Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 09:50 AM EST

PDB ID	:	6PYZ
Title	:	Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PF-06840003 in Active Site
Authors	:	Pham, K.N.; Lewis-Ballester, A.; Yeh, S.R.
Deposited on	:	2019-07-31
Resolution	:	2.02 Å(reported)

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

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

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

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

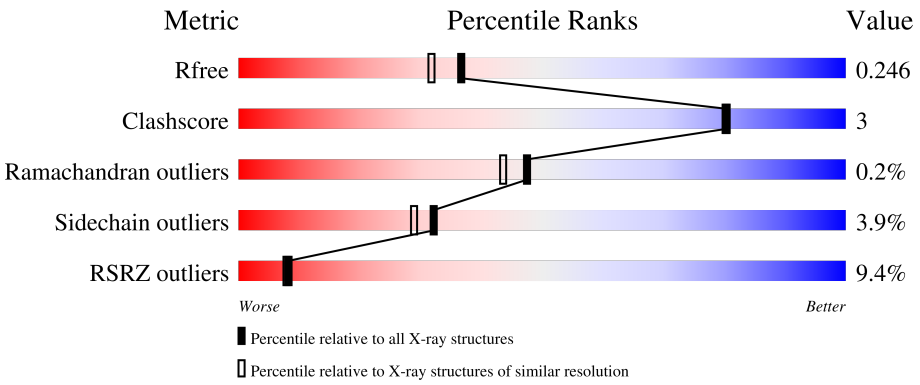
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	380	8%, 84%, 8%, 7%
1	B	380	8%, 88%, •, 8%
1	C	380	11%, 77%, 10%, •, 12%
1	D	380	7%, 81%, 8%, •, 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12971 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
			Total	C	N	O	S			
1	A	353	2975	1908	523	533	11	0	0	0
1	B	348	2920	1877	507	525	11	0	0	0
1	C	333	2799	1802	489	497	11	0	0	0
1	D	342	2899	1864	508	516	11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

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

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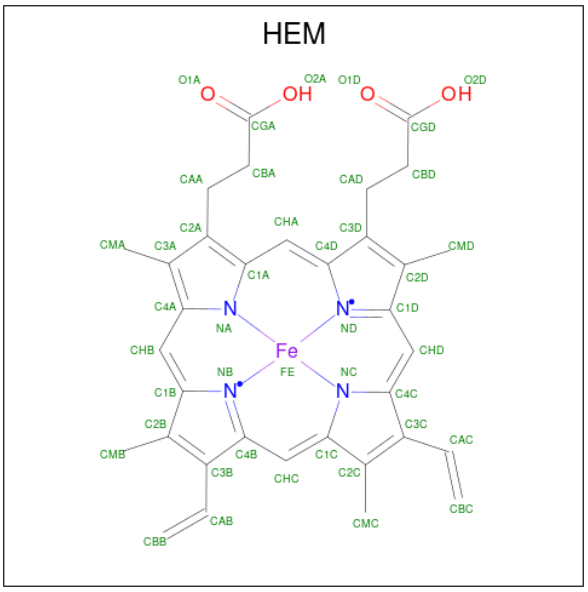
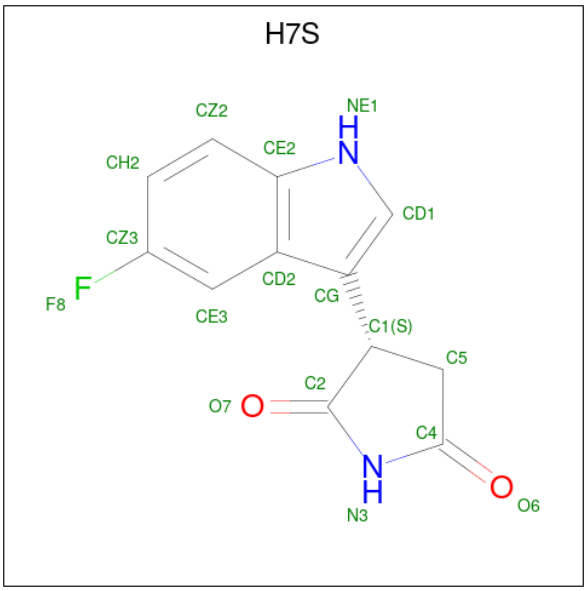
Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression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



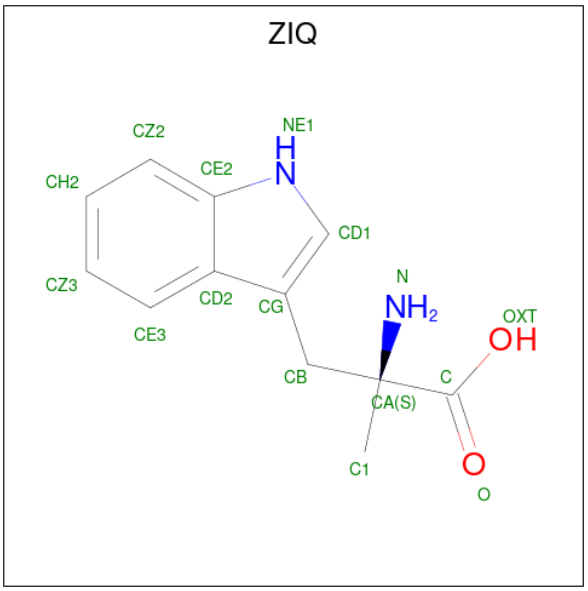
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is (3S)-3-(5-fluoro-1H-indol-3-yl)pyrrolidine-2,5-dione (three-letter code: H7S) (formula: $C_{12}H_9FN_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	17	12	1	2	2	0	0
			Total	C	F	N	O		
3	B	1	17	12	1	2	2	0	0
			Total	C	F	N	O		
3	C	1	17	12	1	2	2	0	0
			Total	C	F	N	O		
3	D	1	17	12	1	2	2	0	0

- Molecule 4 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
			Total	C	N	O		
4	A	1	16	12	2	2	0	0
4	B	1	16	12	2	2	0	0
4	C	1	16	12	2	2	0	0
4	D	1	16	12	2	2	0	0

- Molecule 5 is water.

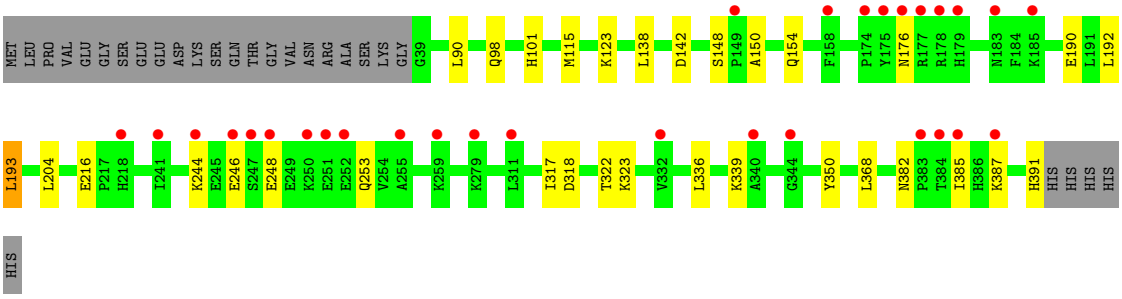
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	285	285	285	0	0
5	B	312	312	312	0	0
5	C	214	214	214	0	0
5	D	263	263	263	0	0

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.

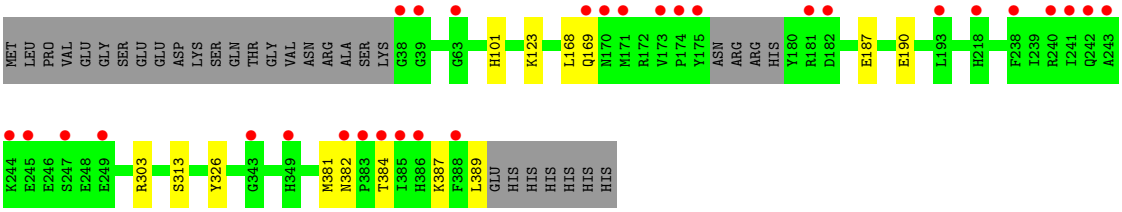
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain A:



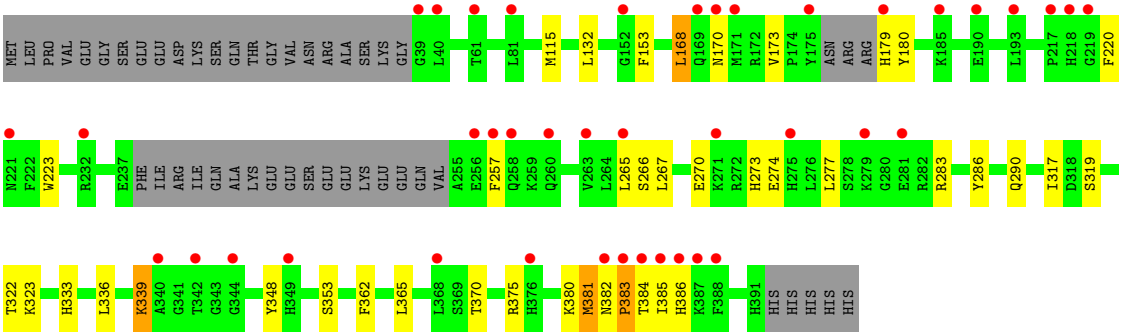
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain B:



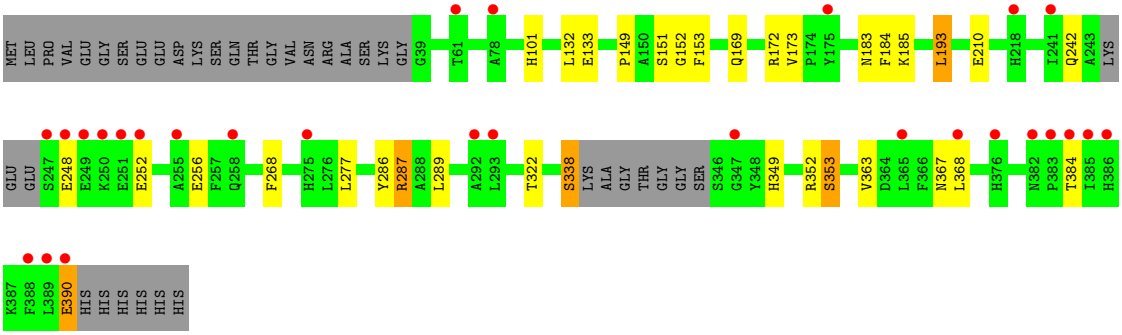
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain C:



• Molecule 1: Tryptophan 2,3-dioxygenase

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	143.65Å 154.16Å 87.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.02 29.86 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.86-2.02) 99.4 (29.86-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.189 , 0.243 0.196 , 0.246	Depositor DCC
R_{free} test set	6380 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12971	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZIQ, HEM, H7S

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.66	0/3045	0.72	0/4098
1	B	0.65	0/2987	0.73	0/4019
1	C	0.66	0/2866	0.73	0/3858
1	D	0.66	0/2966	0.74	0/3991
All	All	0.66	0/11864	0.73	0/15966

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2975	0	2957	14	0
1	B	2920	0	2907	4	0
1	C	2799	0	2782	19	0
1	D	2899	0	2884	18	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	16	0	0	0	0
4	B	16	0	0	1	0
4	C	16	0	0	1	0
4	D	16	0	0	0	0
5	A	285	0	0	4	0
5	B	312	0	0	1	0
5	C	214	0	0	0	0
5	D	263	0	0	3	0
All	All	12971	0	11650	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LEU:O	1:C:339:LYS:HG2	1.83	0.79
1:C:223:TRP:CG	1:C:290:GLN:NE2	2.62	0.68
2:C:401:HEM:HMB1	2:C:401:HEM:HBB2	1.78	0.66
2:A:401:HEM:HMB1	2:A:401:HEM:HBB2	1.82	0.61
1:D:173:VAL:HG21	1:D:353:SER:OG	2.00	0.61
1:A:391:HIS:C	1:D:390:GLU:C	2.62	0.58
1:C:270:GLU:HG2	1:C:286:TYR:CD2	2.38	0.58
1:A:318:ASP:O	1:A:322:THR:HG23	2.04	0.58
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.34	0.57
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.37	0.55
2:A:401:HEM:HBC2	2:A:401:HEM:HHD	1.89	0.55
1:A:176:ASN:ND2	1:A:350:TYR:OH	2.42	0.53
1:C:362:PHE:HB3	1:C:365:LEU:HD12	1.90	0.52
2:B:401:HEM:HBC2	2:B:401:HEM:HHD	1.91	0.52
1:D:151:SER:HB2	3:D:402:H7S:O7	2.10	0.52
1:C:382:ASN:HD22	1:C:383:PRO:HD2	1.75	0.51
3:A:402:H7S:CD1	5:A:547:HOH:O	2.59	0.51
1:B:187:GLU:O	1:B:190:GLU:HB3	2.10	0.51
1:C:381:MET:HB2	1:C:386:HIS:CE1	2.46	0.51
1:B:303:ARG:HD3	1:B:389:LEU:HA	1.94	0.50
1:D:289:LEU:HD11	1:D:368:LEU:HD21	1.93	0.49
1:D:363:VAL:HG22	1:D:367:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:HEM:HBC2	2:C:401:HEM:HHD	1.94	0.49
1:D:248:GLU:O	1:D:252:GLU:HG3	2.13	0.49
1:A:322:THR:HG22	5:A:544:HOH:O	2.12	0.49
1:D:210:GLU:HG2	1:D:287:ARG:HB3	1.94	0.48
1:A:142:ASP:OD2	1:C:375:ARG:NH2	2.47	0.48
1:A:98:GLN:HG2	1:A:204:LEU:HD21	1.95	0.48
1:C:173:VAL:HG21	1:C:353:SER:OG	2.13	0.48
1:D:268:PHE:HA	1:D:286:TYR:OH	2.14	0.47
1:C:223:TRP:CD1	1:C:290:GLN:NE2	2.83	0.47
4:C:403:ZIQ:C	4:C:403:ZIQ:CD1	2.93	0.46
1:B:382:ASN:O	1:B:384:THR:N	2.49	0.45
1:A:150:ALA:HA	1:A:154:GLN:OE1	2.16	0.45
2:C:401:HEM:HBB2	2:C:401:HEM:CMB	2.46	0.45
1:A:336:LEU:O	1:A:339:LYS:HB2	2.16	0.44
1:A:323:LYS:NZ	5:A:516:HOH:O	2.47	0.44
1:C:168:LEU:HB3	1:C:170:ASN:OD1	2.16	0.44
1:C:220:PHE:HB2	1:C:385:ILE:HD12	1.99	0.44
1:C:319:SER:O	1:C:322:THR:HG22	2.18	0.44
1:A:339:LYS:HD3	1:C:370:THR:HA	1.99	0.44
1:C:168:LEU:HD22	1:C:283:ARG:CZ	2.47	0.44
1:D:152:GLY:HA3	2:D:401:HEM:C1D	2.53	0.44
1:D:172:ARG:O	5:D:501:HOH:O	2.21	0.44
1:D:133:GLU:HG2	5:D:550:HOH:O	2.18	0.43
2:A:401:HEM:HBB2	2:A:401:HEM:CMB	2.47	0.43
1:D:193:LEU:HD13	1:D:193:LEU:HA	1.86	0.42
2:D:401:HEM:HMB1	2:D:401:HEM:HBB2	2.01	0.42
1:C:333:HIS:HB2	1:C:348:TYR:CE1	2.54	0.42
1:D:184:PHE:O	1:D:185:LYS:HD2	2.19	0.42
1:D:289:LEU:CD1	1:D:368:LEU:HD21	2.49	0.42
5:B:758:HOH:O	1:D:338:SER:C	2.58	0.42
2:B:401:HEM:HMB1	2:B:401:HEM:HBB2	2.02	0.42
1:A:368:LEU:HD23	1:A:368:LEU:HA	1.93	0.41
1:A:123:LYS:NZ	5:A:510:HOH:O	2.45	0.41
1:C:381:MET:CB	1:C:386:HIS:CE1	3.04	0.41
1:B:326:TYR:OH	1:D:322:THR:CG2	2.69	0.41
2:D:401:HEM:HHD	2:D:401:HEM:HBC2	2.03	0.41
1:C:132:LEU:HD12	1:C:132:LEU:HA	1.93	0.41
1:C:273:HIS:O	1:C:277:LEU:HB2	2.21	0.41
1:A:193:LEU:HD13	1:A:193:LEU:HA	1.93	0.40
4:B:403:ZIQ:CD1	4:B:403:ZIQ:C	3.00	0.40
1:D:132:LEU:HD12	1:D:132:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:THR:HG23	5:D:614:HOH:O	2.21	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	351/380 (92%)	340 (97%)	10 (3%)	1 (0%)	41	36
1	B	344/380 (90%)	336 (98%)	8 (2%)	0	100	100
1	C	327/380 (86%)	316 (97%)	10 (3%)	1 (0%)	41	36
1	D	336/380 (88%)	325 (97%)	10 (3%)	1 (0%)	41	36
All	All	1358/1520 (89%)	1317 (97%)	38 (3%)	3 (0%)	47	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLU
1	D	183	ASN
1	C	383	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/348 (93%)	311 (96%)	14 (4%)	29	25
1	B	319/348 (92%)	312 (98%)	7 (2%)	52	53
1	C	306/348 (88%)	292 (95%)	14 (5%)	27	22
1	D	318/348 (91%)	303 (95%)	15 (5%)	26	22
All	All	1268/1392 (91%)	1218 (96%)	50 (4%)	32	29

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	101	HIS
1	A	138	LEU
1	A	148	SER
1	A	190	GLU
1	A	192	LEU
1	A	193	LEU
1	A	216	GLU
1	A	244	LYS
1	A	248	GLU
1	A	253	GLN
1	A	382	ASN
1	A	385	ILE
1	A	387	LYS
1	B	101	HIS
1	B	123	LYS
1	B	168	LEU
1	B	169	GLN
1	B	313	SER
1	B	381	MET
1	B	387	LYS
1	C	153	PHE
1	C	168	LEU
1	C	179	HIS
1	C	180	TYR
1	C	257	PHE
1	C	265	LEU
1	C	266	SER
1	C	267	LEU
1	C	274	GLU
1	C	323	LYS
1	C	339	LYS
1	C	380	LYS

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Mol	Chain	Res	Type
1	C	381	MET
1	C	384	THR
1	D	101	HIS
1	D	149	PRO
1	D	153	PHE
1	D	169	GLN
1	D	193	LEU
1	D	242	GLN
1	D	256	GLU
1	D	277	LEU
1	D	287	ARG
1	D	338	SER
1	D	349	HIS
1	D	352	ARG
1	D	353	SER
1	D	384	THR
1	D	390	GLU

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

Mol	Chain	Res	Type
1	A	107	ASN
1	B	44	ASN
1	B	197	GLN
1	B	242	GLN
1	B	382	ASN
1	C	258	GLN
1	C	260	GLN
1	C	382	ASN
1	C	386	HIS
1	C	391	HIS

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)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ZIQ	A	403	-	13,17,17	1.64	1 (7%)	14,25,25	1.25	2 (14%)
2	HEM	D	401	1	41,50,50	1.28	6 (14%)	45,82,82	1.99	13 (28%)
3	H7S	C	402	-	17,19,19	0.99	1 (5%)	19,28,28	1.38	4 (21%)
3	H7S	D	402	-	17,19,19	0.92	1 (5%)	19,28,28	1.13	2 (10%)
4	ZIQ	B	403	-	13,17,17	1.71	2 (15%)	14,25,25	1.21	3 (21%)
3	H7S	B	402	-	17,19,19	1.00	1 (5%)	19,28,28	1.54	6 (31%)
2	HEM	B	401	5,1	41,50,50	1.37	5 (12%)	45,82,82	1.92	10 (22%)
2	HEM	A	401	5,1	41,50,50	1.35	5 (12%)	45,82,82	1.78	11 (24%)
2	HEM	C	401	1	41,50,50	1.29	6 (14%)	45,82,82	1.90	14 (31%)
3	H7S	A	402	-	17,19,19	0.91	1 (5%)	19,28,28	1.49	4 (21%)
4	ZIQ	C	403	-	13,17,17	1.65	2 (15%)	14,25,25	1.02	0
4	ZIQ	D	403	-	13,17,17	1.29	1 (7%)	14,25,25	1.32	2 (14%)

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
4	ZIQ	A	403	-	-	4/9/11/11	0/2/2/2
2	HEM	D	401	1	-	2/12/54/54	-
3	H7S	C	402	-	-	0/0/16/16	0/3/3/3
3	H7S	D	402	-	-	0/0/16/16	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ZIQ	B	403	-	-	2/9/11/11	0/2/2/2
3	H7S	B	402	-	-	0/0/16/16	0/3/3/3
2	HEM	B	401	5,1	-	2/12/54/54	-
2	HEM	A	401	5,1	-	2/12/54/54	-
2	HEM	C	401	1	-	2/12/54/54	-
3	H7S	A	402	-	-	0/0/16/16	0/3/3/3
4	ZIQ	C	403	-	-	1/9/11/11	0/2/2/2
4	ZIQ	D	403	-	-	4/9/11/11	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	ZIQ	O-C	3.90	1.34	1.22
2	B	401	HEM	C4D-ND	-3.56	1.34	1.40
4	A	403	ZIQ	O-C	3.53	1.33	1.22
4	C	403	ZIQ	O-C	3.43	1.33	1.22
3	C	402	H7S	CG-CD2	3.27	1.44	1.40
2	B	401	HEM	C1B-NB	-3.26	1.34	1.40
3	B	402	H7S	CG-CD2	3.26	1.44	1.40
2	A	401	HEM	C4D-ND	-3.13	1.34	1.40
2	C	401	HEM	C4D-ND	-2.95	1.35	1.40
2	C	401	HEM	FE-NB	2.91	2.11	1.96
2	A	401	HEM	C1B-NB	-2.91	1.35	1.40
3	D	402	H7S	CG-CD2	2.90	1.44	1.40
2	C	401	HEM	C1B-NB	-2.82	1.35	1.40
2	A	401	HEM	FE-NB	2.77	2.10	1.96
3	A	402	H7S	CG-CD2	2.74	1.43	1.40
2	B	401	HEM	CHB-C1B	2.51	1.41	1.35
2	C	401	HEM	CHB-C1B	2.50	1.41	1.35
2	D	401	HEM	C4B-NB	-2.44	1.33	1.38
2	B	401	HEM	FE-NB	2.43	2.08	1.96
2	A	401	HEM	C4B-NB	-2.43	1.33	1.38
2	D	401	HEM	CHA-C4D	2.35	1.41	1.35
2	D	401	HEM	C1B-NB	-2.32	1.36	1.40
2	D	401	HEM	CHB-C1B	2.32	1.40	1.35
2	B	401	HEM	C4B-NB	-2.28	1.34	1.38
2	D	401	HEM	C4D-ND	-2.26	1.36	1.40
2	A	401	HEM	CHB-C1B	2.23	1.40	1.35
2	D	401	HEM	FE-NB	2.13	2.07	1.96
4	B	403	ZIQ	OXT-C	-2.07	1.22	1.30
4	C	403	ZIQ	CB-CA	-2.05	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C4D-C3D	2.05	1.48	1.45
4	D	403	ZIQ	CB-CA	-2.03	1.52	1.55
2	C	401	HEM	C3B-C4B	2.01	1.48	1.44

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	HEM	CHD-C1D-ND	4.78	129.62	124.43
2	D	401	HEM	C1B-NB-C4B	4.61	109.84	105.07
2	B	401	HEM	CHC-C4B-NB	4.55	129.37	124.43
2	D	401	HEM	CHC-C4B-NB	4.46	129.28	124.43
2	B	401	HEM	CBD-CAD-C3D	-4.32	100.62	112.63
2	B	401	HEM	C1B-NB-C4B	4.22	109.43	105.07
2	C	401	HEM	CHC-C4B-NB	4.21	129.00	124.43
2	C	401	HEM	CBD-CAD-C3D	-4.19	100.98	112.63
2	C	401	HEM	CHD-C1D-ND	4.03	128.81	124.43
2	D	401	HEM	CBD-CAD-C3D	-3.93	101.70	112.63
2	A	401	HEM	CBD-CAD-C3D	-3.89	101.81	112.63
2	A	401	HEM	CHC-C4B-NB	3.89	128.65	124.43
2	D	401	HEM	CHD-C1D-C2D	-3.64	119.30	124.98
2	A	401	HEM	C1B-NB-C4B	3.60	108.80	105.07
2	C	401	HEM	C1B-NB-C4B	3.58	108.77	105.07
2	A	401	HEM	CHA-C4D-ND	3.55	128.77	124.38
3	A	402	H7S	C1-C5-C4	-3.54	102.66	105.58
2	B	401	HEM	CHB-C1B-NB	3.27	128.42	124.38
2	B	401	HEM	CHD-C1D-ND	3.20	127.91	124.43
2	B	401	HEM	O2D-CGD-CBD	3.19	124.27	114.03
2	A	401	HEM	CHD-C1D-ND	3.17	127.88	124.43
2	D	401	HEM	CHA-C4D-ND	3.16	128.28	124.38
2	C	401	HEM	CBA-CAA-C2A	-3.11	107.31	112.62
2	C	401	HEM	CAD-C3D-C4D	3.03	129.95	124.66
3	A	402	H7S	C5-C1-C2	-3.03	102.16	103.64
2	B	401	HEM	CHD-C1D-C2D	-2.96	120.36	124.98
2	C	401	HEM	CHD-C1D-C2D	-2.94	120.39	124.98
2	D	401	HEM	CHB-C1B-NB	2.93	128.00	124.38
3	B	402	H7S	C1-C5-C4	-2.89	103.20	105.58
3	C	402	H7S	C5-C1-C2	-2.88	102.23	103.64
2	A	401	HEM	CHA-C4D-C3D	-2.84	119.99	125.33
3	B	402	H7S	C5-C1-C2	-2.78	102.28	103.64
2	B	401	HEM	CHA-C4D-ND	2.77	127.80	124.38
3	A	402	H7S	CZ3-CE3-CD2	-2.74	116.65	118.80
3	D	402	H7S	CZ3-CE3-CD2	-2.74	116.65	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HEM	CHD-C1D-C2D	-2.72	120.73	124.98
2	C	401	HEM	CHB-C1B-NB	2.70	127.72	124.38
4	A	403	ZIQ	CE3-CD2-CE2	2.62	121.64	118.17
2	C	401	HEM	CHA-C4D-ND	2.59	127.58	124.38
2	B	401	HEM	O2A-CGA-CBA	2.56	122.26	114.03
2	D	401	HEM	C2C-C3C-C4C	-2.56	105.11	106.90
2	C	401	HEM	O2A-CGA-O1A	-2.55	116.93	123.30
3	B	402	H7S	CZ3-CE3-CD2	-2.53	116.82	118.80
2	C	401	HEM	O2A-CGA-CBA	2.53	122.15	114.03
3	C	402	H7S	CZ3-CE3-CD2	-2.51	116.84	118.80
2	A	401	HEM	CHB-C1B-NB	2.49	127.46	124.38
4	D	403	ZIQ	CE3-CD2-CE2	2.46	121.43	118.17
3	A	402	H7S	CH2-CZ2-CE2	-2.46	117.74	120.84
2	D	401	HEM	O2A-CGA-CBA	2.46	121.93	114.03
2	D	401	HEM	CHA-C4D-C3D	-2.45	120.72	125.33
2	D	401	HEM	CAD-C3D-C4D	2.45	128.94	124.66
2	A	401	HEM	O2D-CGD-CBD	2.45	121.89	114.03
3	B	402	H7S	CH2-CZ2-CE2	-2.39	117.83	120.84
3	D	402	H7S	CH2-CZ2-CE2	-2.35	117.88	120.84
3	C	402	H7S	CH2-CZ2-CE2	-2.34	117.89	120.84
2	D	401	HEM	O2A-CGA-O1A	-2.27	117.64	123.30
3	C	402	H7S	C1-C5-C4	-2.26	103.72	105.58
4	B	403	ZIQ	CB-CA-C	2.25	112.20	109.02
4	A	403	ZIQ	CZ3-CE3-CD2	-2.24	117.78	120.89
2	D	401	HEM	O2D-CGD-CBD	2.21	121.14	114.03
3	B	402	H7S	CG-C1-C2	-2.20	106.43	112.14
4	D	403	ZIQ	OXT-C-O	-2.18	116.87	123.82
4	B	403	ZIQ	CZ3-CE3-CD2	-2.18	117.87	120.89
2	C	401	HEM	CAD-C3D-C2D	-2.18	123.83	127.88
2	C	401	HEM	CMD-C2D-C1D	2.17	128.35	125.04
2	A	401	HEM	CMD-C2D-C1D	2.16	128.33	125.04
2	C	401	HEM	O2D-CGD-CBD	2.16	120.97	114.03
2	A	401	HEM	O2A-CGA-O1A	-2.14	117.98	123.30
4	B	403	ZIQ	CE3-CD2-CE2	2.05	120.89	118.17
2	B	401	HEM	O2A-CGA-O1A	-2.05	118.19	123.30
3	B	402	H7S	C5-C1-CG	2.01	119.33	115.14

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	ZIQ	O-C-CA-C1

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Mol	Chain	Res	Type	Atoms
4	A	403	ZIQ	OXT-C-CA-C1
4	D	403	ZIQ	O-C-CA-C1
4	D	403	ZIQ	OXT-C-CA-C1
4	A	403	ZIQ	O-C-CA-CB
4	A	403	ZIQ	OXT-C-CA-CB
4	D	403	ZIQ	O-C-CA-CB
4	D	403	ZIQ	OXT-C-CA-CB
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
4	B	403	ZIQ	O-C-CA-C1
4	B	403	ZIQ	OXT-C-CA-C1
4	C	403	ZIQ	O-C-CA-C1
2	D	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

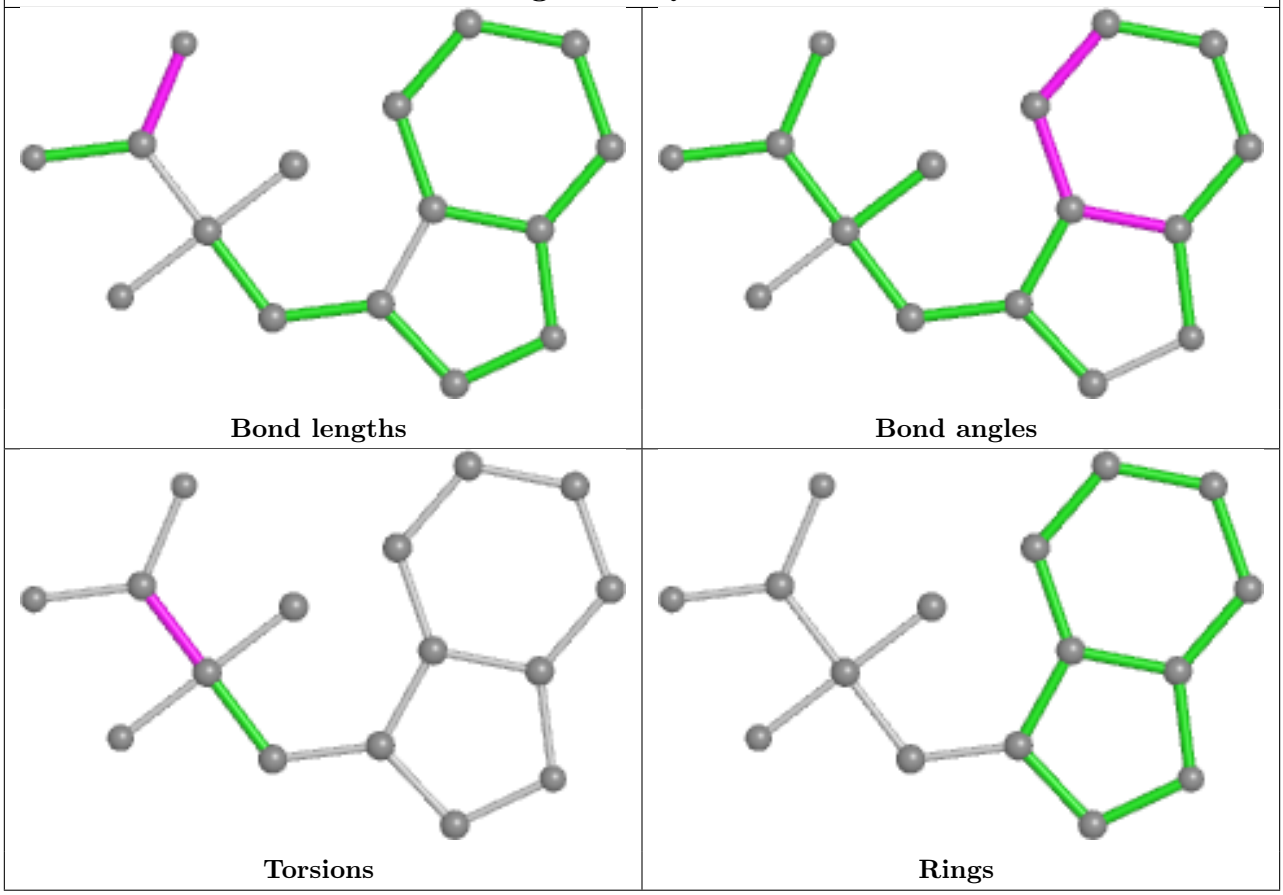
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	3	0
3	D	402	H7S	1	0
4	B	403	ZIQ	1	0
2	B	401	HEM	2	0
2	A	401	HEM	3	0
2	C	401	HEM	3	0
3	A	402	H7S	1	0
4	C	403	ZIQ	1	0

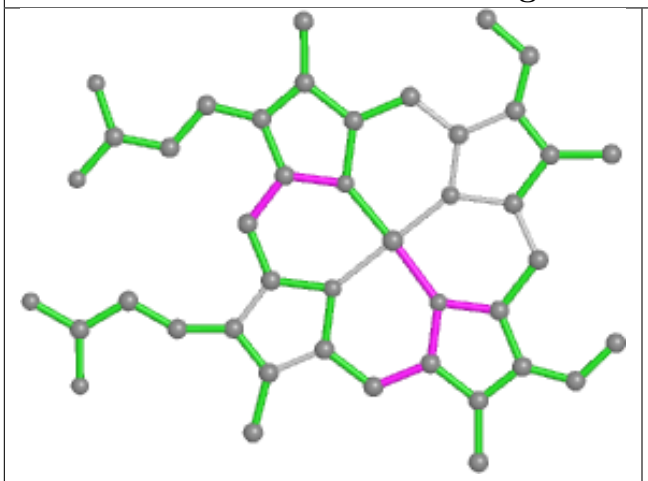
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

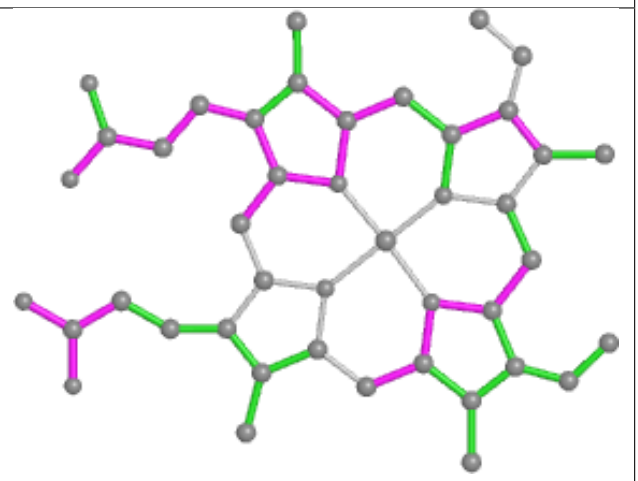
Ligand ZIQ A 403



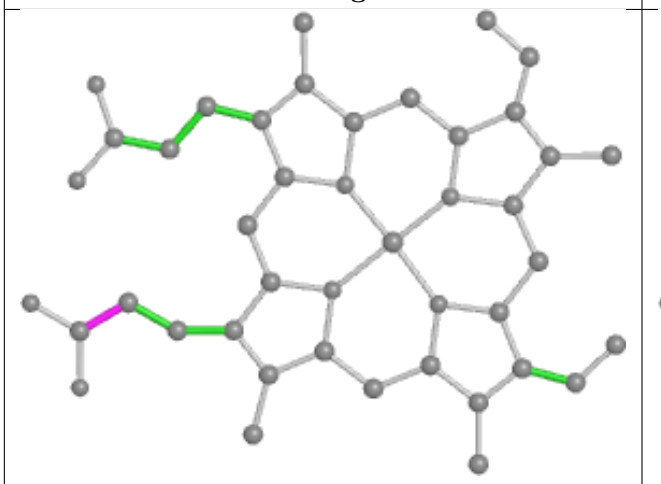
Ligand HEM D 401



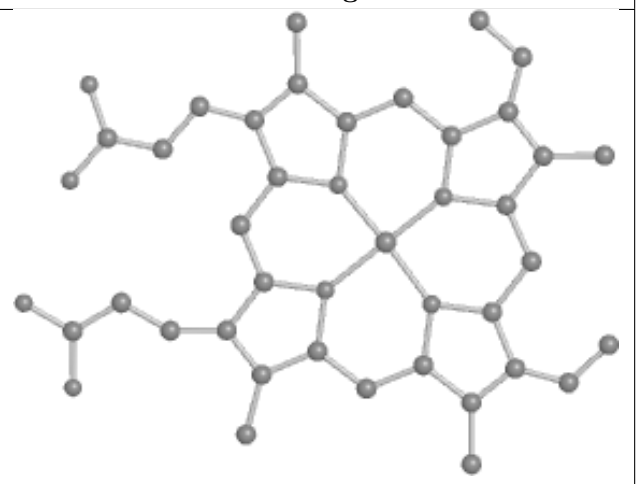
Bond lengths



Bond angles

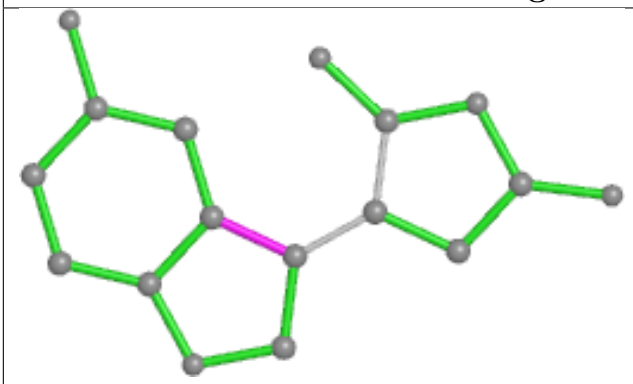


Torsions



Rings

Ligand H7S C 402



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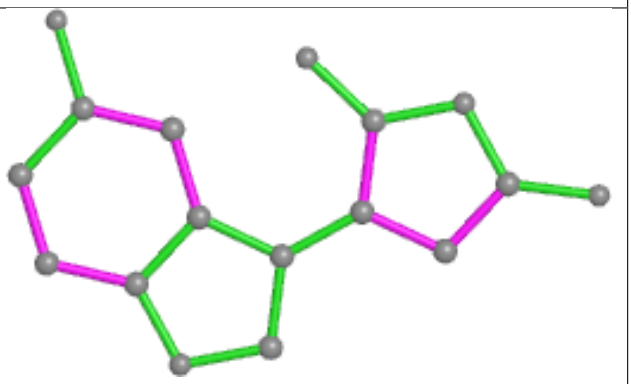
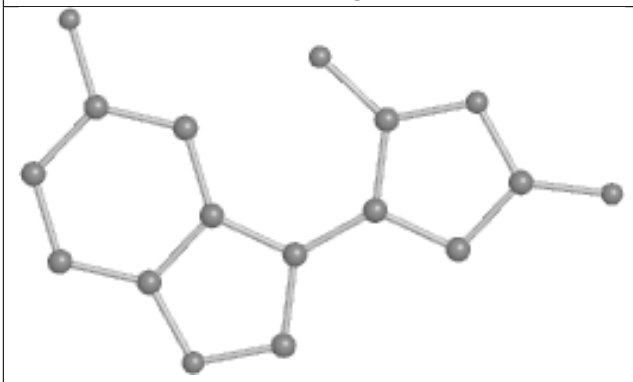
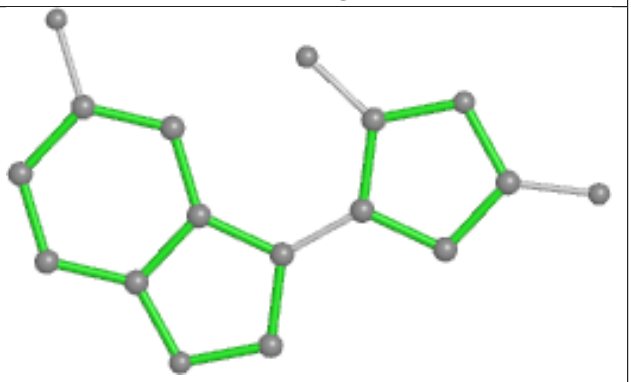


Bond angles

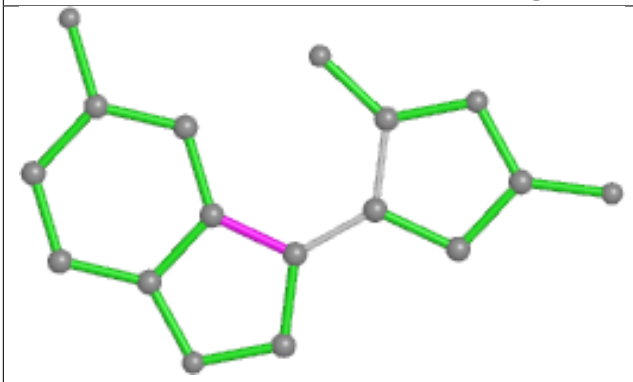


Torsions

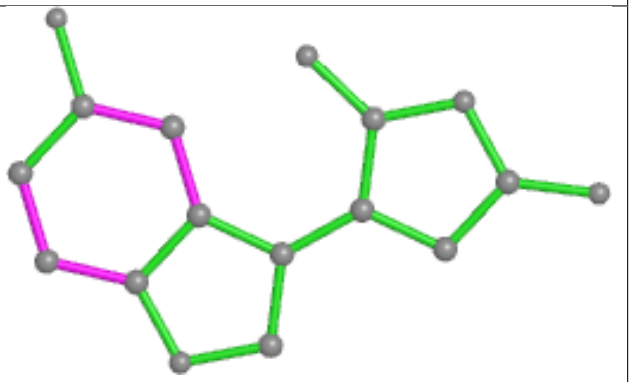


Rings

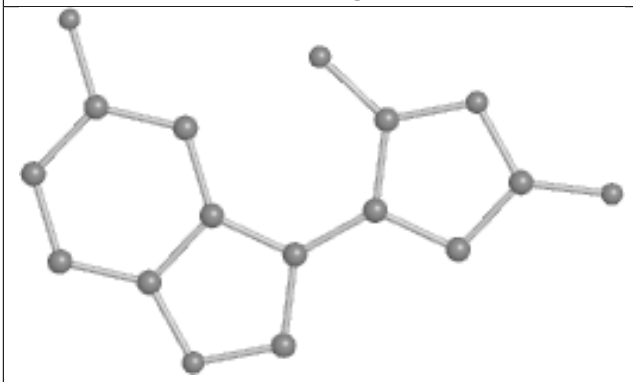
Ligand H7S D 402



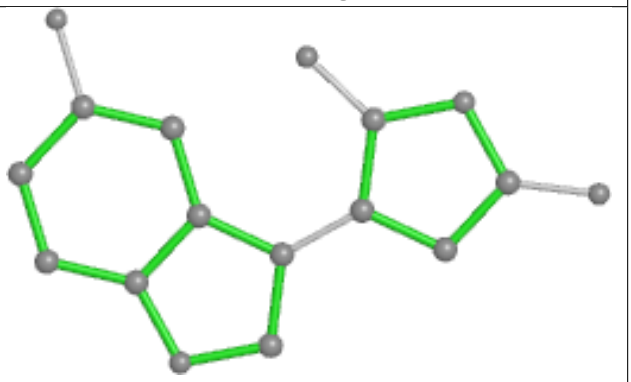
Bond lengths



Bond angles

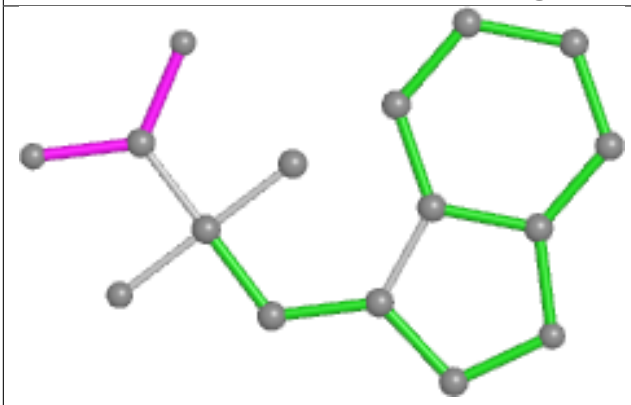


Torsions

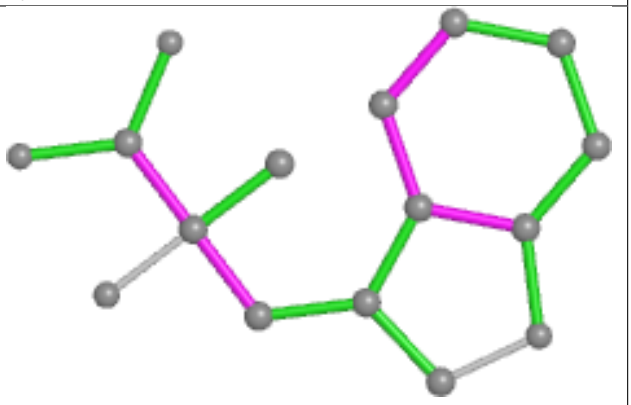


Rings

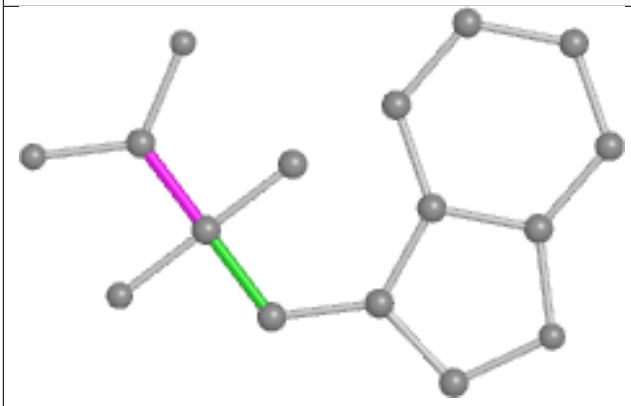
Ligand ZIQ B 403



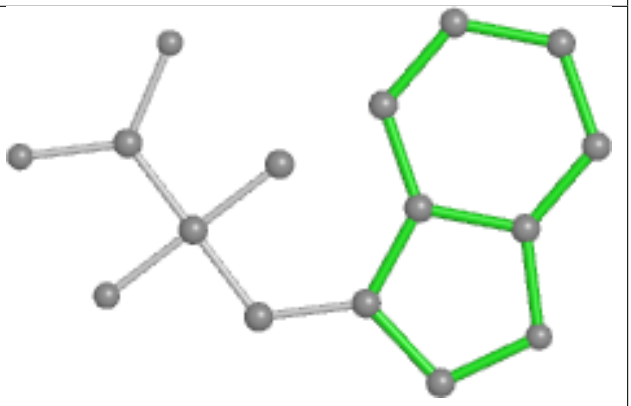
Bond lengths



Bond angles

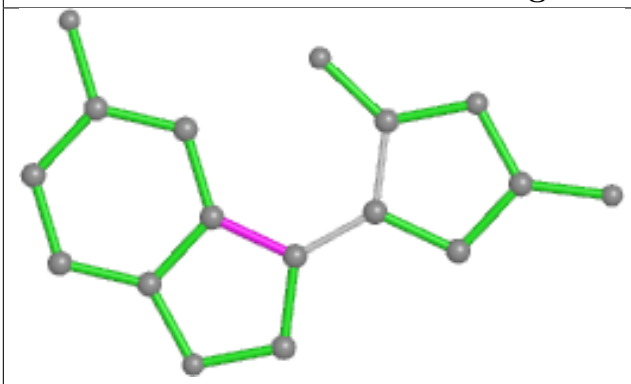


Torsions



Rings

Ligand H7S B 402



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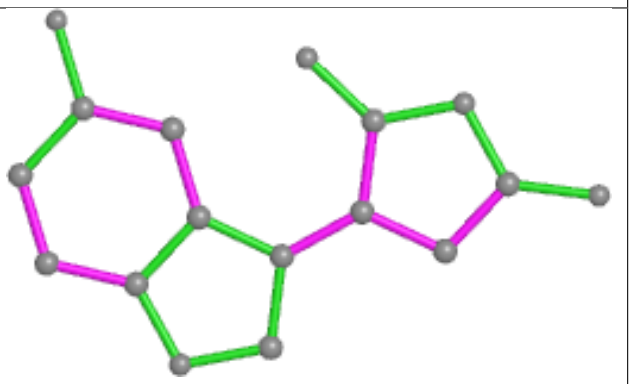
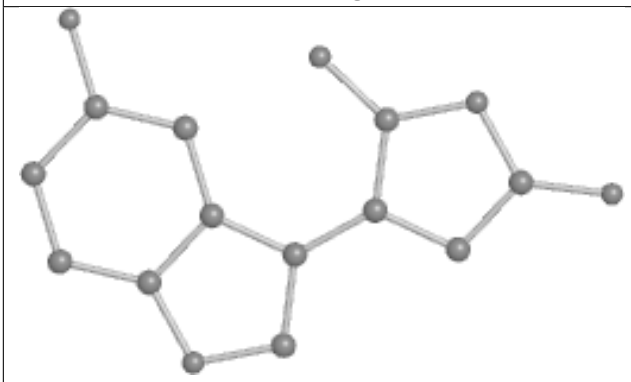


Bond angles



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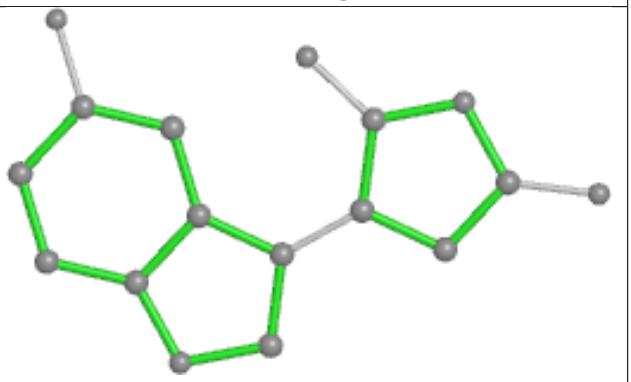
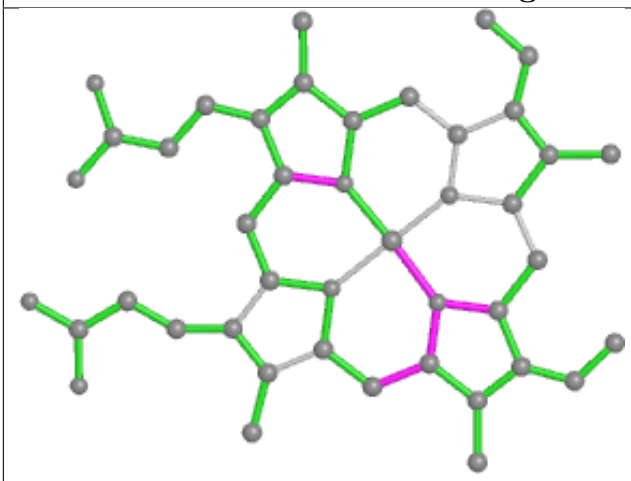


Rings

Ligand HEM B 401



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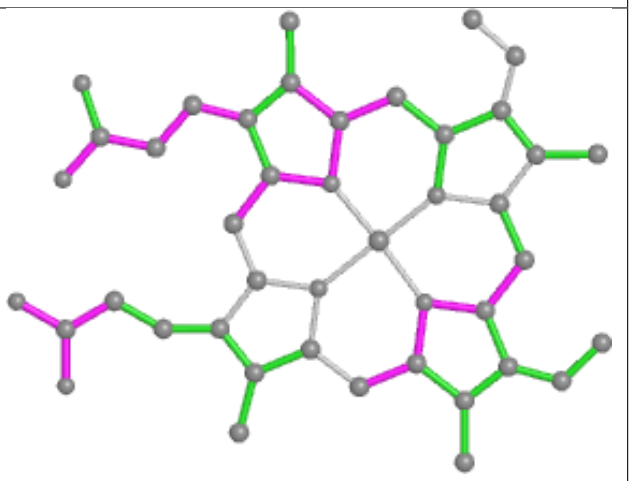
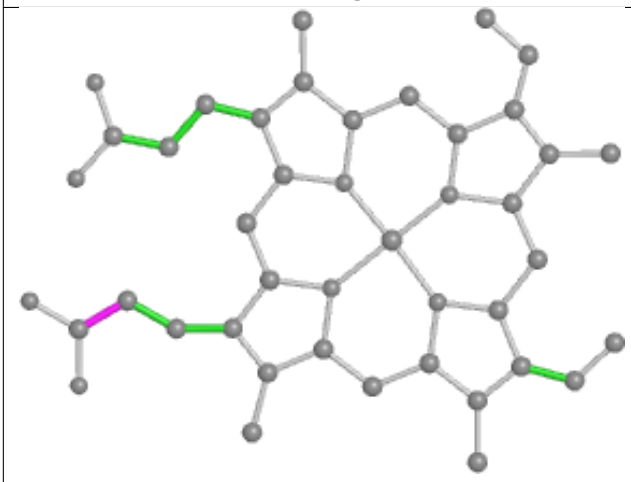
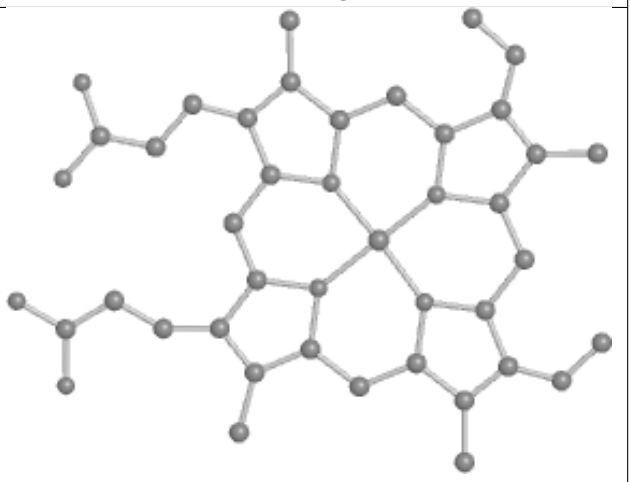


Bond angles

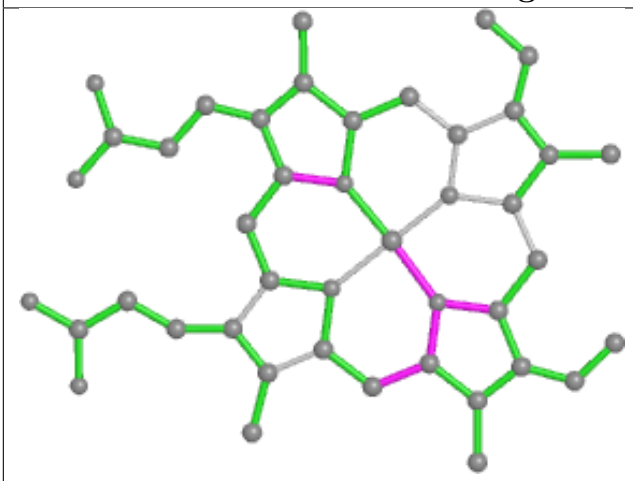


Torsions

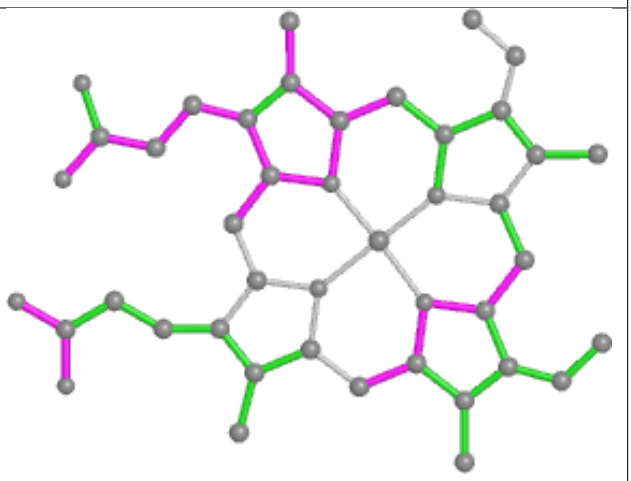


Rings

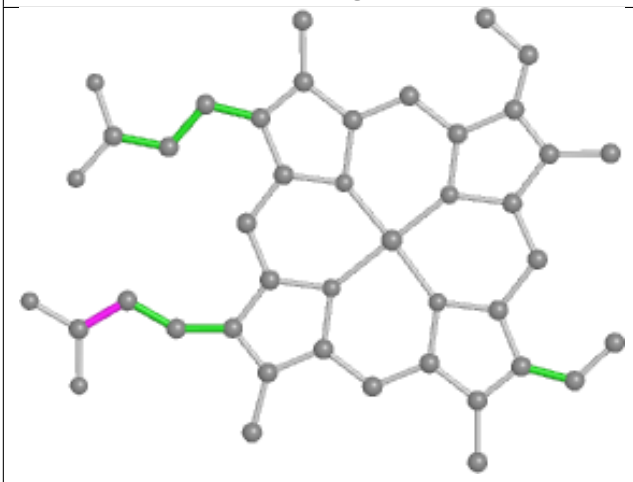
Ligand HEM A 401



Bond lengths



Bond angles



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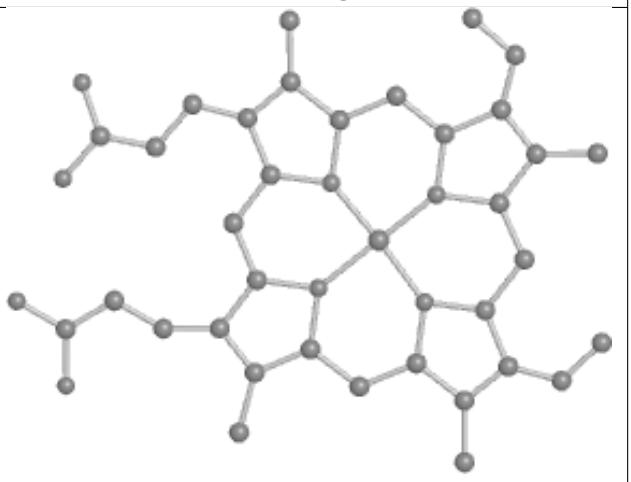
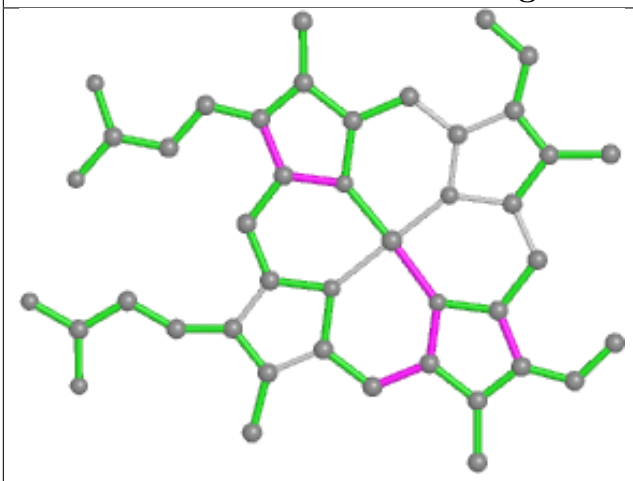


Rings

Ligand HEM C 401



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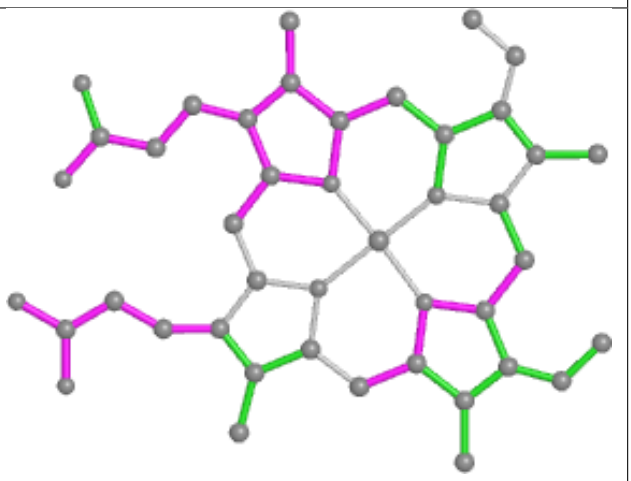
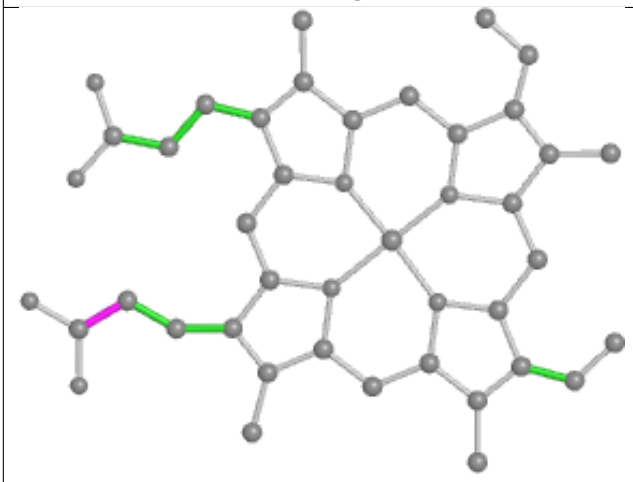


Bond angles



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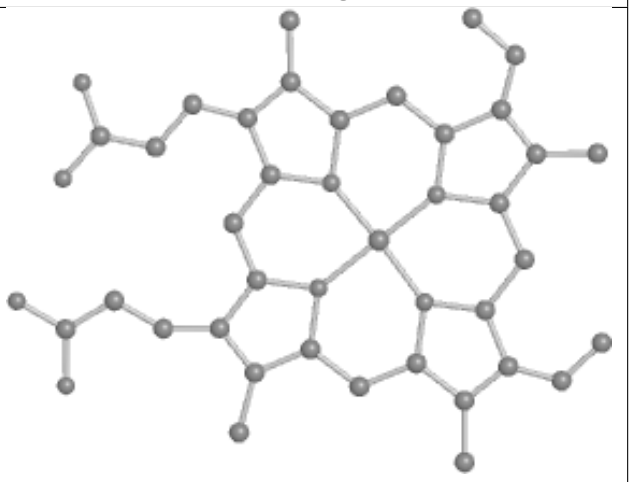
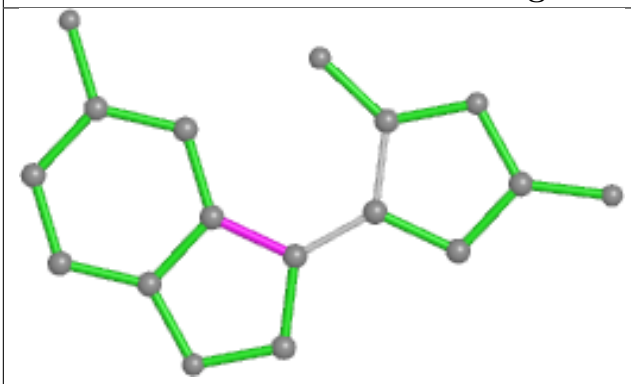
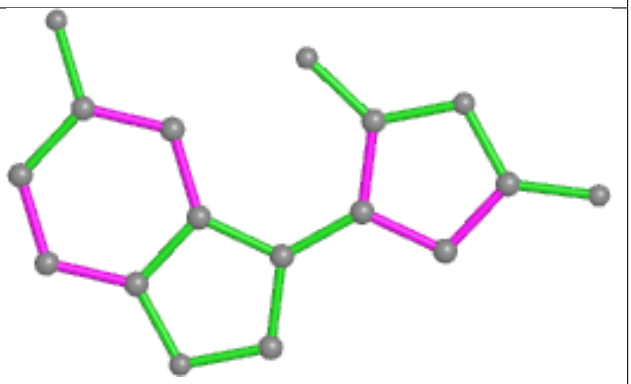


Rings

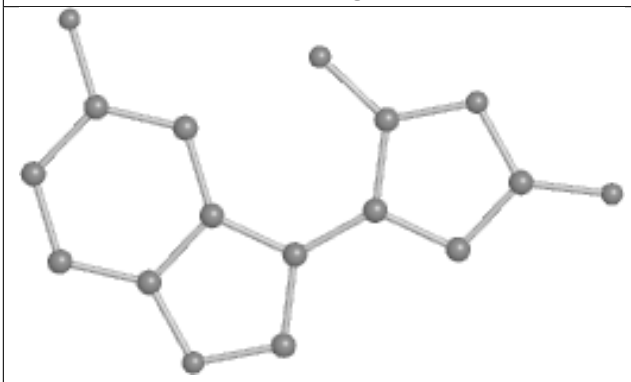
Ligand H7S A 402



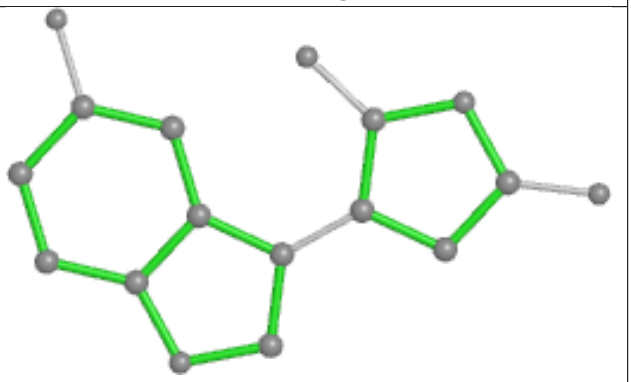
Bond lengths



Bond angles

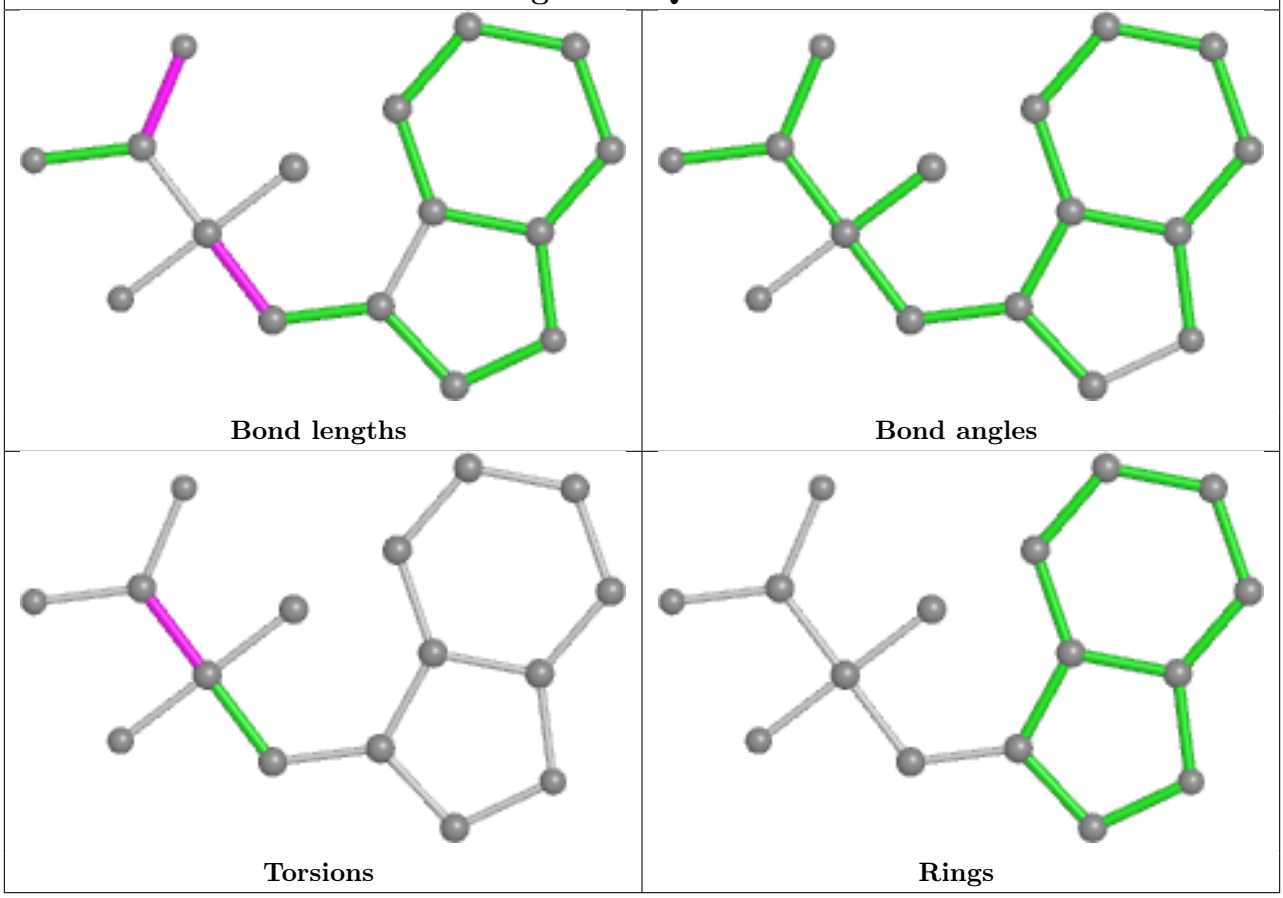


Torsions

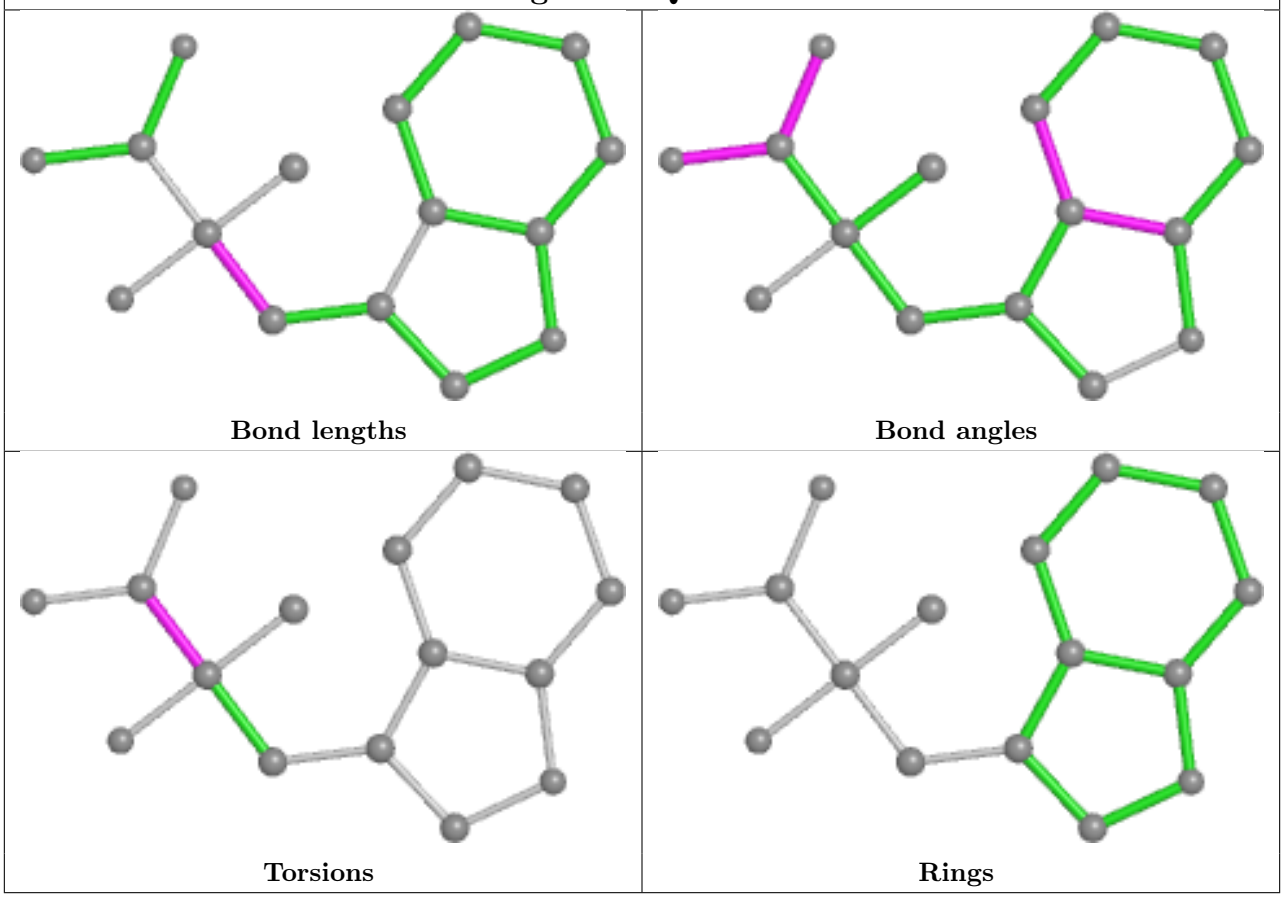


Rings

Ligand ZIQ C 403



Ligand ZIQ D 403



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	353/380 (92%)	0.32	30 (8%)	10	10	29, 46, 86, 113	0
1	B	348/380 (91%)	0.30	30 (8%)	10	10	29, 45, 92, 116	0
1	C	333/380 (87%)	0.56	41 (12%)	4	3	31, 54, 101, 121	0
1	D	342/380 (90%)	0.38	28 (8%)	11	11	31, 49, 91, 127	0
All	All	1376/1520 (90%)	0.39	129 (9%)	8	8	29, 49, 94, 127	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	175	TYR	9.0
1	B	243	ALA	7.7
1	B	388	PHE	7.7
1	D	384	THR	7.6
1	C	257	PHE	6.1
1	B	174	PRO	6.1
1	B	175	TYR	5.8
1	B	38	GLY	5.8
1	D	383	PRO	5.7
1	C	218	HIS	5.5
1	B	384	THR	5.4
1	C	385	ILE	5.2
1	D	390	GLU	4.9
1	B	245	GLU	4.8
1	A	248	GLU	4.7
1	D	388	PHE	4.6
1	B	173	VAL	4.6
1	B	242	GLN	4.5
1	D	248	GLU	4.5
1	B	39	GLY	4.4
1	C	384	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	247	SER	4.2
1	C	382	ASN	4.2
1	C	171	MET	4.2
1	C	256	GLU	4.2
1	C	386	HIS	4.2
1	D	385	ILE	4.1
1	C	271	LYS	4.1
1	D	218	HIS	4.1
1	C	383	PRO	3.9
1	A	241	ILE	3.8
1	B	349	HIS	3.8
1	C	258	GLN	3.6
1	A	176	ASN	3.6
1	B	182	ASP	3.6
1	A	246	GLU	3.6
1	C	193	LEU	3.6
1	A	251	GLU	3.6
1	A	252	GLU	3.4
1	D	252	GLU	3.4
1	C	170	ASN	3.3
1	D	382	ASN	3.2
1	B	383	PRO	3.2
1	A	255	ALA	3.2
1	C	39	GLY	3.2
1	B	63	GLY	3.1
1	C	179	HIS	3.1
1	A	384	THR	3.0
1	A	179	HIS	3.0
1	D	275	HIS	3.0
1	D	389	LEU	3.0
1	A	259	LYS	3.0
1	D	365	LEU	2.9
1	D	247	SER	2.9
1	C	275	HIS	2.9
1	B	385	ILE	2.9
1	B	386	HIS	2.9
1	A	174	PRO	2.9
1	C	217	PRO	2.8
1	B	249	GLU	2.8
1	B	382	ASN	2.8
1	A	385	ILE	2.8
1	C	219	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	258	GLN	2.7
1	A	185	LYS	2.7
1	B	238	PHE	2.7
1	C	81	LEU	2.7
1	C	260	GLN	2.6
1	D	251	GLU	2.6
1	D	292	ALA	2.6
1	C	387	LYS	2.6
1	A	183	ASN	2.6
1	A	344	GLY	2.5
1	A	250	LYS	2.5
1	C	232	ARG	2.5
1	A	383	PRO	2.5
1	B	193	LEU	2.5
1	D	241	ILE	2.5
1	D	249	GLU	2.5
1	C	40	LEU	2.4
1	B	181	ARG	2.4
1	C	388	PHE	2.4
1	C	376	HIS	2.4
1	C	185	LYS	2.4
1	D	61	THR	2.4
1	C	368	LEU	2.4
1	D	386	HIS	2.3
1	D	347	GLY	2.3
1	B	241	ILE	2.3
1	A	311	LEU	2.3
1	D	368	LEU	2.3
1	C	265	LEU	2.3
1	B	244	LYS	2.3
1	B	247	SER	2.3
1	B	171	MET	2.3
1	A	218	HIS	2.3
1	D	250	LYS	2.2
1	C	349	HIS	2.2
1	C	281	GLU	2.2
1	D	255	ALA	2.2
1	D	293	LEU	2.2
1	C	169	GLN	2.2
1	B	240	ARG	2.2
1	A	175	TYR	2.2
1	C	152	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	169	GLN	2.2
1	D	376	HIS	2.2
1	C	221	ASN	2.1
1	A	279	LYS	2.1
1	A	387	LYS	2.1
1	A	177	ARG	2.1
1	B	343	GLY	2.1
1	C	344	GLY	2.1
1	C	340	ALA	2.1
1	A	158	PHE	2.1
1	C	263	VAL	2.1
1	B	170	ASN	2.1
1	B	218	HIS	2.1
1	A	149	PRO	2.1
1	A	332	VAL	2.1
1	C	190	GLU	2.1
1	C	61	THR	2.1
1	A	178	ARG	2.0
1	A	244	LYS	2.0
1	A	340	ALA	2.0
1	C	342	THR	2.0
1	D	78	ALA	2.0
1	D	175	TYR	2.0
1	C	279	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

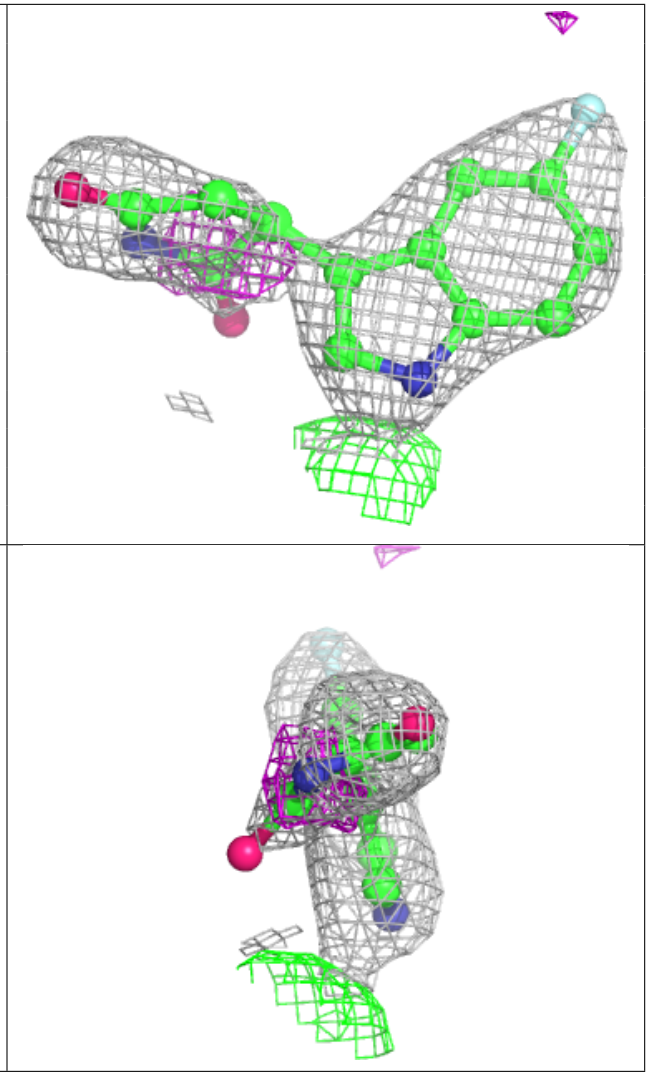
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

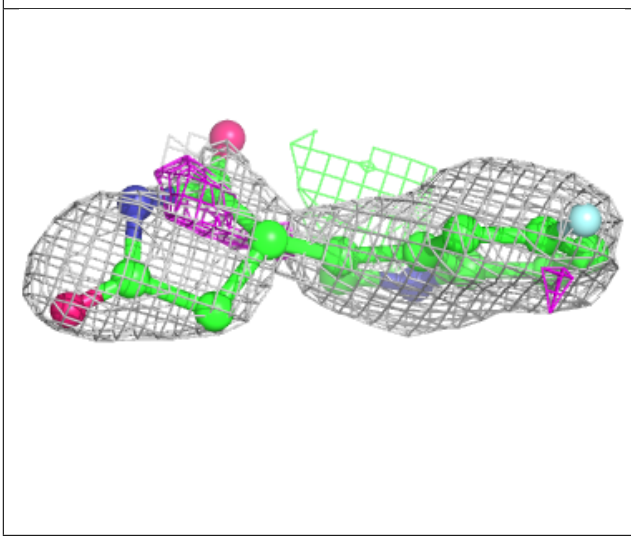
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	H7S	C	402	17/17	0.84	0.21	71,79,91,97	0
3	H7S	A	402	17/17	0.87	0.25	76,80,85,89	0
3	H7S	D	402	17/17	0.87	0.20	61,66,72,72	0
4	ZIQ	D	403	16/16	0.89	0.14	46,51,62,65	0
3	H7S	B	402	17/17	0.93	0.15	65,68,74,77	0
4	ZIQ	B	403	16/16	0.95	0.11	38,43,51,51	0
4	ZIQ	C	403	16/16	0.95	0.10	45,53,64,70	0
4	ZIQ	A	403	16/16	0.95	0.15	35,38,47,48	0
2	HEM	A	401	43/43	0.96	0.15	35,43,50,57	0
2	HEM	D	401	43/43	0.97	0.11	33,42,50,56	0
2	HEM	B	401	43/43	0.97	0.12	35,41,48,51	0
2	HEM	C	401	43/43	0.97	0.12	41,48,54,60	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 H7S C 402:

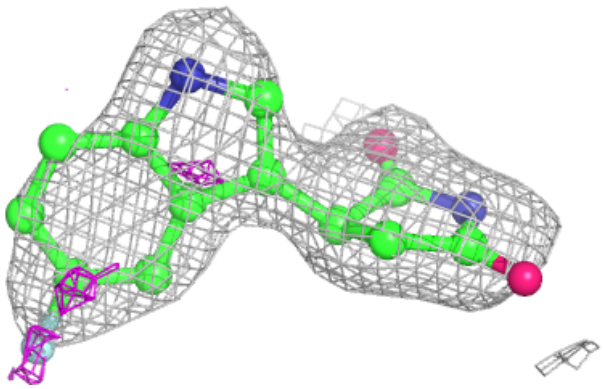
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

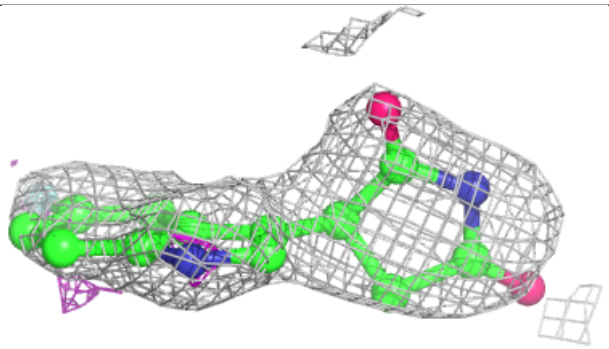


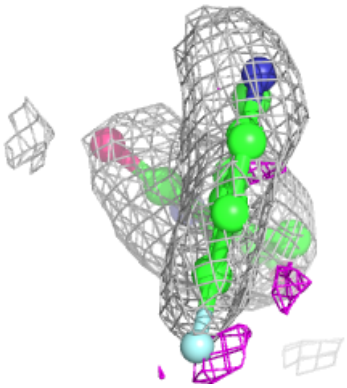


Electron density around H7S A 402:

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

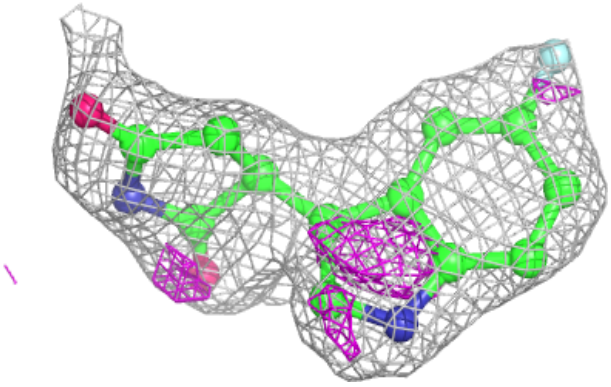


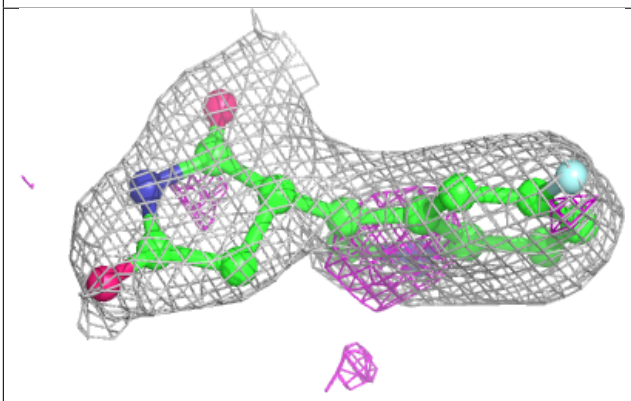


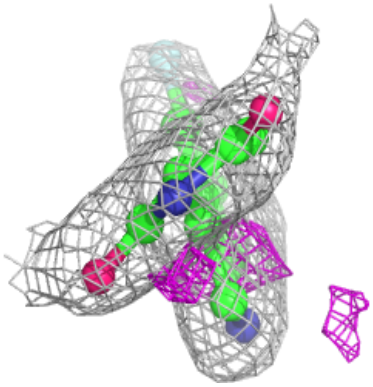


Electron density around H7S D 402:

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

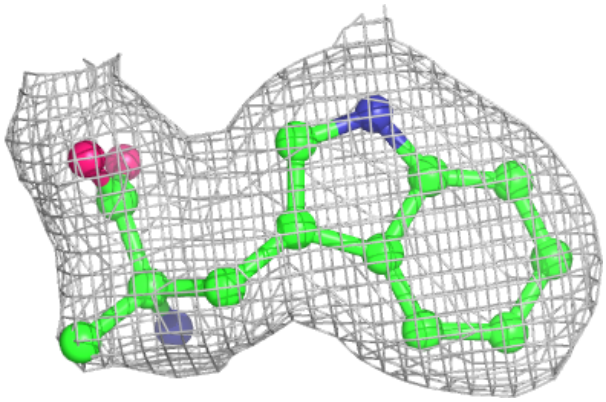


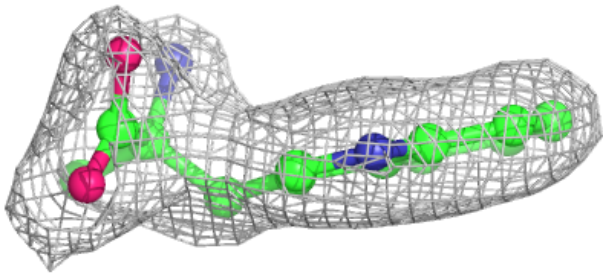


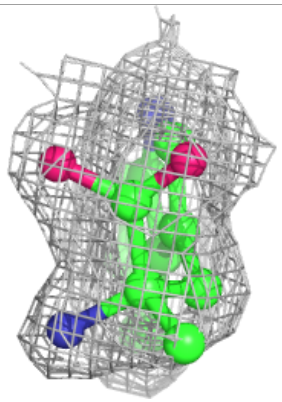


Electron density around ZIQ D 403:

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

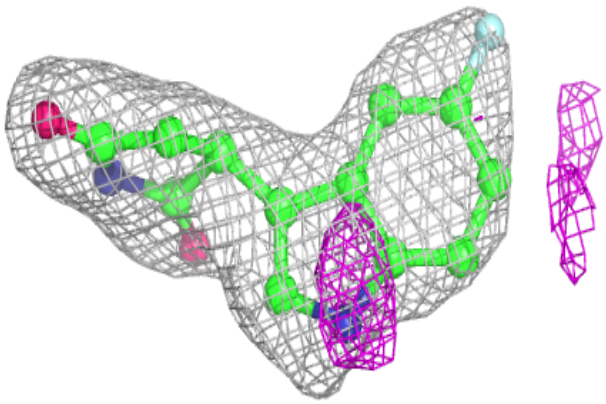


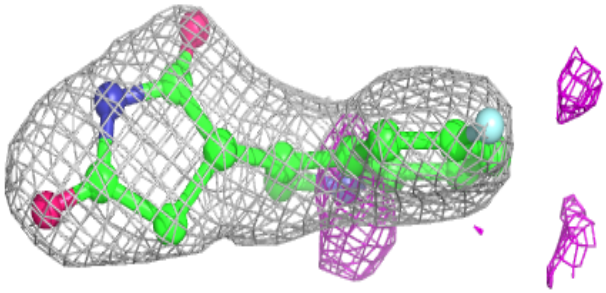


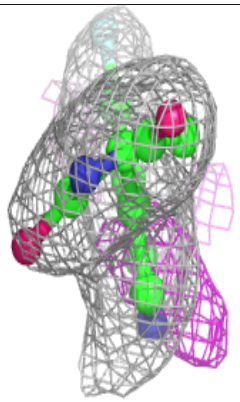


Electron density around H7S B 402:

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

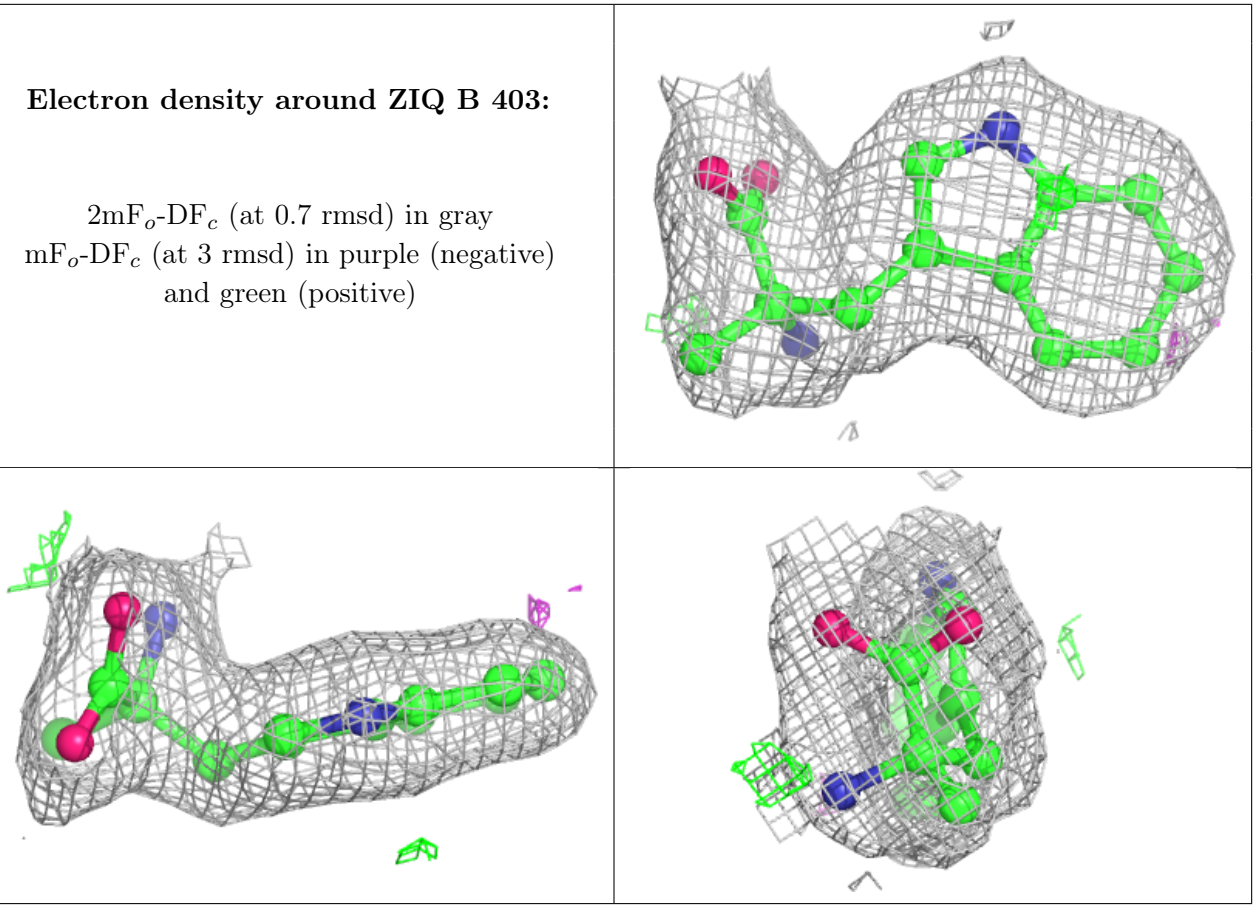






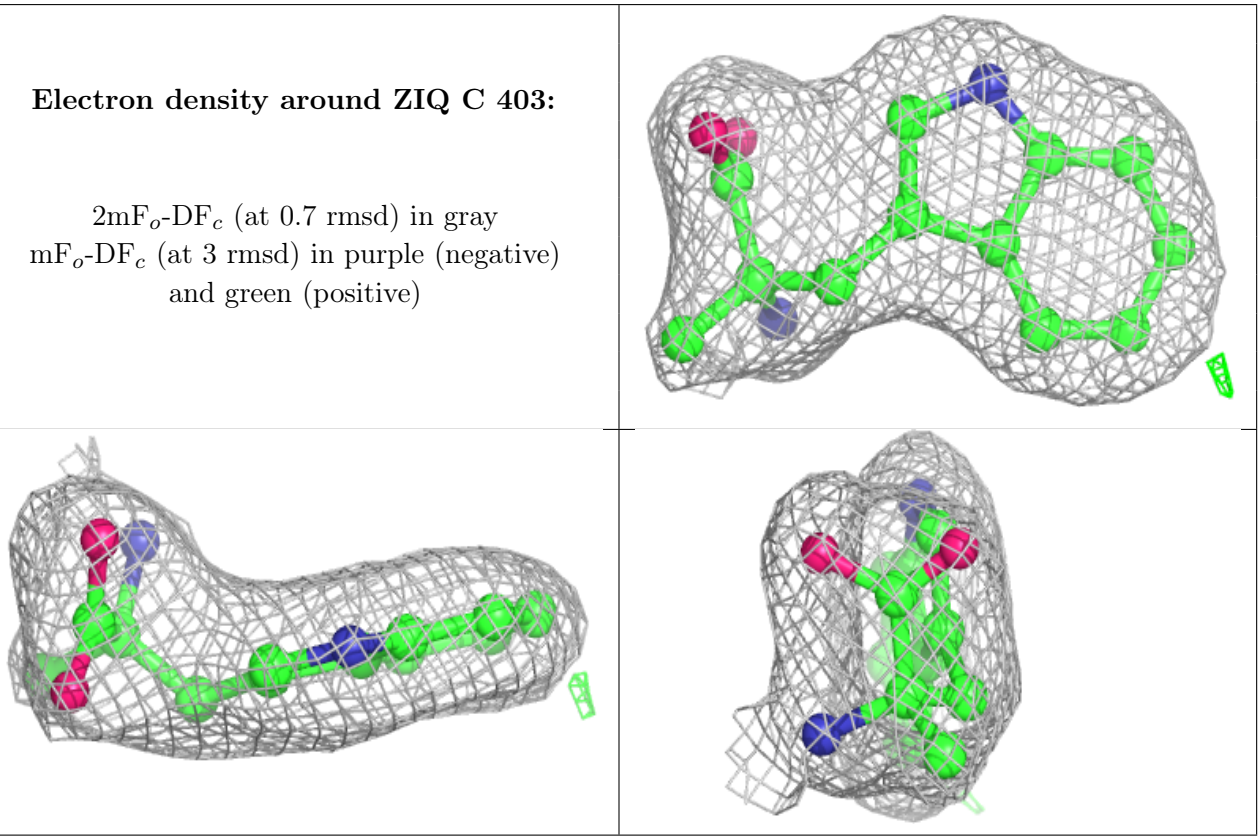
Electron density around ZIQ B 403:

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



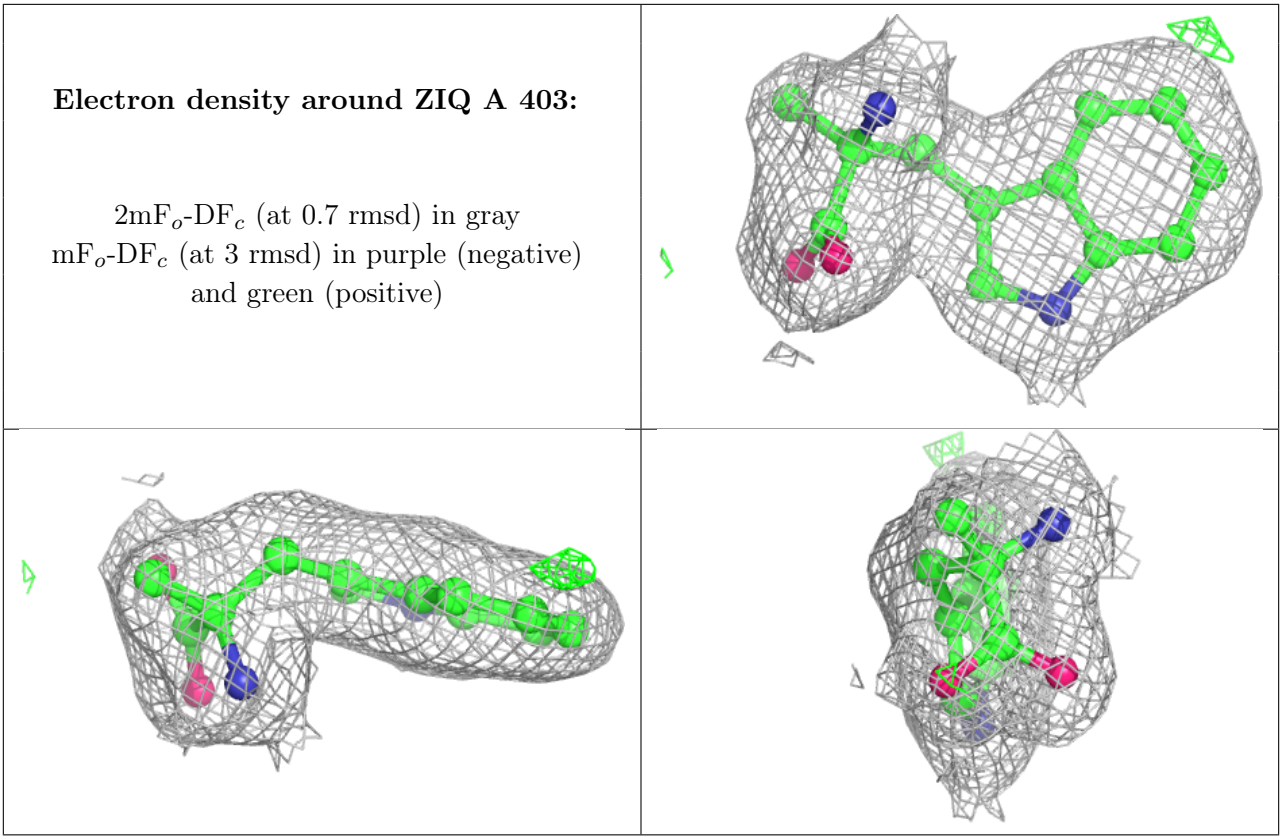
Electron density around ZIQ C 403:

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



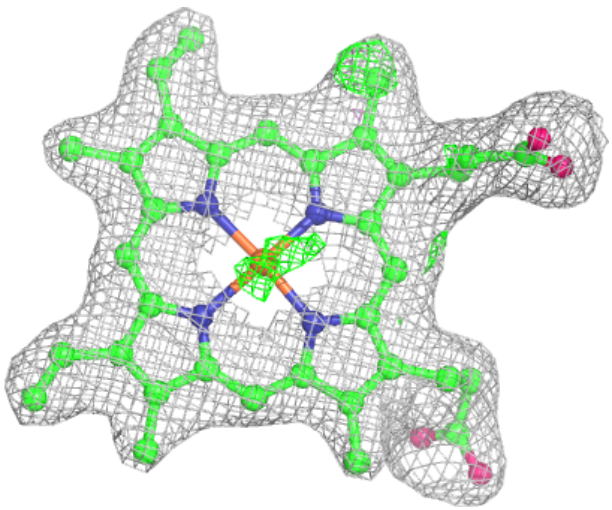
Electron density around ZIQ A 403:

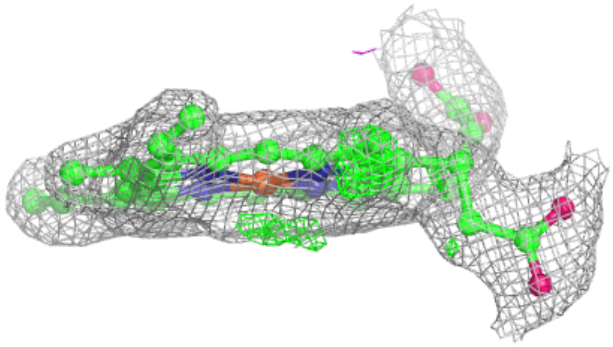
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

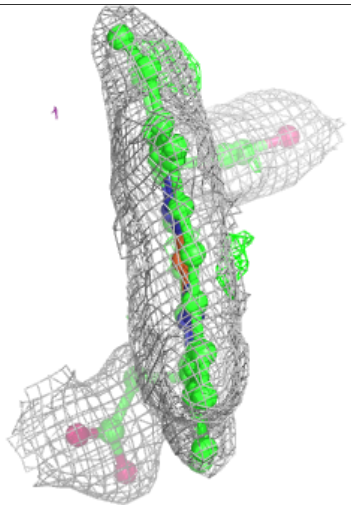


Electron density around HEM A 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

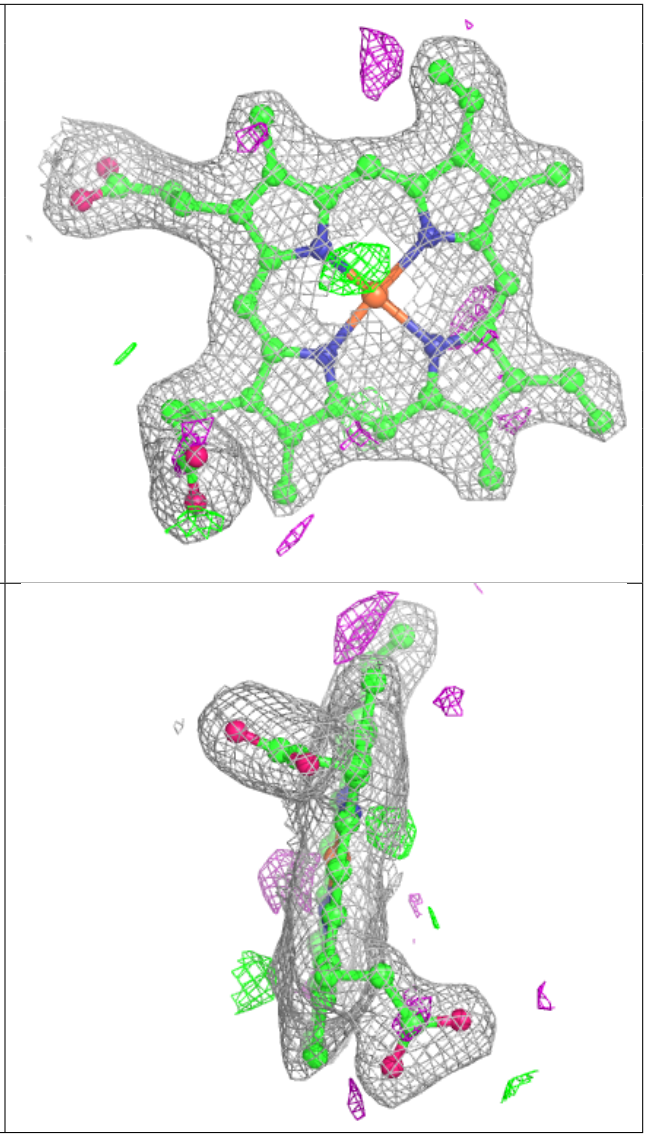






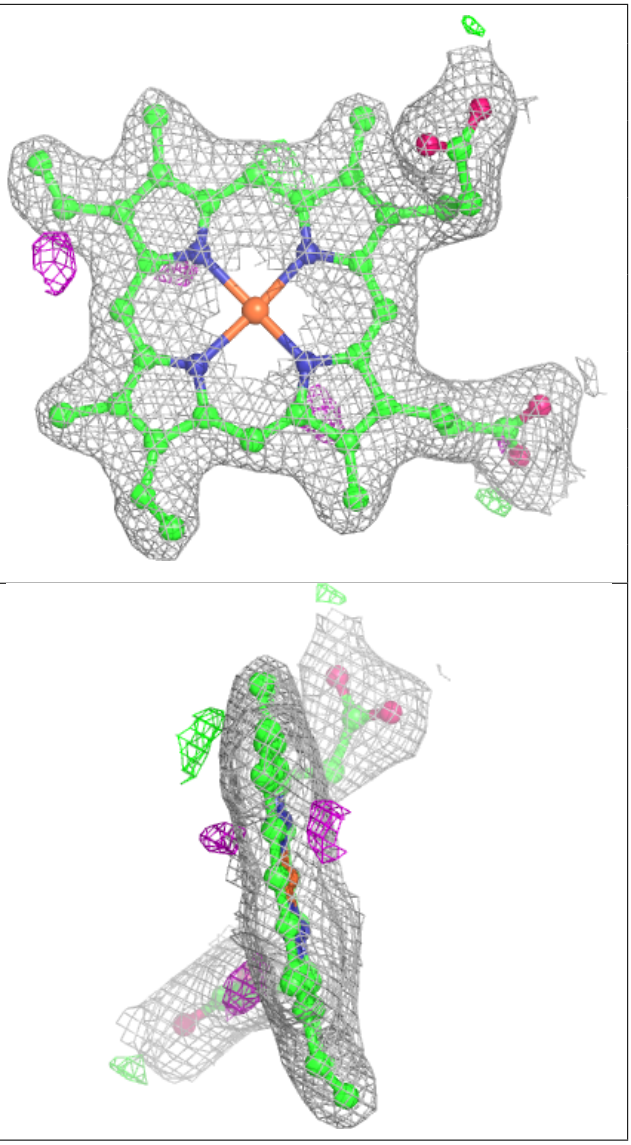
Electron density around HEM D 401:

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



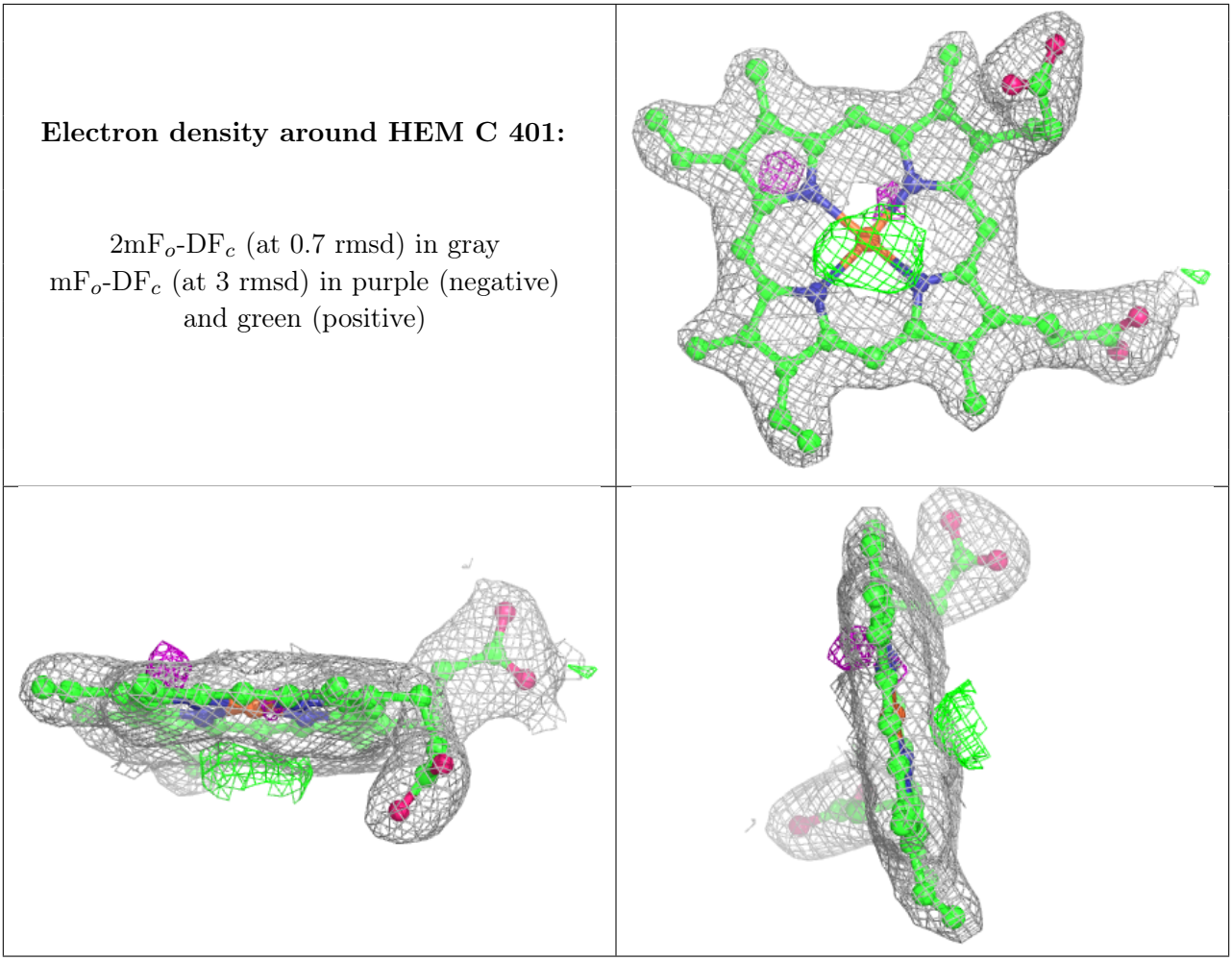
Electron density around HEM B 401:

$2mF_o$-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 C 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.