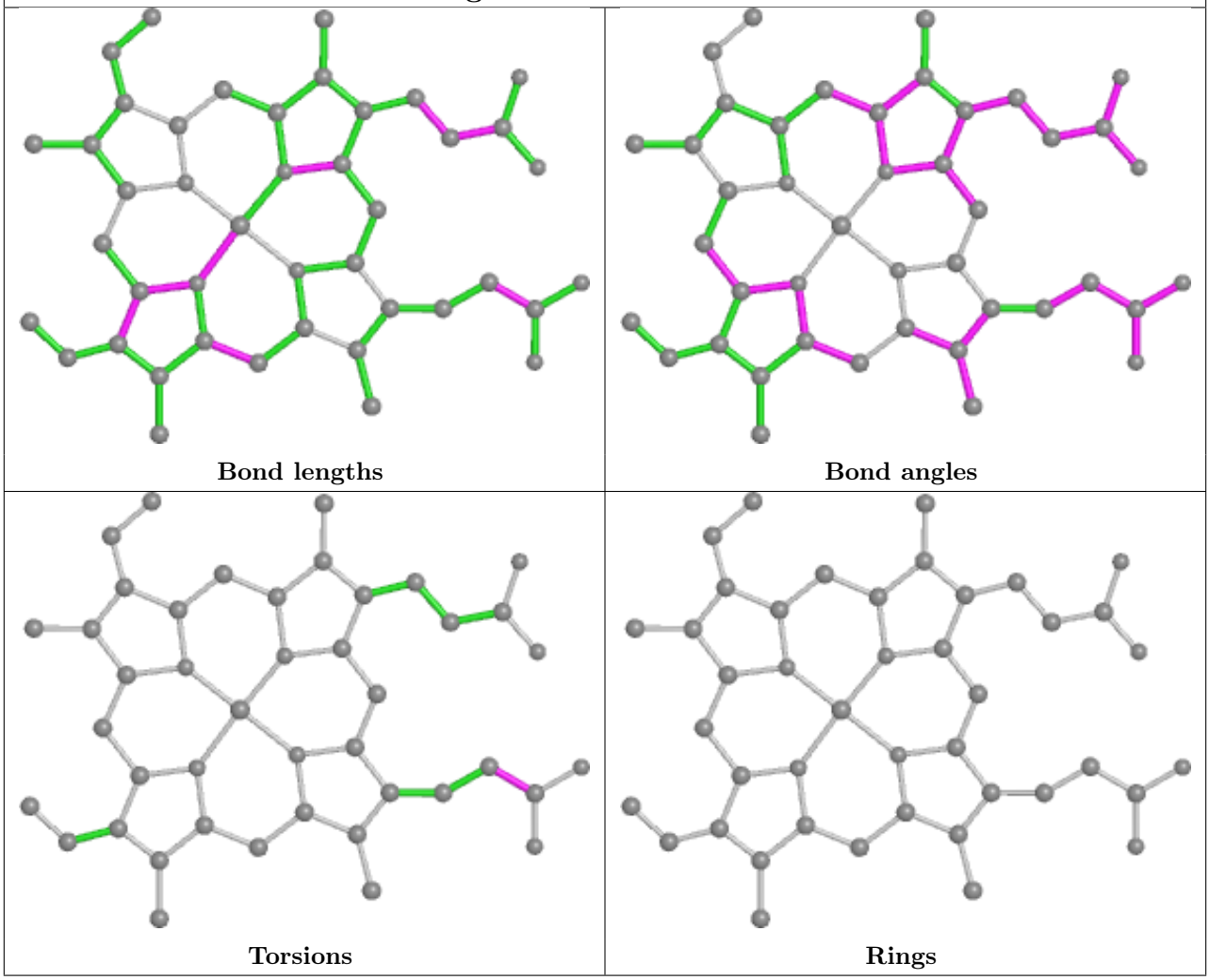


Torsions



Rings

Ligand HEM BBB 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	AAA	344/380 (90%)	0.36	30 (8%) 10 14	30, 53, 117, 141	0
1	BBB	344/380 (90%)	0.16	28 (8%) 12 16	29, 46, 112, 136	0
1	CCC	326/380 (85%)	0.45	44 (13%) 3 4	31, 61, 118, 152	0
1	DDD	343/380 (90%)	0.22	28 (8%) 11 15	31, 53, 104, 147	0
All	All	1357/1520 (89%)	0.29	130 (9%) 8 10	29, 53, 115, 152	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	385	ILE	5.8
1	BBB	384	THR	5.7
1	DDD	248	GLU	5.6
1	CCC	385	ILE	5.4
1	CCC	252	GLU	5.2
1	AAA	247	SER	5.0
1	CCC	383	PRO	4.9
1	AAA	384	THR	4.9
1	CCC	384	THR	4.9
1	BBB	173	VAL	4.8
1	CCC	218	HIS	4.7
1	CCC	254	VAL	4.6
1	AAA	245	GLU	4.6
1	BBB	181	ARG	4.5
1	BBB	38	GLY	4.5
1	AAA	246	GLU	4.5
1	AAA	259	LYS	4.4
1	BBB	174	PRO	4.4
1	BBB	386	HIS	4.3
1	AAA	255	ALA	4.3
1	CCC	257	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	CCC	271	LYS	4.2
1	BBB	39	GLY	4.1
1	DDD	384	THR	4.1
1	BBB	383	PRO	4.0
1	DDD	247	SER	4.0
1	DDD	218	HIS	4.0
1	CCC	275	HIS	3.9
1	DDD	388	PHE	3.8
1	DDD	252	GLU	3.8
1	AAA	388	PHE	3.8
1	DDD	390	GLU	3.7
1	CCC	368	LEU	3.7
1	AAA	248	GLU	3.7
1	DDD	241	ILE	3.7
1	BBB	382	ASN	3.5
1	BBB	245	GLU	3.5
1	BBB	175	TYR	3.5
1	AAA	382	ASN	3.5
1	DDD	275	HIS	3.5
1	CCC	169	GLN	3.3
1	CCC	278	SER	3.3
1	DDD	250	LYS	3.3
1	BBB	385	ILE	3.3
1	AAA	252	GLU	3.3
1	CCC	232	ARG	3.3
1	AAA	383	PRO	3.3
1	DDD	254	VAL	3.3
1	DDD	383	PRO	3.3
1	BBB	388	PHE	3.3
1	CCC	258	GLN	3.2
1	AAA	386	HIS	3.2
1	BBB	247	SER	3.2
1	BBB	180	TYR	3.2
1	AAA	251	GLU	3.2
1	DDD	61	THR	3.2
1	DDD	255	ALA	3.2
1	AAA	250	LYS	3.2
1	DDD	368	LEU	3.2
1	BBB	240	ARG	3.1
1	CCC	279	LYS	3.1
1	CCC	61	THR	3.1
1	DDD	251	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	253	GLN	3.0
1	CCC	193	LEU	3.0
1	AAA	389	LEU	3.0
1	BBB	170	ASN	3.0
1	CCC	255	ALA	3.0
1	DDD	338	SER	3.0
1	DDD	257	PHE	3.0
1	AAA	149	PRO	3.0
1	DDD	39	GLY	2.9
1	CCC	182	ASP	2.9
1	DDD	258	GLN	2.9
1	BBB	249	GLU	2.9
1	CCC	235	GLU	2.9
1	DDD	385	ILE	2.9
1	CCC	349	HIS	2.8
1	AAA	275	HIS	2.8
1	CCC	234	LEU	2.8
1	CCC	233	GLY	2.8
1	CCC	380	LYS	2.8
1	DDD	387	LYS	2.8
1	BBB	246	GLU	2.7
1	CCC	372	LEU	2.7
1	BBB	248	GLU	2.6
1	BBB	340	ALA	2.6
1	DDD	179	HIS	2.6
1	DDD	182	ASP	2.6
1	AAA	279	LYS	2.6
1	CCC	179	HIS	2.6
1	DDD	389	LEU	2.6
1	CCC	39	GLY	2.6
1	DDD	193	LEU	2.5
1	BBB	193	LEU	2.5
1	BBB	241	ILE	2.5
1	AAA	387	LYS	2.5
1	CCC	190	GLU	2.5
1	AAA	244	LYS	2.5
1	CCC	170	ASN	2.4
1	AAA	280	GLY	2.4
1	BBB	169	GLN	2.4
1	BBB	63	GLY	2.4
1	DDD	365	LEU	2.4
1	AAA	253	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	173	VAL	2.4
1	BBB	182	ASP	2.3
1	CCC	219	GLY	2.3
1	BBB	389	LEU	2.3
1	AAA	146	TYR	2.3
1	CCC	171	MET	2.3
1	DDD	219	GLY	2.3
1	CCC	256	GLU	2.3
1	AAA	276	LEU	2.3
1	CCC	187	GLU	2.3
1	AAA	311	LEU	2.3
1	CCC	326	TYR	2.3
1	CCC	63	GLY	2.3
1	AAA	257	PHE	2.3
1	AAA	241	ILE	2.3
1	CCC	236	GLU	2.2
1	CCC	98	GLN	2.2
1	CCC	181	ARG	2.1
1	AAA	165	ILE	2.1
1	CCC	389	LEU	2.1
1	CCC	276	LEU	2.1
1	CCC	296	TYR	2.1
1	CCC	272	ARG	2.0
1	BBB	238	PHE	2.0
1	AAA	249	GLU	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)

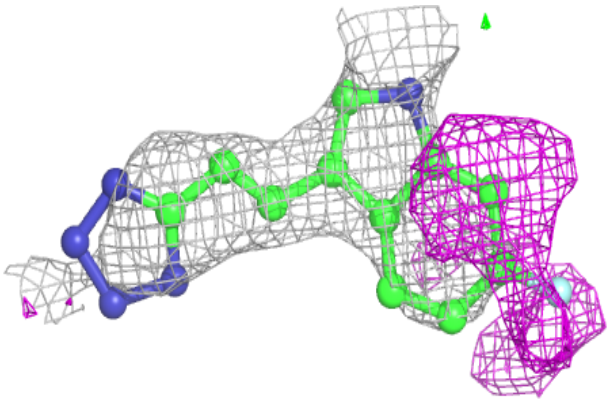
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

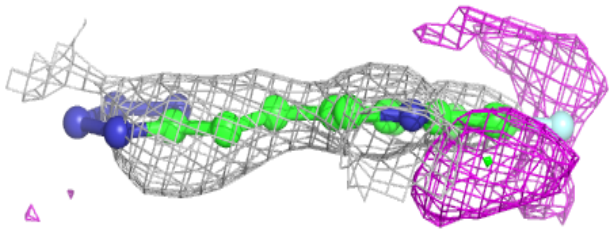
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	A1AER	AAA	403	17/17	0.81	0.41	94,103,122,123	0
4	A1AER	BBB	403	17/17	0.84	0.25	79,90,123,124	0
4	A1AER	DDD	403	17/17	0.92	0.22	80,90,100,117	0
3	ZIQ	CCC	402	16/16	0.96	0.10	45,51,62,68	0
2	HEM	CCC	401	43/43	0.96	0.12	47,61,71,85	0
3	ZIQ	DDD	402	16/16	0.97	0.10	42,47,54,57	0
3	ZIQ	AAA	402	16/16	0.97	0.13	32,37,53,64	0
3	ZIQ	BBB	402	16/16	0.97	0.08	33,36,38,41	0
2	HEM	AAA	401	43/43	0.97	0.13	40,51,64,74	0
2	HEM	DDD	401	43/43	0.98	0.11	36,44,66,81	0
2	HEM	BBB	401	43/43	0.98	0.10	37,45,61,63	0

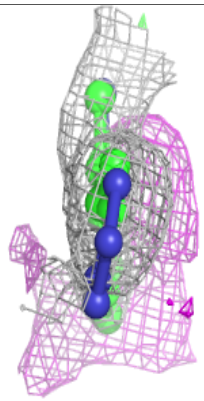
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AER AAA 403:

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

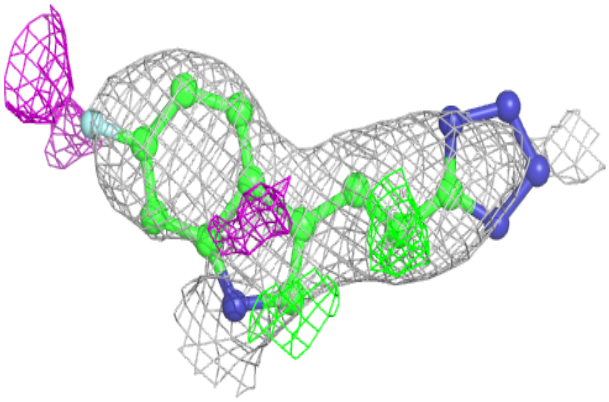


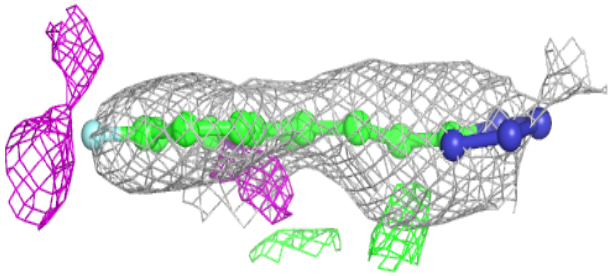


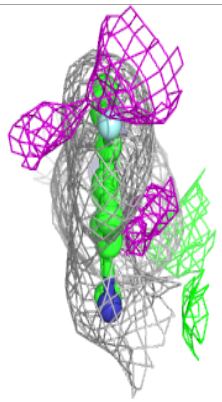


Electron density around A1AER BBB 403:

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

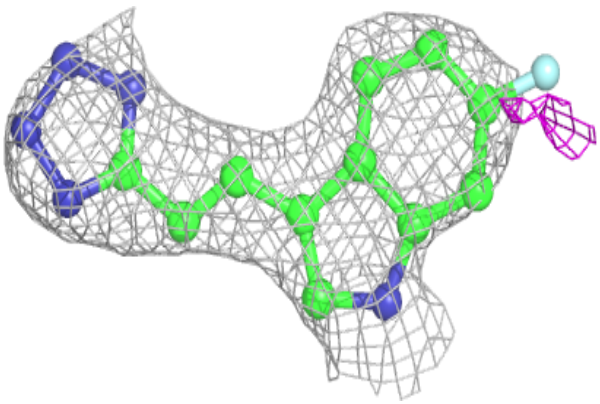


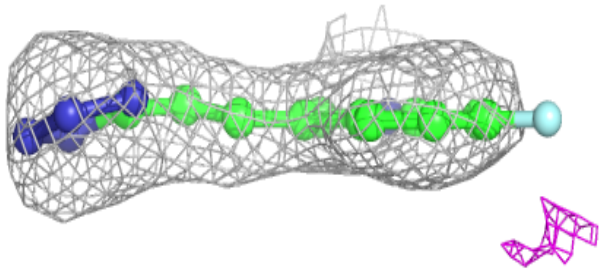


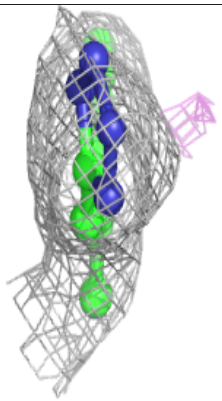


Electron density around A1AER DDD 403:

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

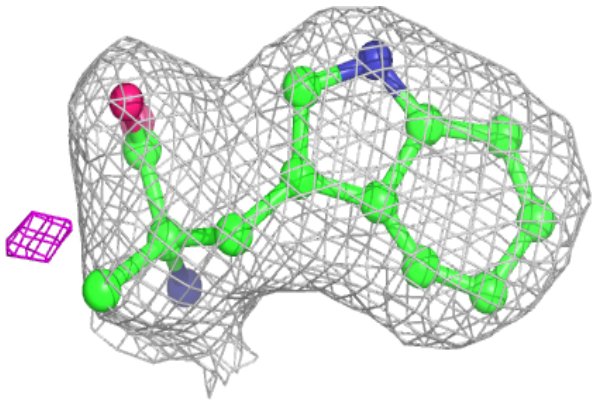


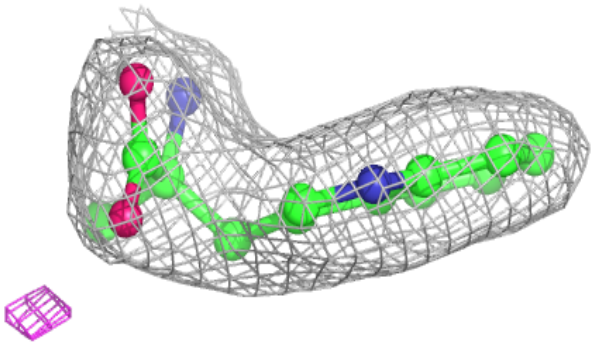


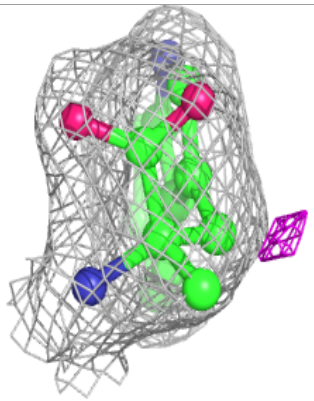


Electron density around ZIQ CCC 402:

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

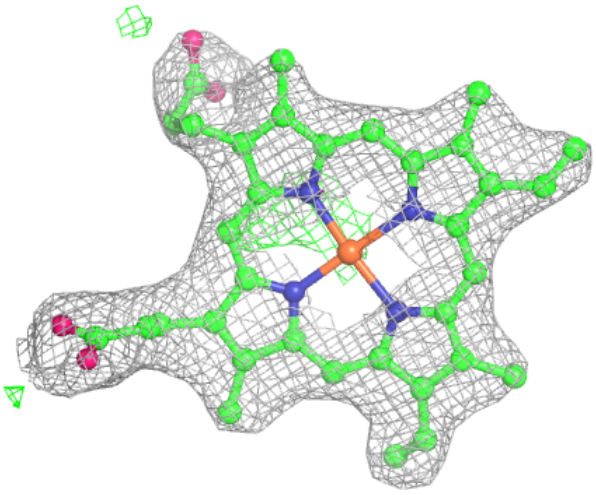


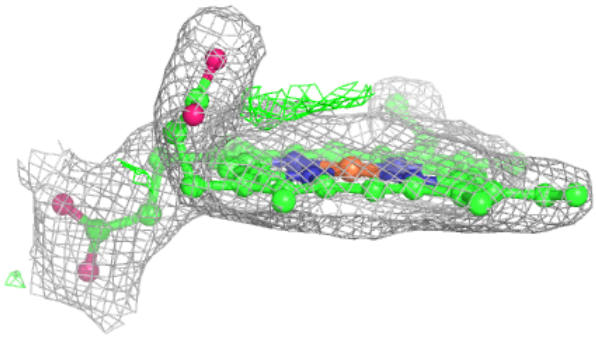


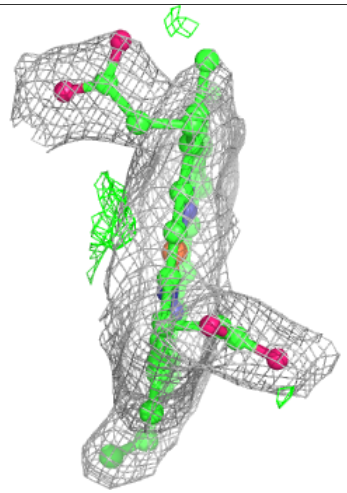


Electron density around HEM CCC 401:

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

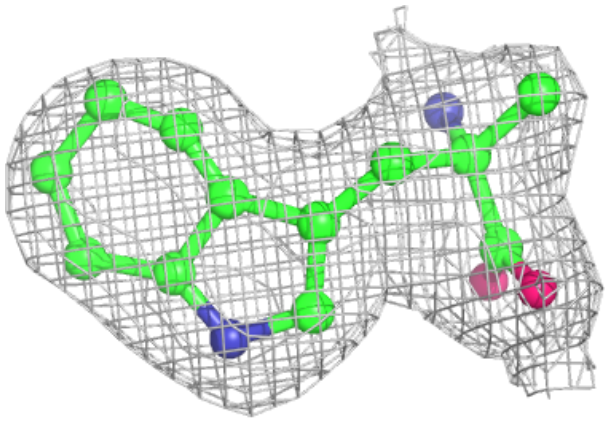


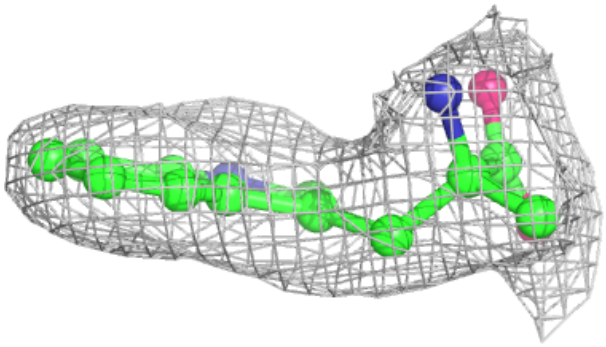


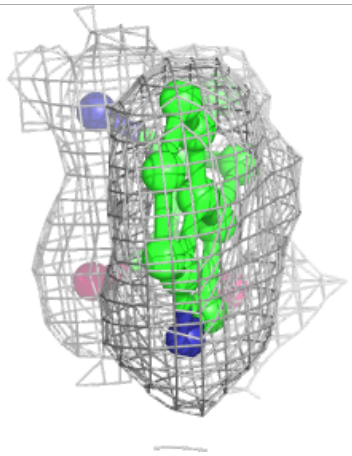


Electron density around ZIQ DDD 402:

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

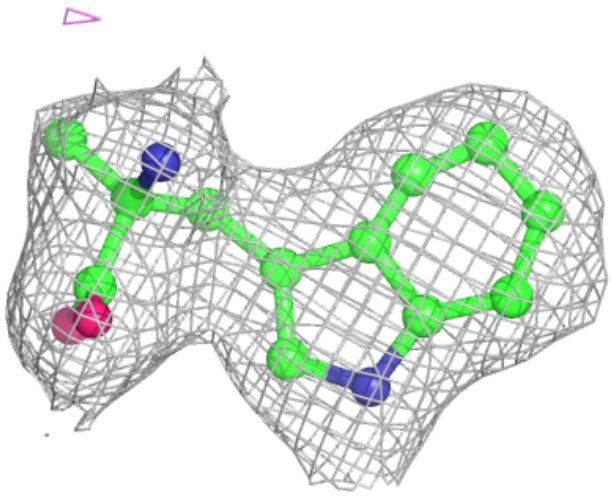


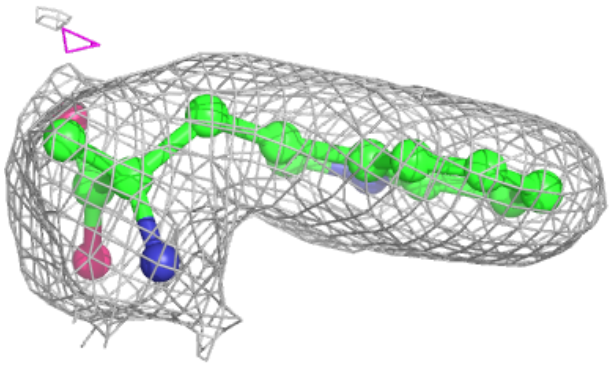


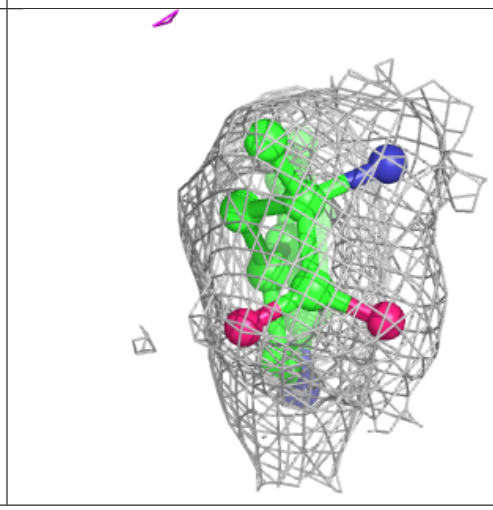


Electron density around ZIQ AAA 402:

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

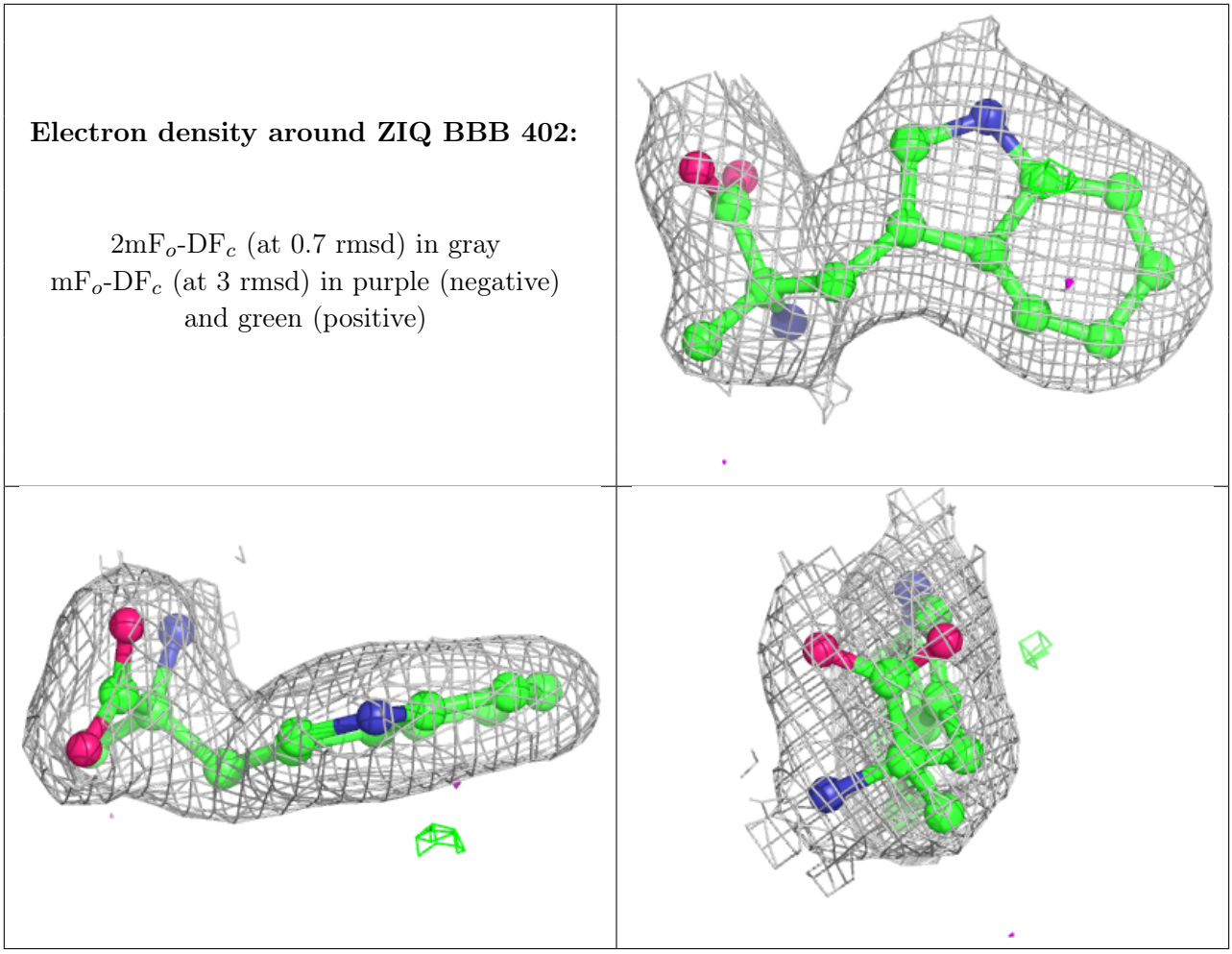






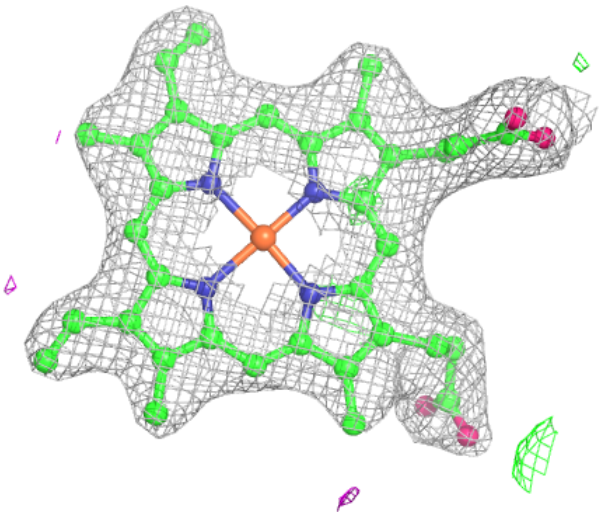
Electron density around ZIQ BBB 402:

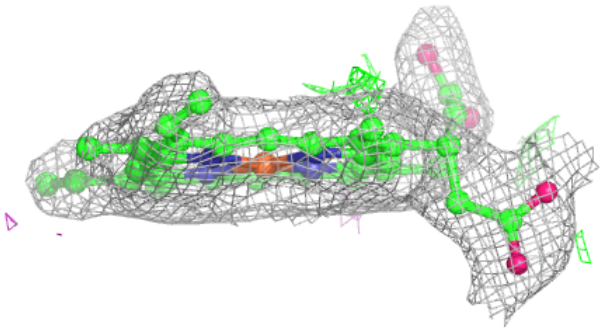
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

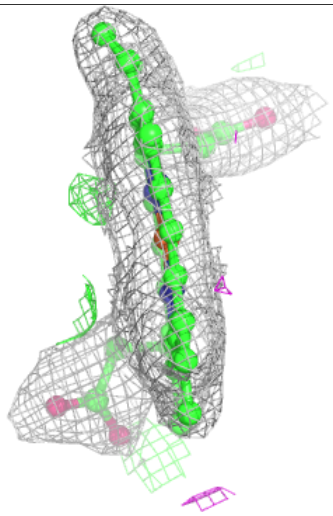


Electron density around HEM AAA 401:

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

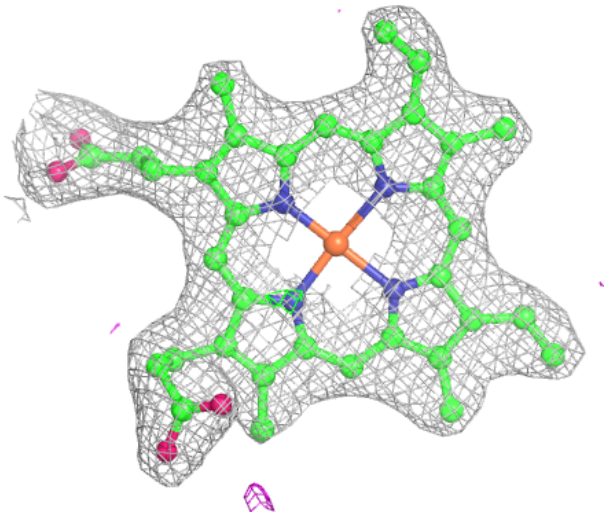


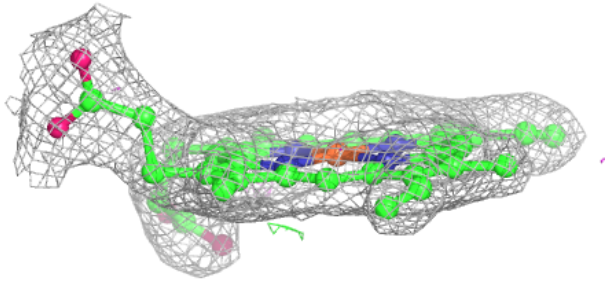


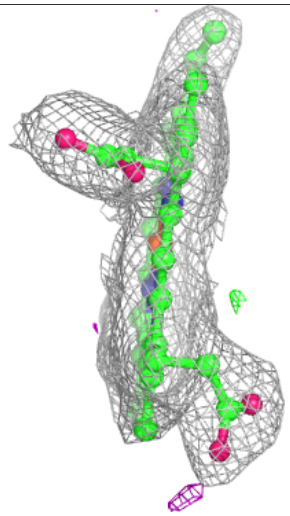


Electron density around HEM DDD 401:

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

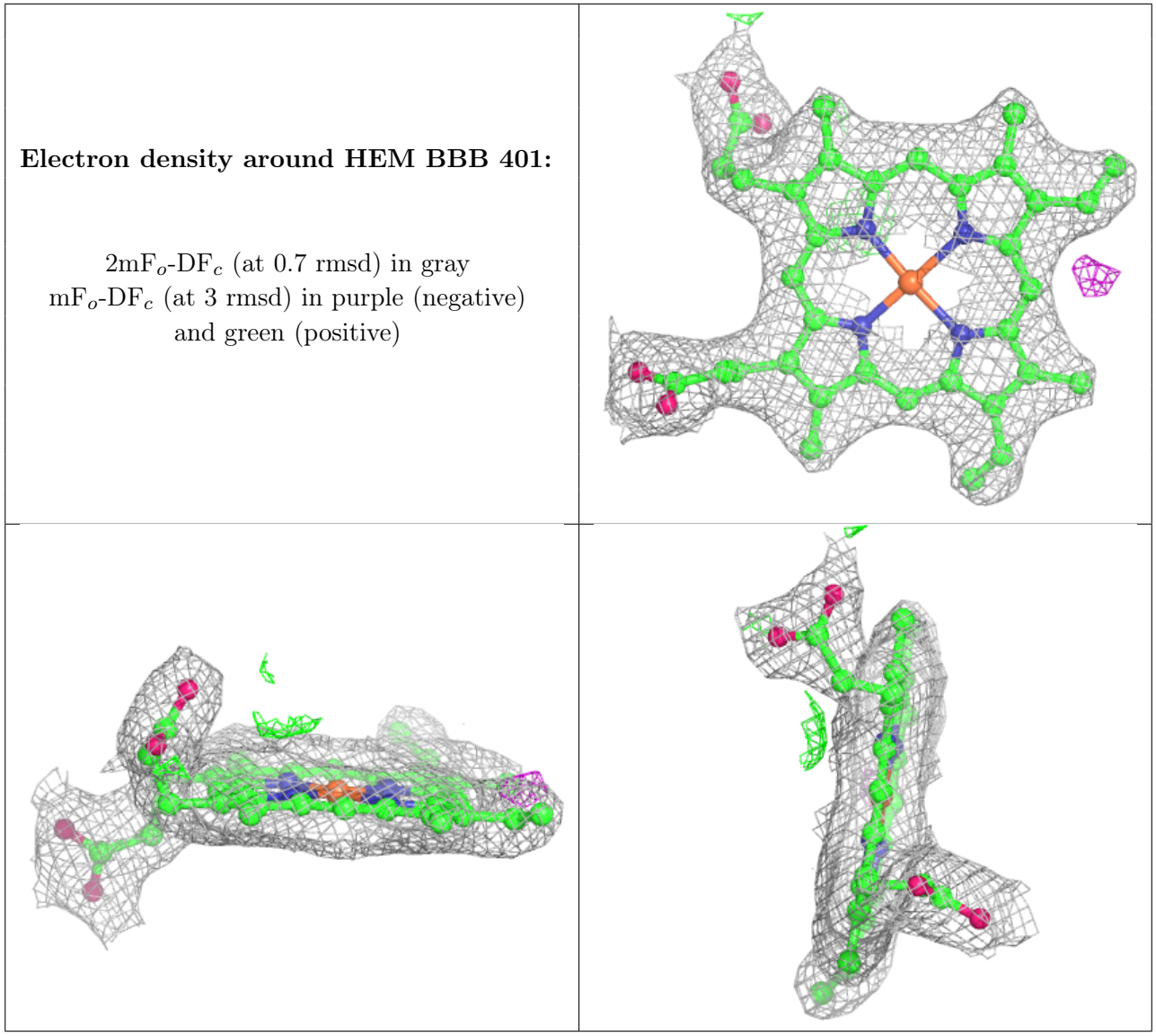






Electron density around HEM BBB 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.