Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2025 – 12:10 pm GMT

PDB ID	:	9ESF
Title	:	Holo IDO with a bound inhibitor
Authors	:	Wicki, M.; Mac Sweeney, A.
Deposited on	:	2024-03-26
Resolution	:	2.50 Å(reported)

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

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

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

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

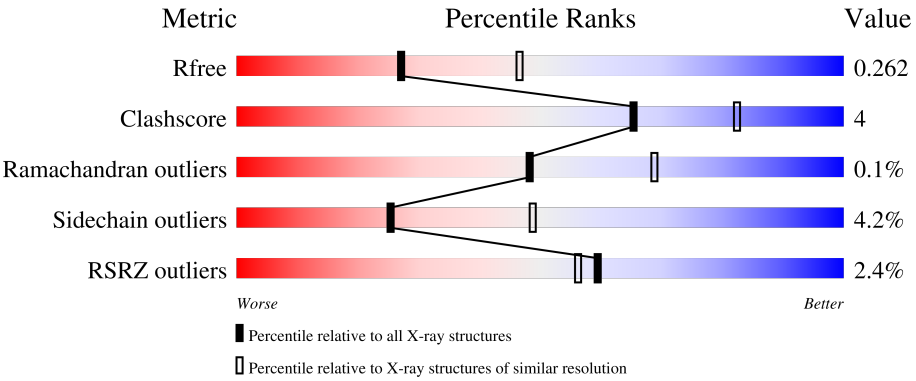
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	365	79% 9% • 11%
1	B	365	3% 79% 11% • 10%
1	C	365	3% 79% 11% • 10%
1	D	365	2% 80% 9% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11162 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	A	324	Total	C	N	O	S	0	0	0
			2706	1732	465	497	12			
1	B	328	Total	C	N	O	S	0	1	0
			2734	1749	472	501	12			
1	C	330	Total	C	N	O	S	0	0	0
			2735	1751	469	503	12			
1	D	331	Total	C	N	O	S	0	0	0
			2741	1753	472	504	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P20351
A	380	LEU	-	expression tag	UNP P20351
A	381	GLU	-	expression tag	UNP P20351
A	382	HIS	-	expression tag	UNP P20351
A	383	HIS	-	expression tag	UNP P20351
A	384	HIS	-	expression tag	UNP P20351
A	385	HIS	-	expression tag	UNP P20351
A	386	HIS	-	expression tag	UNP P20351
A	387	HIS	-	expression tag	UNP P20351
B	23	MET	-	initiating methionine	UNP P20351
B	380	LEU	-	expression tag	UNP P20351
B	381	GLU	-	expression tag	UNP P20351
B	382	HIS	-	expression tag	UNP P20351
B	383	HIS	-	expression tag	UNP P20351
B	384	HIS	-	expression tag	UNP P20351
B	385	HIS	-	expression tag	UNP P20351
B	386	HIS	-	expression tag	UNP P20351
B	387	HIS	-	expression tag	UNP P20351
C	23	MET	-	initiating methionine	UNP P20351
C	380	LEU	-	expression tag	UNP P20351
C	381	GLU	-	expression tag	UNP P20351

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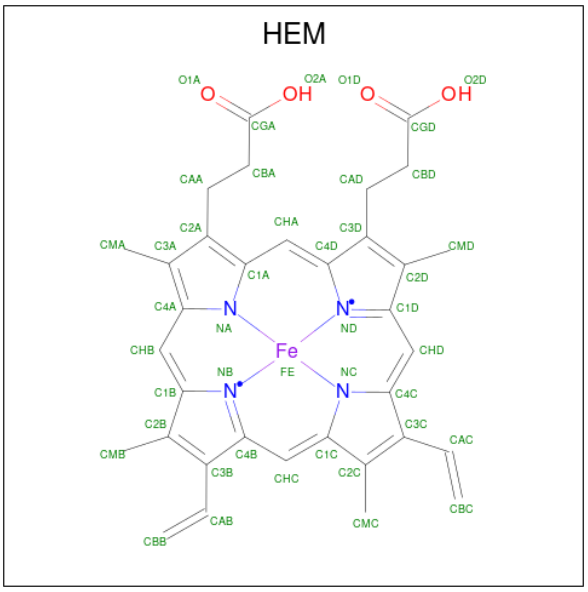
Chain	Residue	Modelled	Actual	Comment	Reference
C	382	HIS	-	expression tag	UNP P20351
C	383	HIS	-	expression tag	UNP P20351
C	384	HIS	-	expression tag	UNP P20351
C	385	HIS	-	expression tag	UNP P20351
C	386	HIS	-	expression tag	UNP P20351
C	387	HIS	-	expression tag	UNP P20351
D	23	MET	-	initiating methionine	UNP P20351
D	380	LEU	-	expression tag	UNP P20351
D	381	GLU	-	expression tag	UNP P20351
D	382	HIS	-	expression tag	UNP P20351
D	383	HIS	-	expression tag	UNP P20351
D	384	HIS	-	expression tag	UNP P20351
D	385	HIS	-	expression tag	UNP P20351
D	386	HIS	-	expression tag	UNP P20351
D	387	HIS	-	expression tag	UNP P20351

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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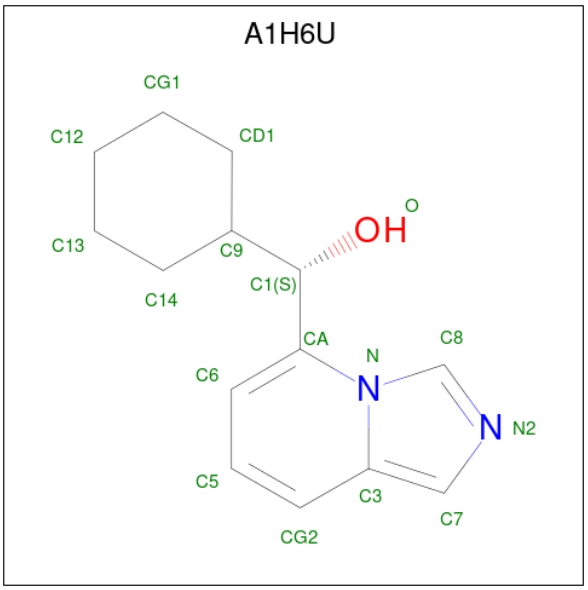
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ({S})-cyclohexyl(imidazo[1,5-a]pyridin-5-yl)methanol (three-letter code: A1H6U) (formula: $C_{14}H_{18}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			17	14	2	1			
3	B	1	Total	C	N	O		0	0
			17	14	2	1			
3	C	1	Total	C	N	O		0	0
			17	14	2	1			
3	D	1	Total	C	N	O		0	0
			17	14	2	1			

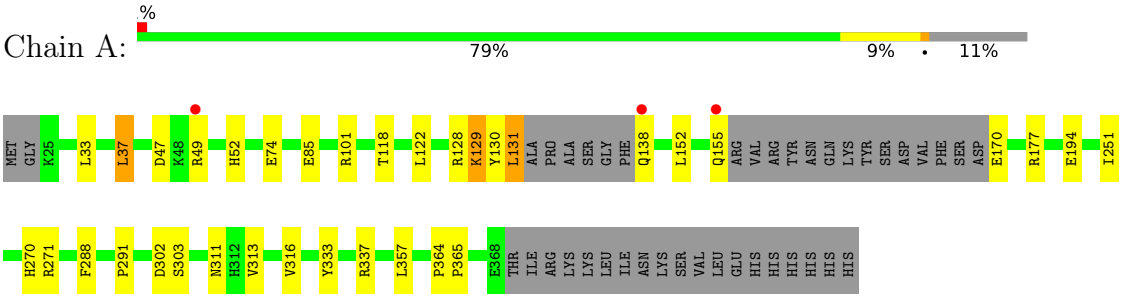
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		

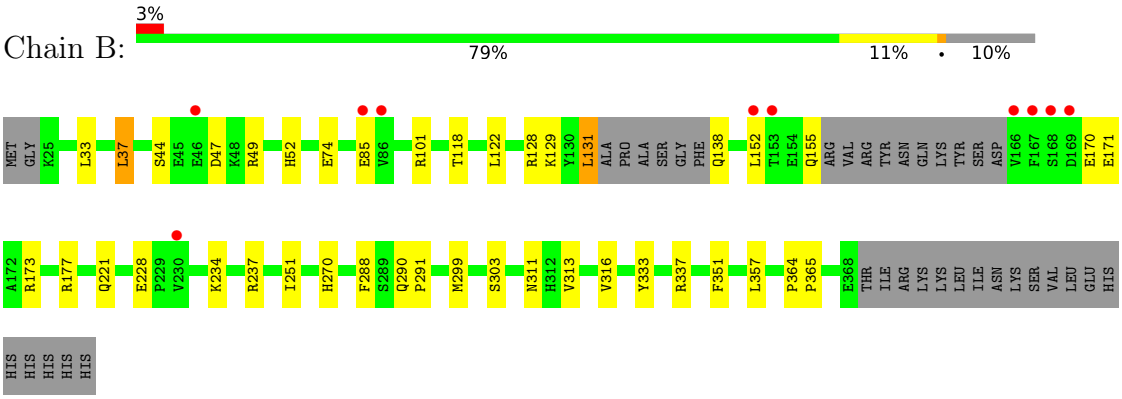
3 Residue-property plots (i)

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.

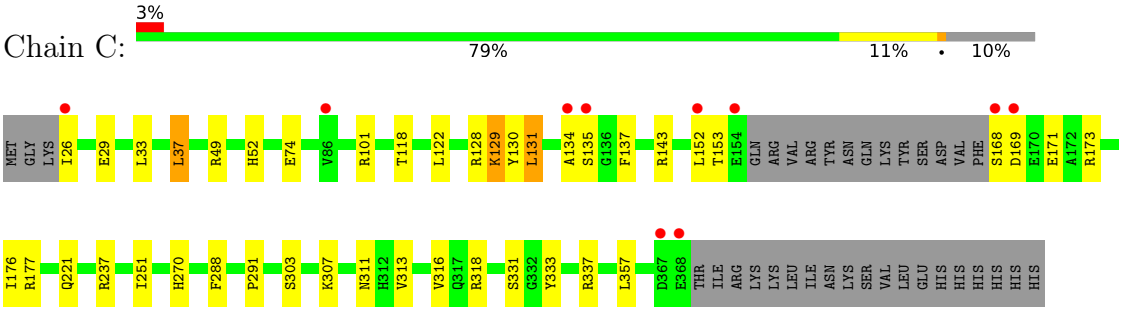
• Molecule 1: Tryptophan 2,3-dioxygenase



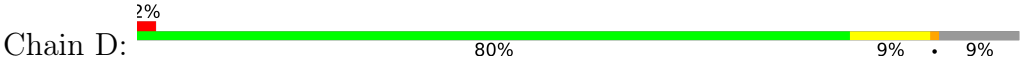
• Molecule 1: Tryptophan 2,3-dioxygenase

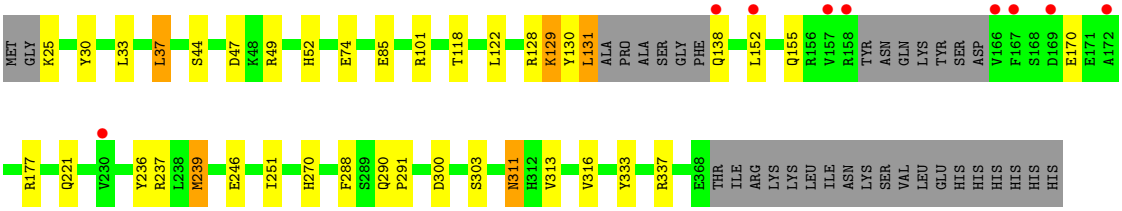


• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase




MET GLY K25 Y30 L33 L37 S44 D47 K48 R49 H52 E74 E85 R101 T118 L122 R128 K129 Y130 L131 ALA PRO ALA SER GLY PHE Q138 L152 Q155 R156 V157 R158 TYR ASN GLN LYS TYR SER ASP V166 F167 S168 D169 E170 E171 A172
R177 Q221 V230 Y236 R237 L238 M239 E246 I251 H270 F288 S289 Q290 P291 D300 S303 N311 H312 V313 V316 Y333 R337 E368 THR ILE ARG LYS LYS LEU ILE ASN LYS SER VAL LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	143.77Å 143.77Å 141.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.06 – 2.50 47.06 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.06-2.50) 99.9 (47.06-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.245 , 0.274 0.238 , 0.262	Depositor DCC
R_{free} test set	2882 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 17.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.060 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11162	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 4.55% 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, A1H6U

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	0.36	0/2759	0.49	0/3718
1	B	0.36	0/2790	0.49	0/3760
1	C	0.38	0/2791	0.53	1/3766 (0.0%)
1	D	0.36	0/2794	0.49	0/3767
All	All	0.36	0/11134	0.50	1/15011 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168	SER	C-N-CA	5.29	134.93	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2706	0	2713	24	0
1	B	2734	0	2734	22	0
1	C	2735	0	2729	26	0
1	D	2741	0	2727	28	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	17	0	0	1	0
3	B	17	0	0	1	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
All	All	11162	0	11023	81	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 (81) 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:D:49:ARG:HH22	1:D:129:LYS:NZ	1.55	1.04
1:C:49:ARG:HH22	1:C:129:LYS:NZ	1.58	1.01
1:A:49:ARG:HH22	1:A:129:LYS:NZ	1.56	1.01
1:C:49:ARG:HH22	1:C:129:LYS:HZ2	1.18	0.90
1:A:49:ARG:HH22	1:A:129:LYS:HZ3	1.24	0.82
1:A:49:ARG:NH2	1:A:129:LYS:NZ	2.28	0.81
1:D:49:ARG:NH2	1:D:129:LYS:NZ	2.28	0.81
1:C:49:ARG:NH2	1:C:129:LYS:NZ	2.29	0.80
1:D:49:ARG:HH22	1:D:129:LYS:HZ3	1.35	0.72
1:C:49:ARG:NH1	1:C:130:TYR:OH	2.23	0.71
1:D:49:ARG:NH1	1:D:130:TYR:OH	2.24	0.70
1:A:49:ARG:NH1	1:A:130:TYR:OH	2.25	0.70
1:D:49:ARG:HH22	1:D:129:LYS:HZ2	1.44	0.64
1:A:118:THR:HG21	1:D:101:ARG:HB2	1.80	0.63
1:A:52:HIS:HE1	1:D:74:GLU:OE1	1.82	0.63
1:A:74:GLU:OE1	1:D:52:HIS:HE1	1.82	0.63
1:B:74:GLU:OE1	1:C:52:HIS:HE1	1.84	0.60
1:B:101:ARG:HB2	1:C:118:THR:HG21	1.85	0.57
1:C:307:LYS:NZ	1:D:311:ASN:HD21	2.01	0.56
1:B:52:HIS:HE1	1:C:74:GLU:OE1	1.88	0.56
1:C:251:ILE:O	1:C:270:HIS:HE1	1.89	0.55
1:B:118:THR:HG21	1:C:101:ARG:HB2	1.91	0.53
1:D:25:LYS:HD3	1:D:30:TYR:HA	1.90	0.53
1:B:251:ILE:O	1:B:270:HIS:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:O	1:A:270:HIS:HE1	1.92	0.52
1:C:169:ASP:O	1:C:173:ARG:HB2	2.10	0.51
1:D:251:ILE:O	1:D:270:HIS:HE1	1.94	0.50
1:B:316:VAL:HG22	2:B:401:HEM:C1B	2.47	0.49
1:C:357:LEU:HD21	1:D:122:LEU:HG	1.94	0.49
1:D:33:LEU:HB3	1:D:37:LEU:HD22	1.95	0.49
1:A:122:LEU:HG	1:B:357:LEU:HD21	1.96	0.48
1:A:357:LEU:HD21	1:B:122:LEU:HG	1.96	0.48
1:B:101:ARG:HE	1:C:118:THR:CG2	2.27	0.48
1:C:333:TYR:CZ	1:C:337:ARG:HD2	2.50	0.47
1:D:316:VAL:HG22	2:D:401:HEM:C1B	2.50	0.46
1:A:316:VAL:HG22	2:A:401:HEM:C1B	2.51	0.46
1:A:118:THR:CG2	1:D:101:ARG:HE	2.29	0.46
1:B:101:ARG:HH21	1:C:118:THR:HG22	1.80	0.45
1:C:316:VAL:HG22	2:C:401:HEM:C1B	2.52	0.45
1:A:33:LEU:HB3	1:A:37:LEU:HD22	1.99	0.45
1:D:128:ARG:HA	1:D:131:LEU:HD22	1.99	0.45
1:C:122:LEU:H	1:C:122:LEU:HD12	1.80	0.45
1:D:221:GLN:NE2	1:D:237:ARG:HH21	2.15	0.45
1:C:49:ARG:NH2	1:C:129:LYS:HZ1	2.12	0.44
1:D:152:LEU:HB2	1:D:155:GLN:HG2	2.00	0.44
1:B:101:ARG:HE	1:C:118:THR:HG21	1.81	0.44
1:A:101:ARG:HH21	1:D:118:THR:HG22	1.83	0.44
1:D:236:TYR:O	1:D:239:MET:HG3	2.18	0.44
1:C:128:ARG:HA	1:C:131:LEU:HD22	2.00	0.44
1:A:122:LEU:HD12	1:A:122:LEU:H	1.82	0.43
1:C:318:ARG:NH2	1:D:300:ASP:OD1	2.51	0.43
1:B:33:LEU:HB3	1:B:37:LEU:HD22	1.99	0.43
1:C:288:PHE:C	1:C:291:PRO:HD2	2.38	0.43
1:A:128:ARG:HA	1:A:131:LEU:HD22	2.01	0.43
1:D:122:LEU:HD12	1:D:122:LEU:H	1.84	0.43
1:A:138:GLN:NE2	3:A:402:A1H6U:O	2.52	0.43
1:B:152:LEU:HB2	1:B:155:GLN:HG2	2.01	0.43
1:C:137:PHE:CB	1:C:143:ARG:HG3	2.49	0.43
1:D:138:GLN:NE2	3:D:402:A1H6U:O	2.51	0.43
1:A:288:PHE:C	1:A:291:PRO:HD2	2.39	0.43
1:A:333:TYR:CZ	1:A:337:ARG:HD2	2.54	0.43
1:D:288:PHE:C	1:D:291:PRO:HD2	2.40	0.43
1:B:138:GLN:NE2	3:B:402:A1H6U:O	2.49	0.42
1:B:128:ARG:HA	1:B:131:LEU:HD22	2.02	0.42
1:C:33:LEU:HB3	1:C:37:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:PHE:CE2	1:C:176:ILE:HD12	2.55	0.42
1:B:333:TYR:CZ	1:B:337:ARG:HD2	2.55	0.42
1:B:364:PRO:HA	1:B:365:PRO:HD3	1.92	0.41
1:C:221:GLN:NE2	1:C:237:ARG:HH21	2.18	0.41
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.91	0.41
1:A:101:ARG:HB2	1:D:118:THR:HG21	2.02	0.41
1:D:333:TYR:CZ	1:D:337:ARG:HD2	2.56	0.41
1:B:221:GLN:NE2	1:B:237:ARG:HH21	2.18	0.41
1:B:299:MET:HE3	1:B:351:PHE:HA	2.02	0.41
1:A:118:THR:HG21	1:D:101:ARG:HE	1.86	0.41
1:B:228:GLU:HB3	1:B:234:LYS:HB2	2.03	0.41
1:A:152:LEU:HB2	1:A:155:GLN:HG2	2.04	0.41
1:B:44:SER:HB2	1:B:49:ARG:O	2.21	0.41
1:A:194:GLU:HG2	1:A:271:ARG:HB3	2.03	0.40
1:D:44:SER:HB2	1:D:49:ARG:O	2.21	0.40
1:B:288:PHE:C	1:B:291:PRO:HD2	2.41	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	318/365 (87%)	310 (98%)	8 (2%)	0	100	100
1	B	323/365 (88%)	317 (98%)	6 (2%)	0	100	100
1	C	326/365 (89%)	314 (96%)	11 (3%)	1 (0%)	37	56
1	D	325/365 (89%)	317 (98%)	8 (2%)	0	100	100
All	All	1292/1460 (88%)	1258 (97%)	33 (3%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	134	ALA

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	300/337 (89%)	289 (96%)	11 (4%)	29	55
1	B	301/337 (89%)	288 (96%)	13 (4%)	25	48
1	C	301/337 (89%)	287 (95%)	14 (5%)	22	44
1	D	300/337 (89%)	287 (96%)	13 (4%)	25	48
All	All	1202/1348 (89%)	1151 (96%)	51 (4%)	25	49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	47	ASP
1	A	85	GLU
1	A	129	LYS
1	A	131	LEU
1	A	170	GLU
1	A	177	ARG
1	A	302	ASP
1	A	303	SER
1	A	311	ASN
1	A	313	VAL
1	B	37	LEU
1	B	47	ASP
1	B	85	GLU
1	B	129	LYS
1	B	131	LEU
1	B	170	GLU
1	B	171	GLU
1	B	173	ARG
1	B	177	ARG
1	B	290	GLN

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Mol	Chain	Res	Type
1	B	303	SER
1	B	311	ASN
1	B	313	VAL
1	C	26	ILE
1	C	29	GLU
1	C	37	LEU
1	C	129	LYS
1	C	131	LEU
1	C	135	SER
1	C	152	LEU
1	C	153	THR
1	C	171	GLU
1	C	177	ARG
1	C	303	SER
1	C	311	ASN
1	C	313	VAL
1	C	331	SER
1	D	37	LEU
1	D	47	ASP
1	D	85	GLU
1	D	129	LYS
1	D	131	LEU
1	D	170	GLU
1	D	177	ARG
1	D	239	MET
1	D	246	GLU
1	D	290	GLN
1	D	303	SER
1	D	311	ASN
1	D	313	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	141	GLN
1	A	221	GLN
1	A	270	HIS
1	A	274	GLN
1	A	311	ASN
1	B	52	HIS
1	B	141	GLN

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Mol	Chain	Res	Type
1	B	221	GLN
1	B	270	HIS
1	B	274	GLN
1	B	311	ASN
1	C	52	HIS
1	C	141	GLN
1	C	221	GLN
1	C	270	HIS
1	C	274	GLN
1	C	311	ASN
1	D	52	HIS
1	D	100	ASN
1	D	141	GLN
1	D	190	GLN
1	D	221	GLN
1	D	270	HIS
1	D	274	GLN
1	D	311	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	A1H6U	B	402	2	16,19,19	1.21	2 (12%)	16,26,26	1.08	1 (6%)
3	A1H6U	C	402	2	16,19,19	1.29	2 (12%)	16,26,26	1.23	1 (6%)
3	A1H6U	A	402	2	16,19,19	1.26	2 (12%)	16,26,26	0.94	1 (6%)
2	HEM	D	401	1,3	41,50,50	0.95	2 (4%)	45,82,82	1.15	3 (6%)
3	A1H6U	D	402	2	16,19,19	1.26	2 (12%)	16,26,26	1.13	1 (6%)
2	HEM	B	401	1,3	41,50,50	0.95	2 (4%)	45,82,82	1.08	3 (6%)
2	HEM	A	401	1,3	41,50,50	0.97	2 (4%)	45,82,82	1.13	3 (6%)
2	HEM	C	401	1,3	41,50,50	0.95	1 (2%)	45,82,82	1.12	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H6U	B	402	2	-	1/8/16/16	0/3/3/3
3	A1H6U	C	402	2	-	1/8/16/16	0/3/3/3
3	A1H6U	A	402	2	-	1/8/16/16	0/3/3/3
2	HEM	D	401	1,3	-	6/12/54/54	-
3	A1H6U	D	402	2	-	1/8/16/16	0/3/3/3
2	HEM	B	401	1,3	-	6/12/54/54	-
2	HEM	A	401	1,3	-	6/12/54/54	-
2	HEM	C	401	1,3	-	6/12/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	CHB-C1B	3.05	1.42	1.35
3	B	402	A1H6U	C6-CA	-3.04	1.34	1.39
3	C	402	A1H6U	C6-CA	-3.03	1.34	1.39
2	B	401	HEM	CHB-C1B	3.00	1.42	1.35
3	A	402	A1H6U	C6-CA	-2.98	1.34	1.39
3	D	402	A1H6U	C6-CA	-2.93	1.34	1.39
2	A	401	HEM	CHB-C1B	2.88	1.42	1.35
2	D	401	HEM	CHB-C1B	2.73	1.42	1.35
3	A	402	A1H6U	C5-C6	2.50	1.44	1.38
3	C	402	A1H6U	C5-C6	2.45	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	A1H6U	C5-C6	2.38	1.43	1.38
2	B	401	HEM	C1B-NB	-2.34	1.36	1.40
2	A	401	HEM	C1B-NB	-2.29	1.36	1.40
3	B	402	A1H6U	C5-C6	2.20	1.43	1.38
2	D	401	HEM	C1B-NB	-2.14	1.36	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HEM	C4C-CHD-C1D	3.79	127.56	122.56
2	D	401	HEM	C4C-CHD-C1D	3.71	127.45	122.56
3	D	402	A1H6U	C5-CG2-C3	-3.69	119.16	121.25
3	C	402	A1H6U	C5-CG2-C3	-3.63	119.19	121.25
2	B	401	HEM	C4C-CHD-C1D	3.60	127.31	122.56
2	C	401	HEM	C4C-CHD-C1D	3.59	127.29	122.56
3	A	402	A1H6U	C5-CG2-C3	-2.86	119.63	121.25
2	C	401	HEM	C4B-CHC-C1C	2.72	126.15	122.56
2	D	401	HEM	C4B-CHC-C1C	2.71	126.14	122.56
2	A	401	HEM	C4B-CHC-C1C	2.68	126.09	122.56
2	B	401	HEM	C4B-CHC-C1C	2.66	126.07	122.56
2	D	401	HEM	CMC-C2C-C3C	2.38	129.13	124.68
2	C	401	HEM	CMC-C2C-C3C	2.38	129.12	124.68
2	B	401	HEM	CMC-C2C-C3C	2.31	129.01	124.68
2	A	401	HEM	CMC-C2C-C3C	2.27	128.93	124.68
3	B	402	A1H6U	C5-CG2-C3	-2.12	120.05	121.25

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1H6U	O-C1-CA-C6
3	C	402	A1H6U	O-C1-CA-C6
2	A	401	HEM	C2B-C3B-CAB-CBB
2	B	401	HEM	C2B-C3B-CAB-CBB
2	C	401	HEM	C2B-C3B-CAB-CBB
2	D	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C4B-C3B-CAB-CBB
2	C	401	HEM	C4B-C3B-CAB-CBB
2	D	401	HEM	C4B-C3B-CAB-CBB
3	B	402	A1H6U	O-C1-CA-C6
3	D	402	A1H6U	O-C1-CA-C6
2	B	401	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	C	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D

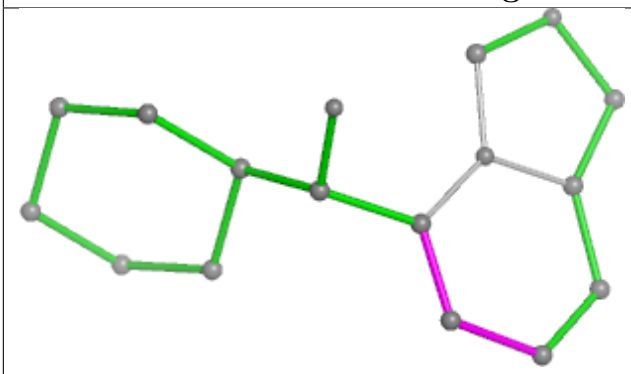
There are no ring outliers.

7 monomers are involved in 7 short contacts:

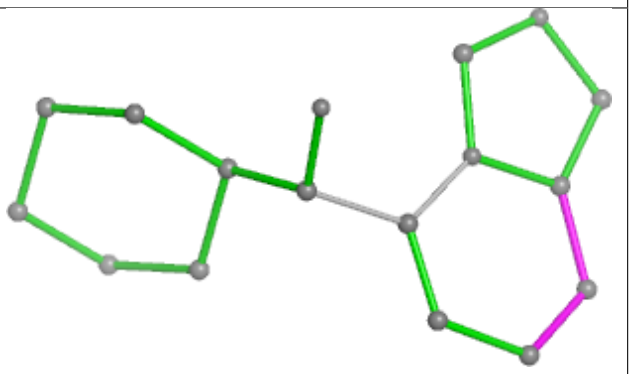
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	A1H6U	1	0
3	A	402	A1H6U	1	0
2	D	401	HEM	1	0
3	D	402	A1H6U	1	0
2	B	401	HEM	1	0
2	A	401	HEM	1	0
2	C	401	HEM	1	0

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.

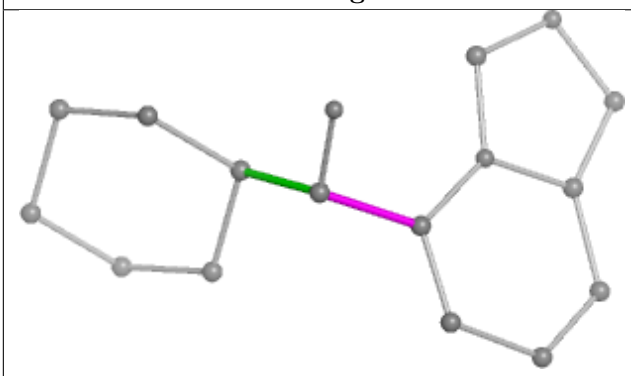
Ligand A1H6U B 402



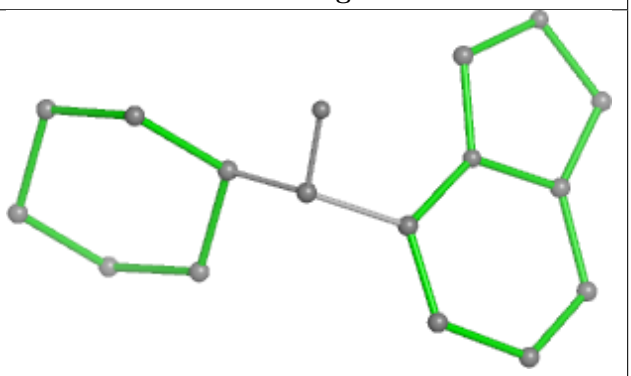
Bond lengths



Bond angles

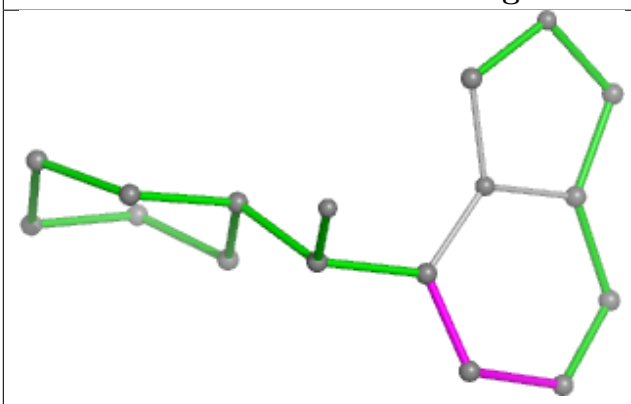


Torsions



Rings

Ligand A1H6U C 402



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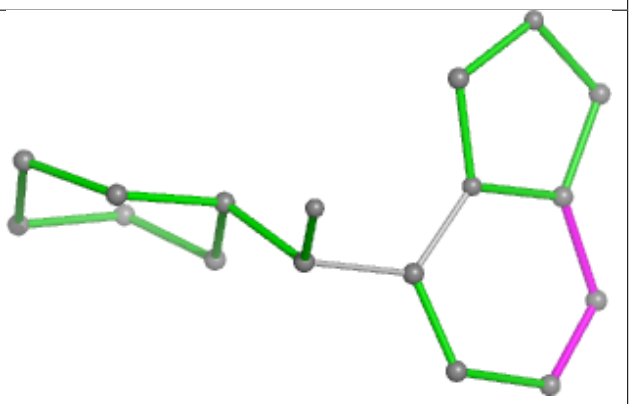

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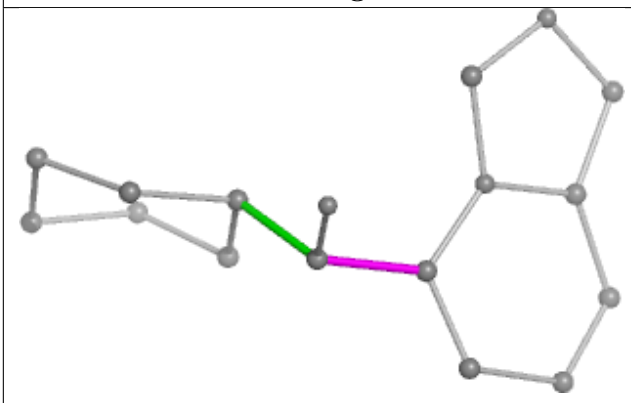

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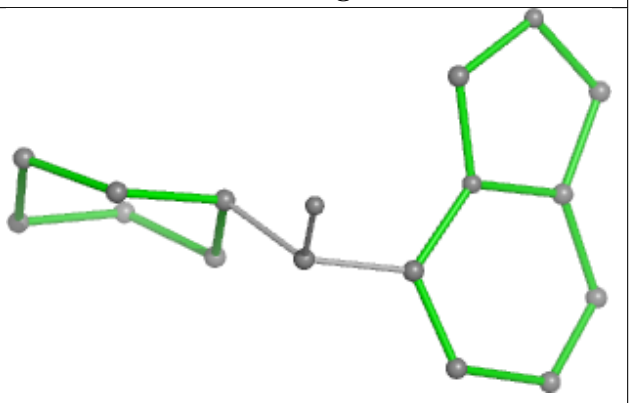
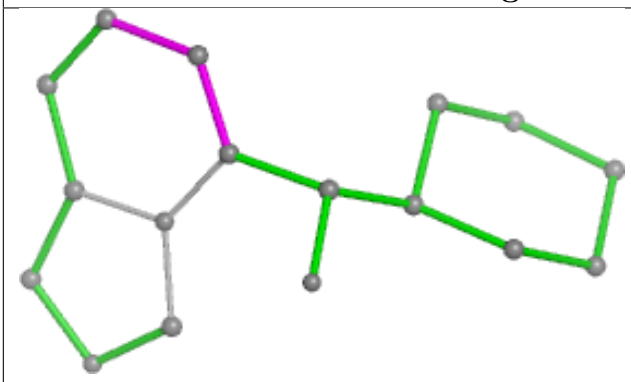


Rings

Ligand A1H6U A 402



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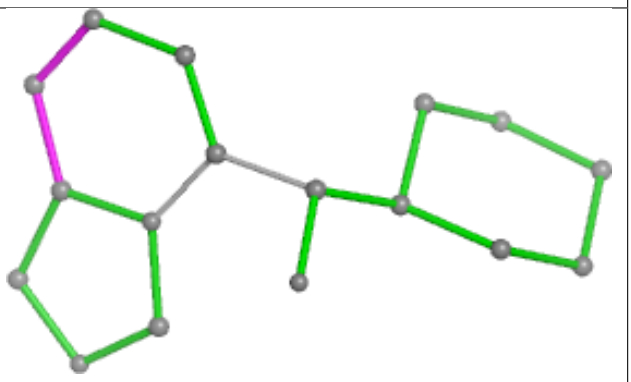

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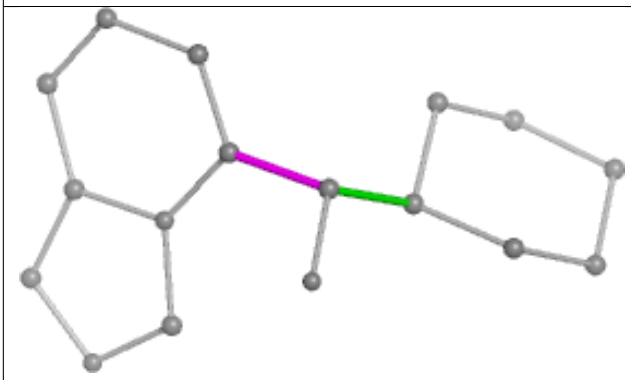

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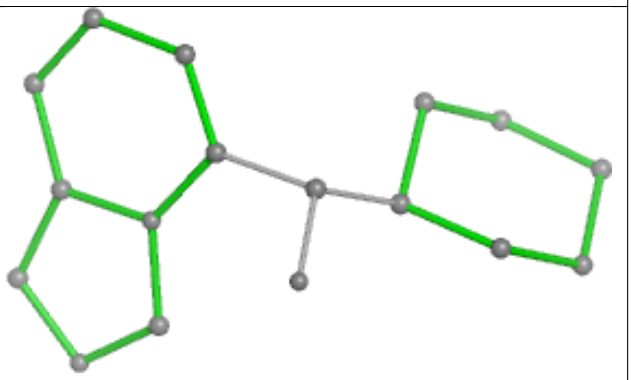
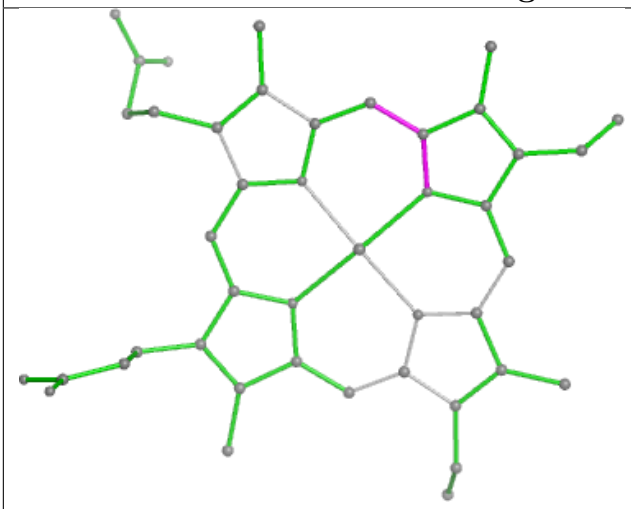
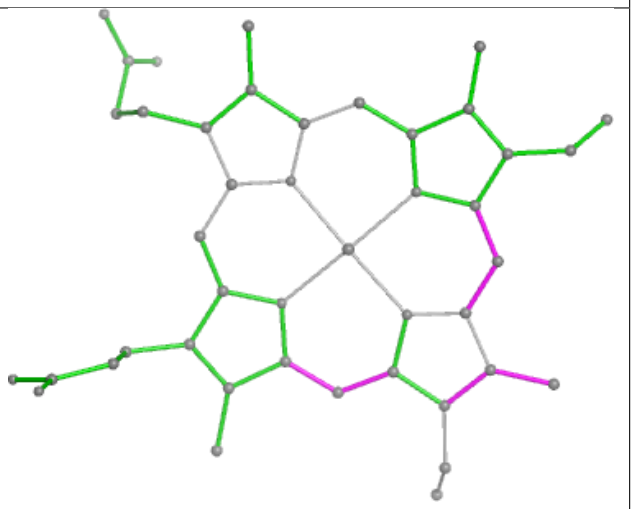


Rings

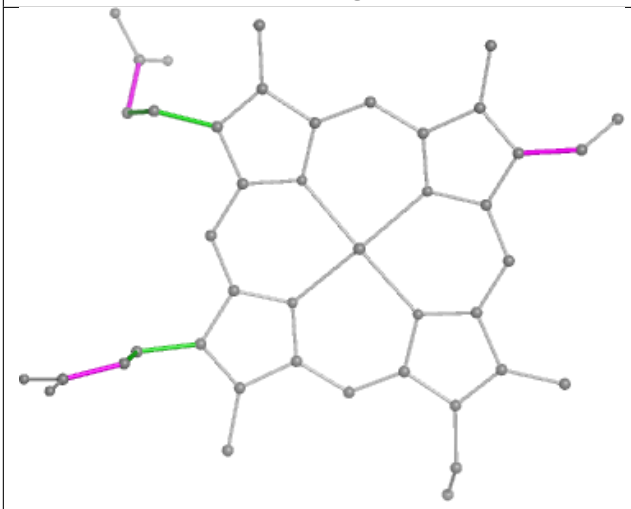
Ligand HEM D 401



Bond lengths



Bond angles



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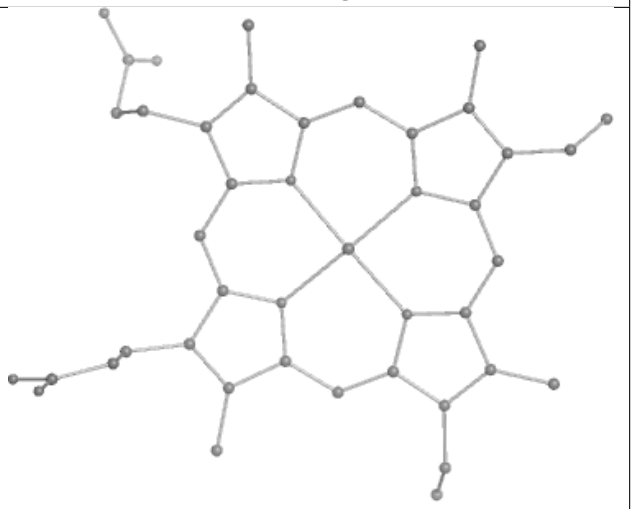
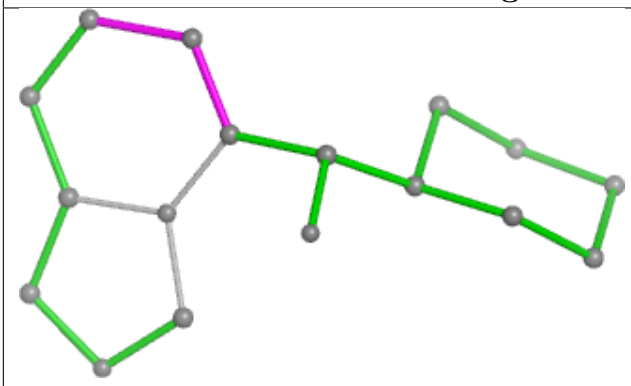


Rings

Ligand A1H6U D 402



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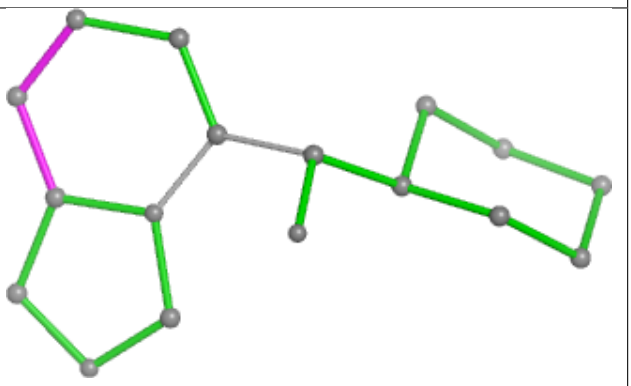
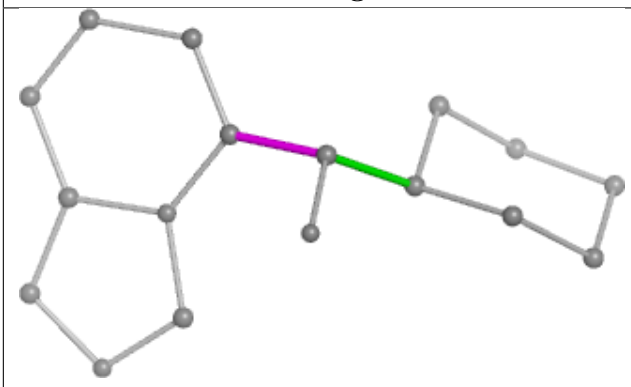


Bond angles



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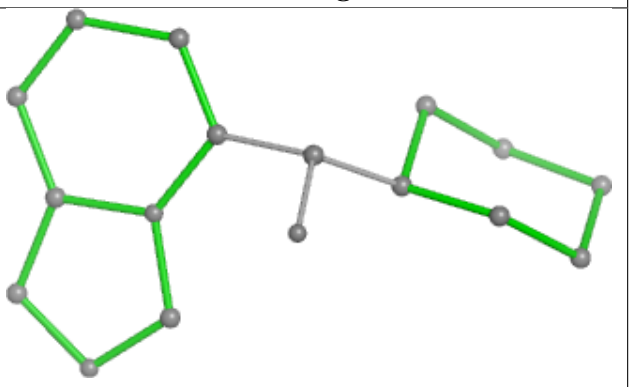
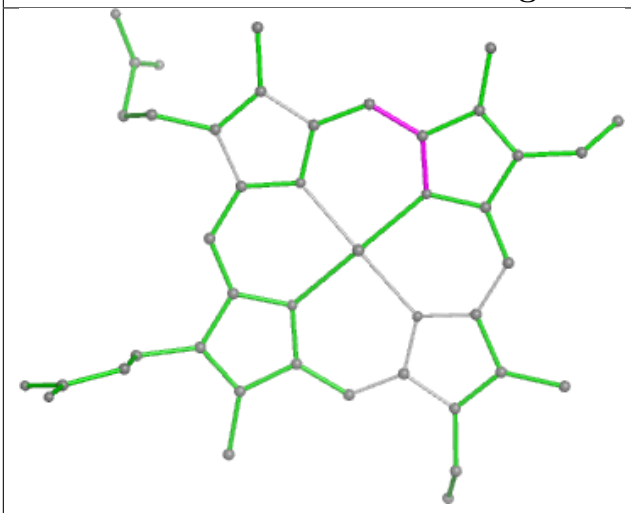
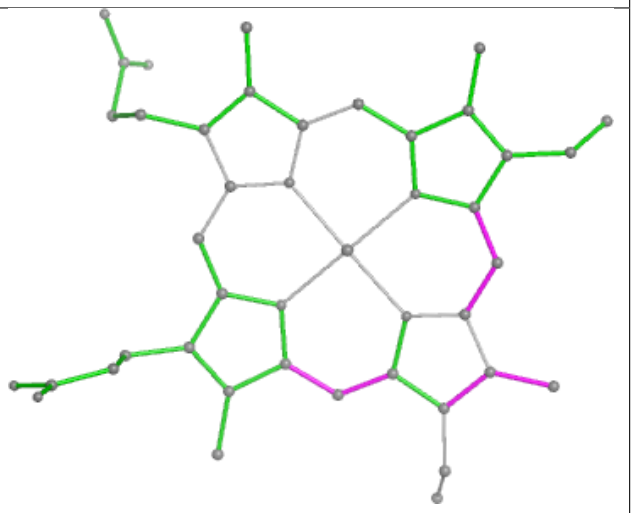


Rings

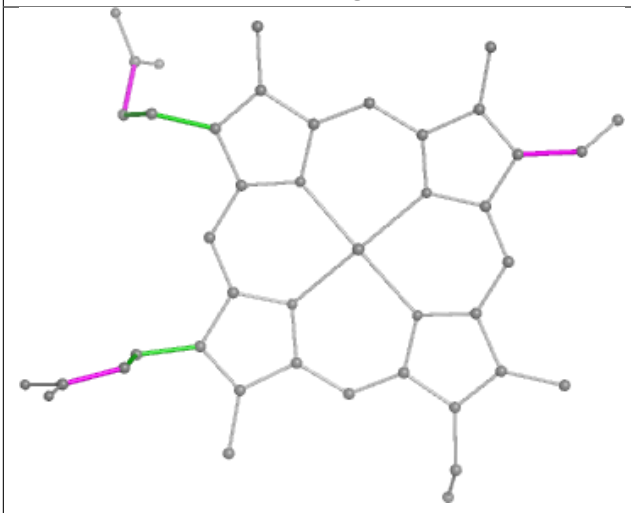
Ligand HEM B 401



Bond lengths



Bond angles



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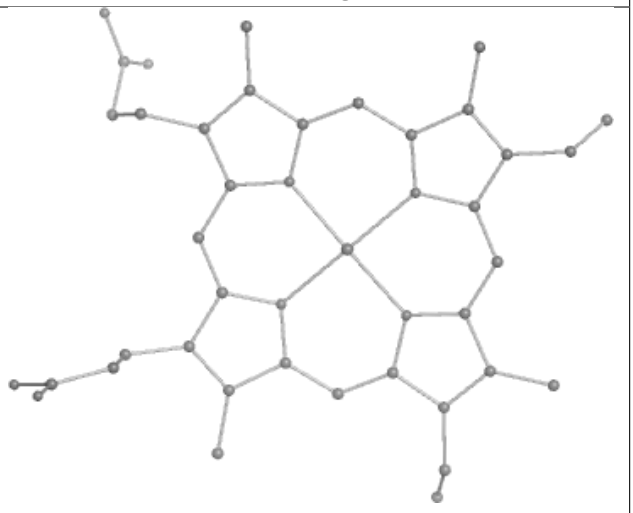
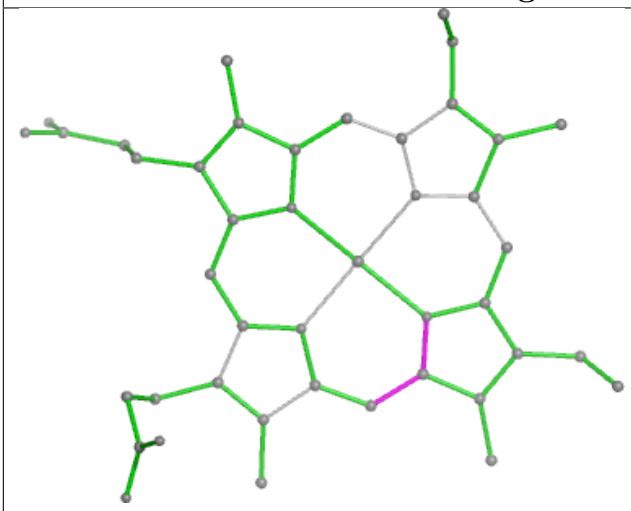
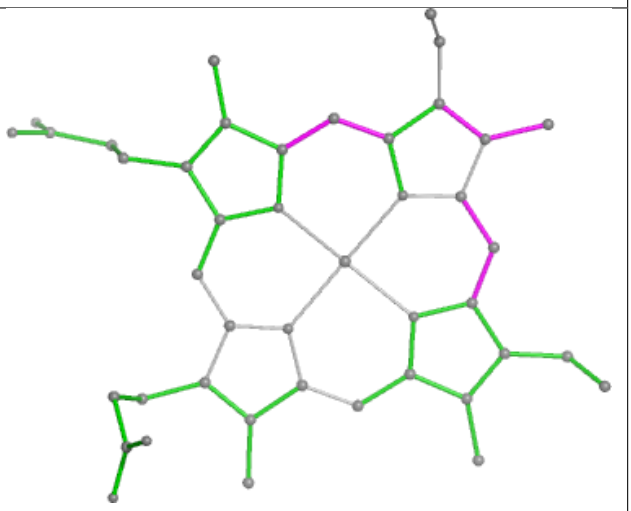


Rings

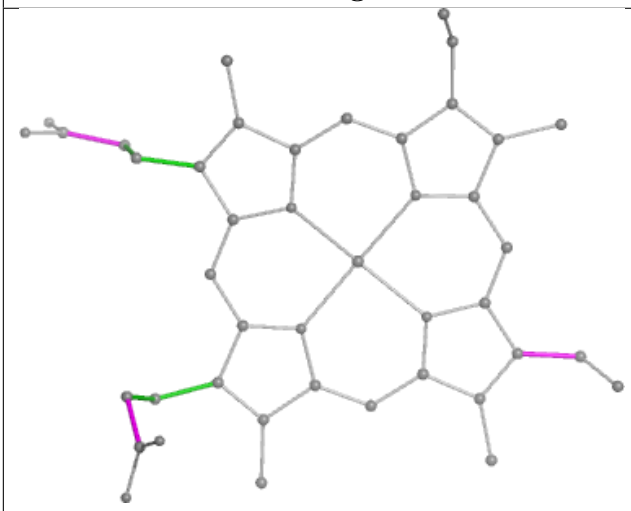
Ligand HEM A 401



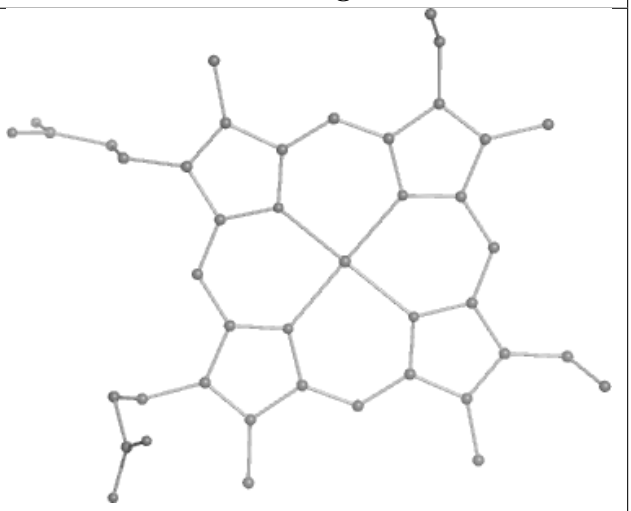
Bond lengths



Bond angles

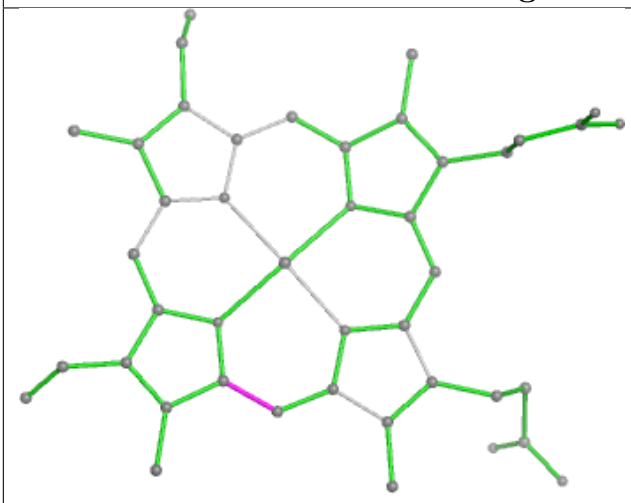


Torsions

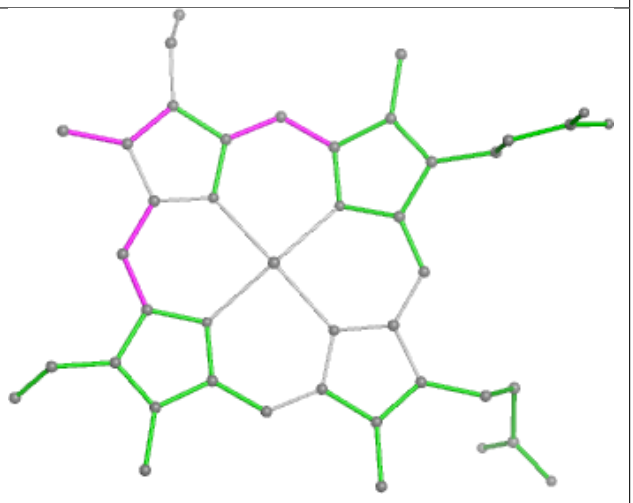


Rings

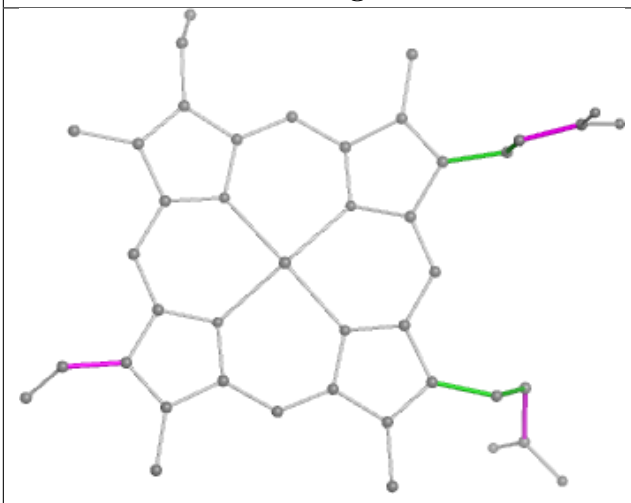
Ligand HEM C 401



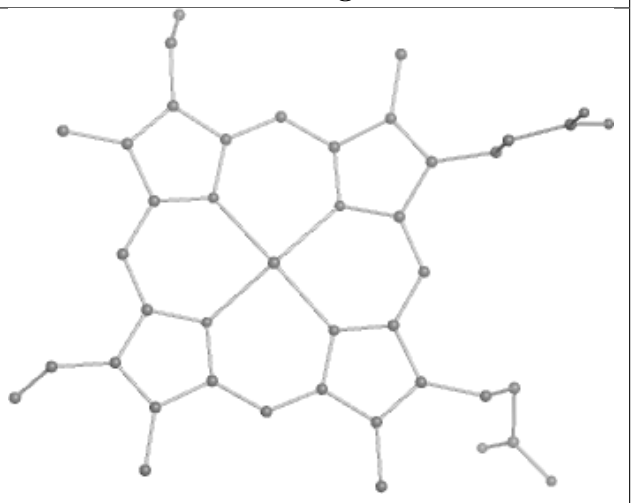
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	324/365 (88%)	-0.05	3 (0%)	81	78	34, 54, 77, 92	0
1	B	328/365 (89%)	0.09	10 (3%)	52	49	29, 53, 80, 105	1 (0%)
1	C	330/365 (90%)	0.04	10 (3%)	52	49	33, 51, 73, 95	0
1	D	331/365 (90%)	0.08	9 (2%)	56	52	34, 52, 83, 100	0
All	All	1313/1460 (89%)	0.04	32 (2%)	59	56	29, 52, 79, 105	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	VAL	4.9
1	C	168	SER	4.6
1	D	166	VAL	4.0
1	B	152	LEU	3.6
1	B	166	VAL	3.6
1	C	86	VAL	3.2
1	B	169	ASP	3.0
1	D	158	ARG	2.9
1	B	168	SER	2.9
1	C	368	GLU	2.7
1	B	167	PHE	2.7
1	C	152	LEU	2.6
1	C	135	SER	2.6
1	C	134	ALA	2.5
1	D	157	VAL	2.5
1	A	138	GLN	2.5
1	B	153	THR	2.5
1	A	49	ARG	2.5
1	D	169	ASP	2.4
1	B	85	GLU	2.3
1	D	138	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	46	GLU	2.3
1	C	154	GLU	2.3
1	D	152	LEU	2.3
1	D	172	ALA	2.2
1	C	169	ASP	2.2
1	B	230	VAL	2.1
1	C	367	ASP	2.1
1	D	230	VAL	2.1
1	D	167	PHE	2.1
1	C	26	ILE	2.0
1	A	155	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

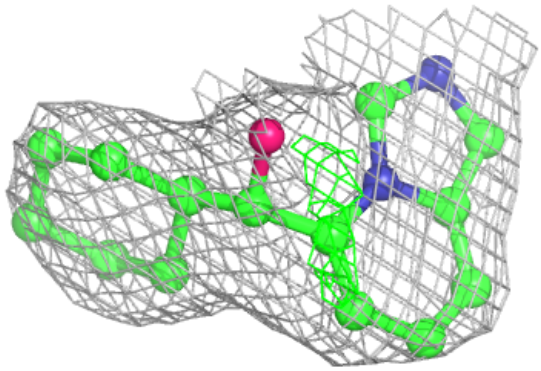
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

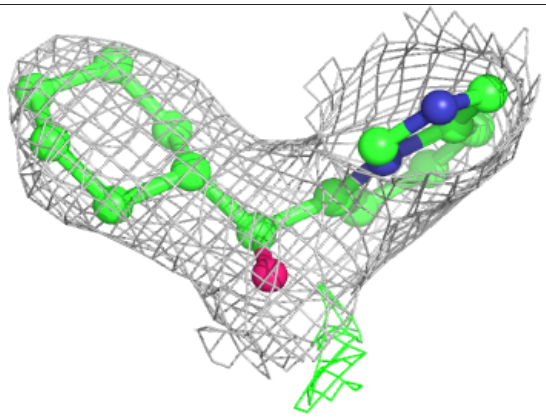
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1H6U	A	402	17/17	0.91	0.10	53,53,54,54	0
3	A1H6U	D	402	17/17	0.93	0.09	40,42,43,43	0
3	A1H6U	C	402	17/17	0.95	0.09	53,54,54,54	0
2	HEM	C	401	43/43	0.96	0.09	47,48,52,54	0
3	A1H6U	B	402	17/17	0.96	0.06	36,37,37,37	0
2	HEM	B	401	43/43	0.97	0.08	50,51,55,56	0
2	HEM	D	401	43/43	0.97	0.08	49,50,51,52	0
2	HEM	A	401	43/43	0.98	0.07	47,48,51,51	0

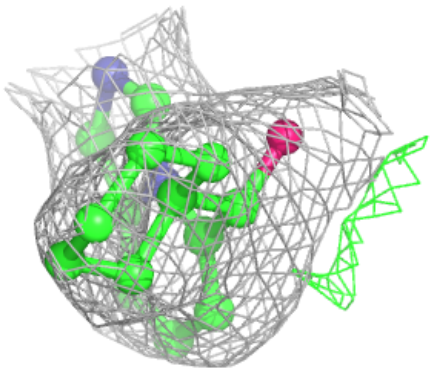
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H6U 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)

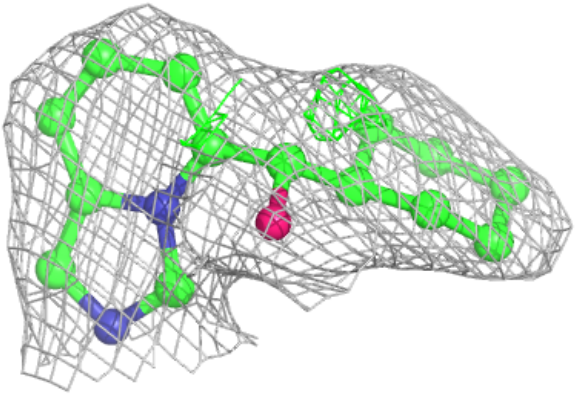


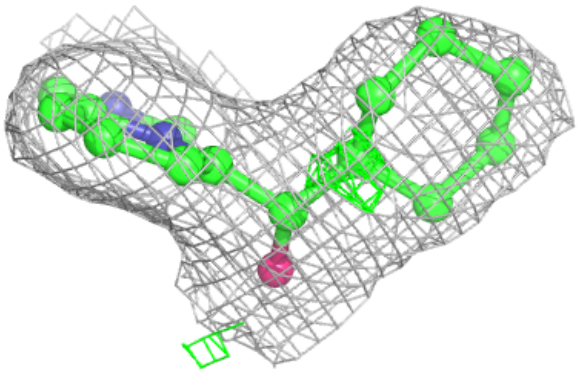


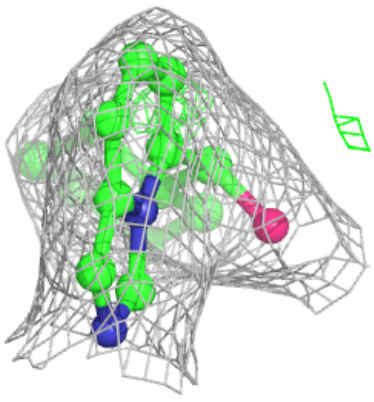


Electron density around A1H6U D 402:

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

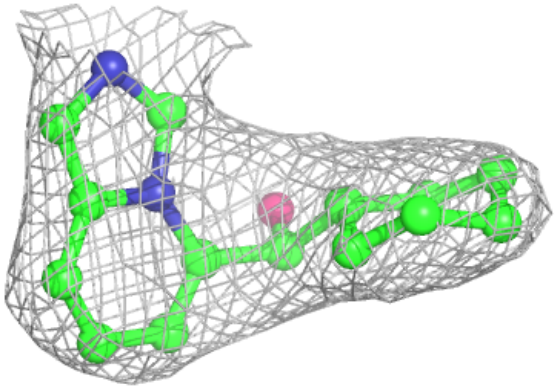


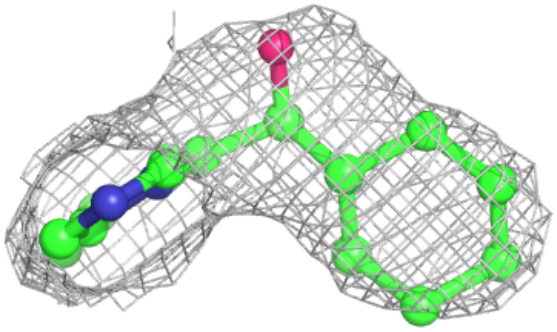


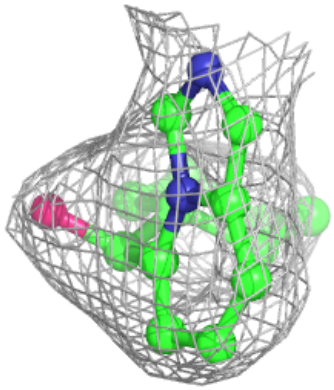


Electron density around A1H6U C 402:

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

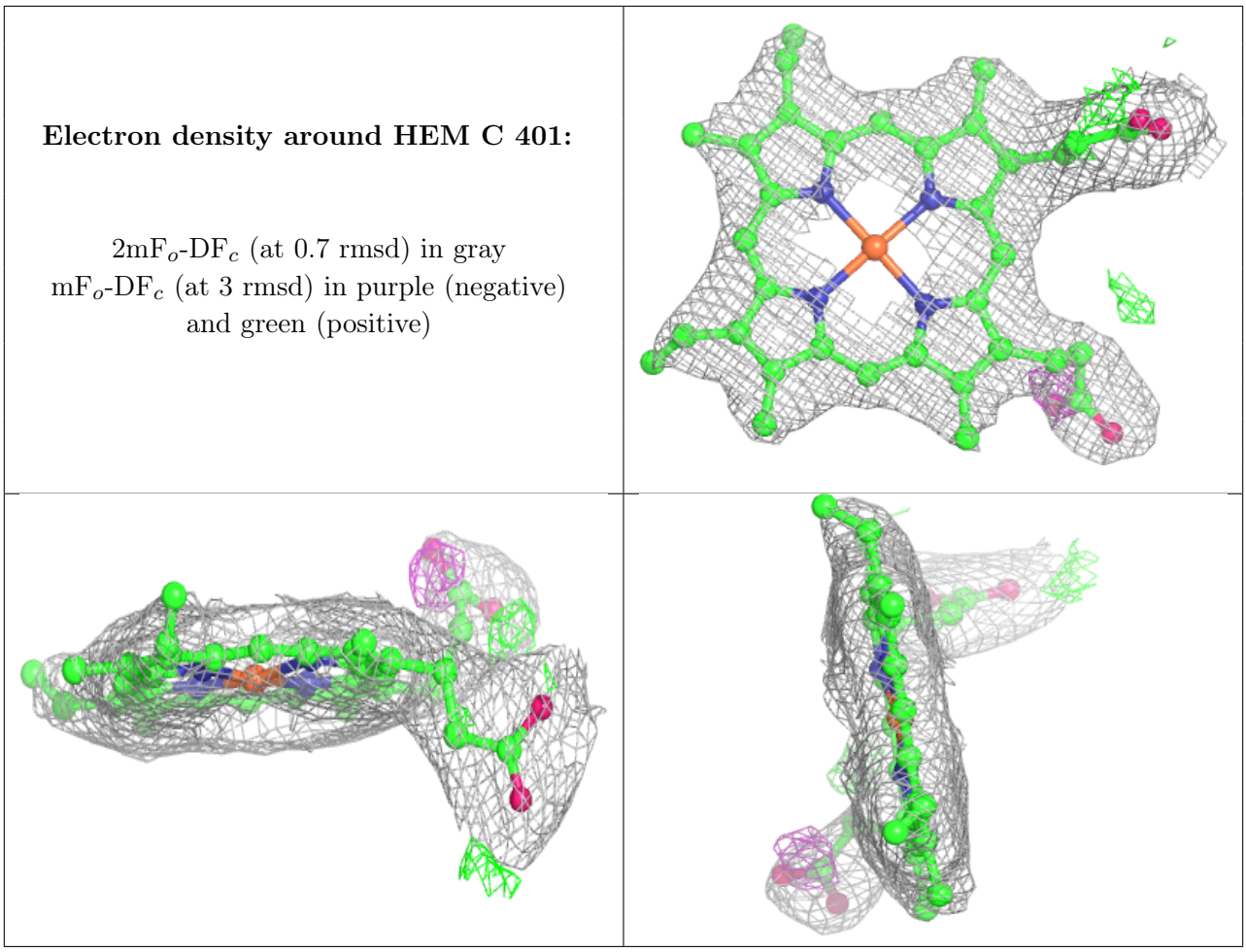






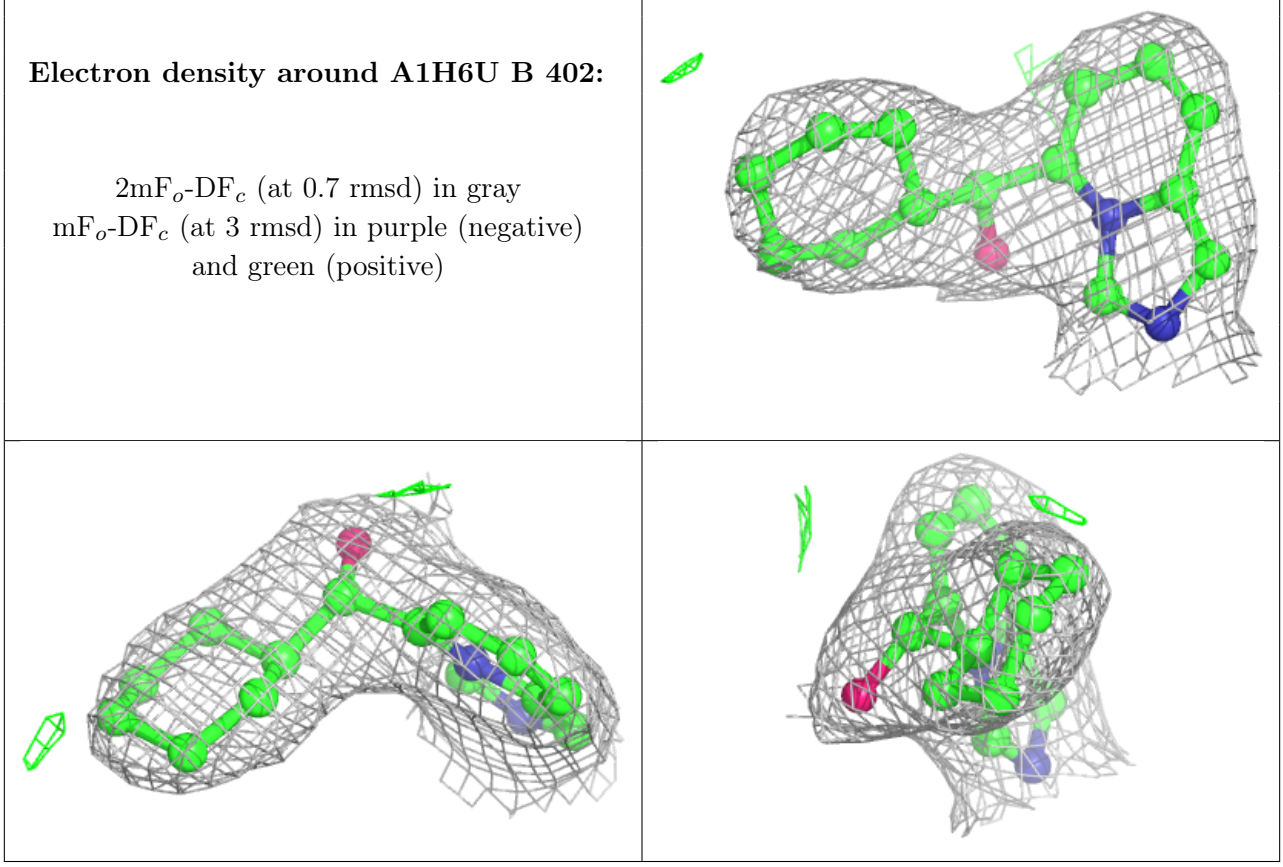
Electron density around HEM C 401:

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



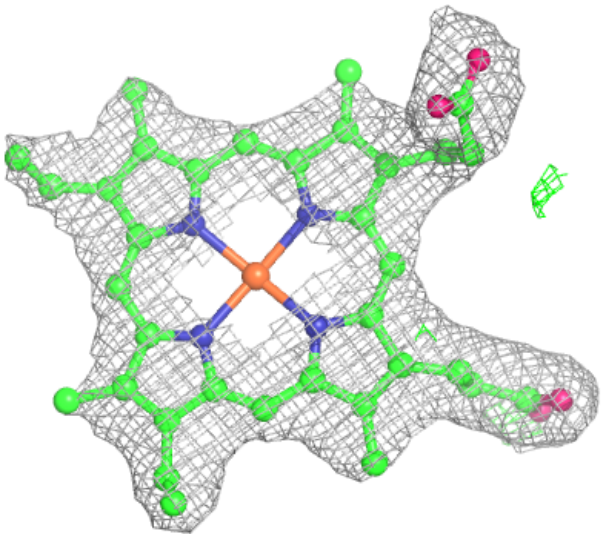
Electron density around A1H6U B 402:

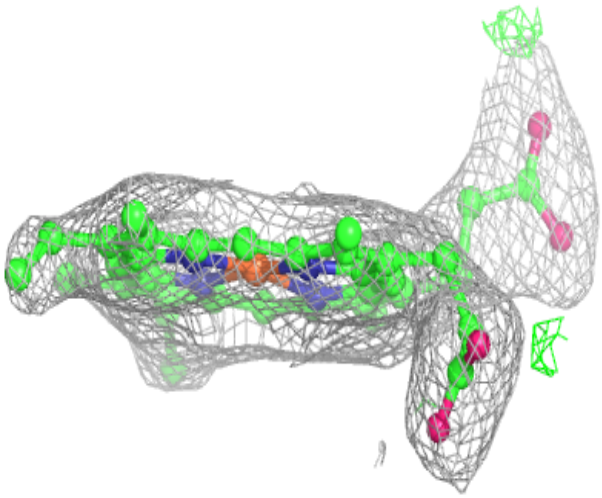
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

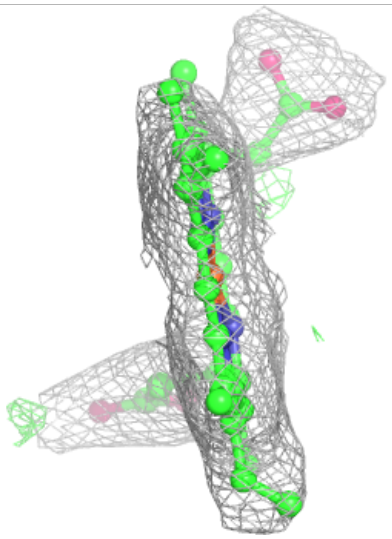


Electron density around HEM B 401:

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

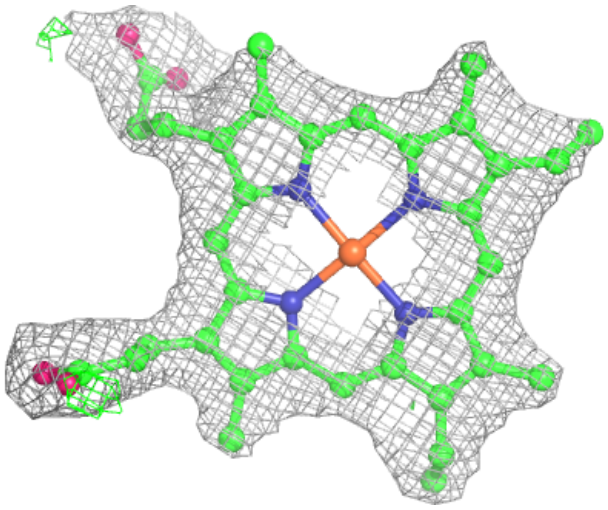


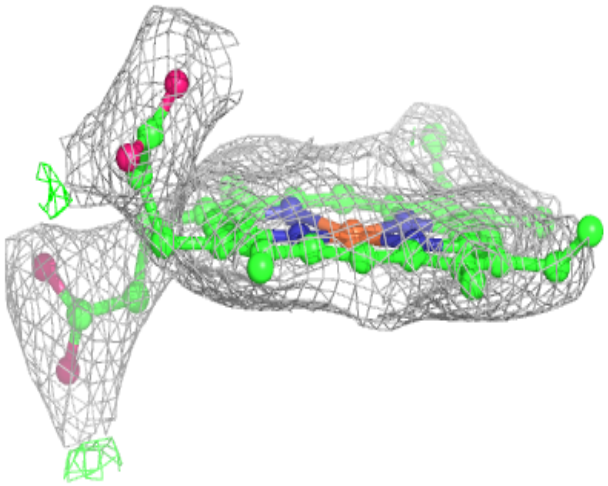


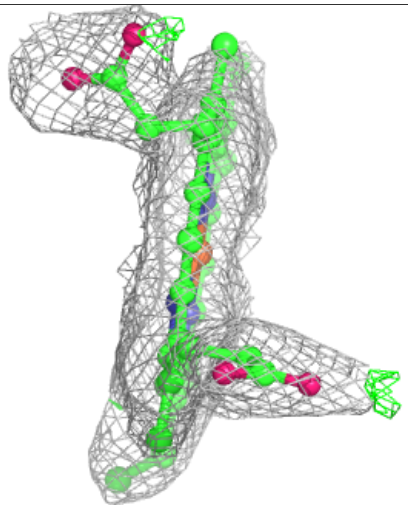


Electron density around HEM D 401:

$2mF_o$-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 A 401:

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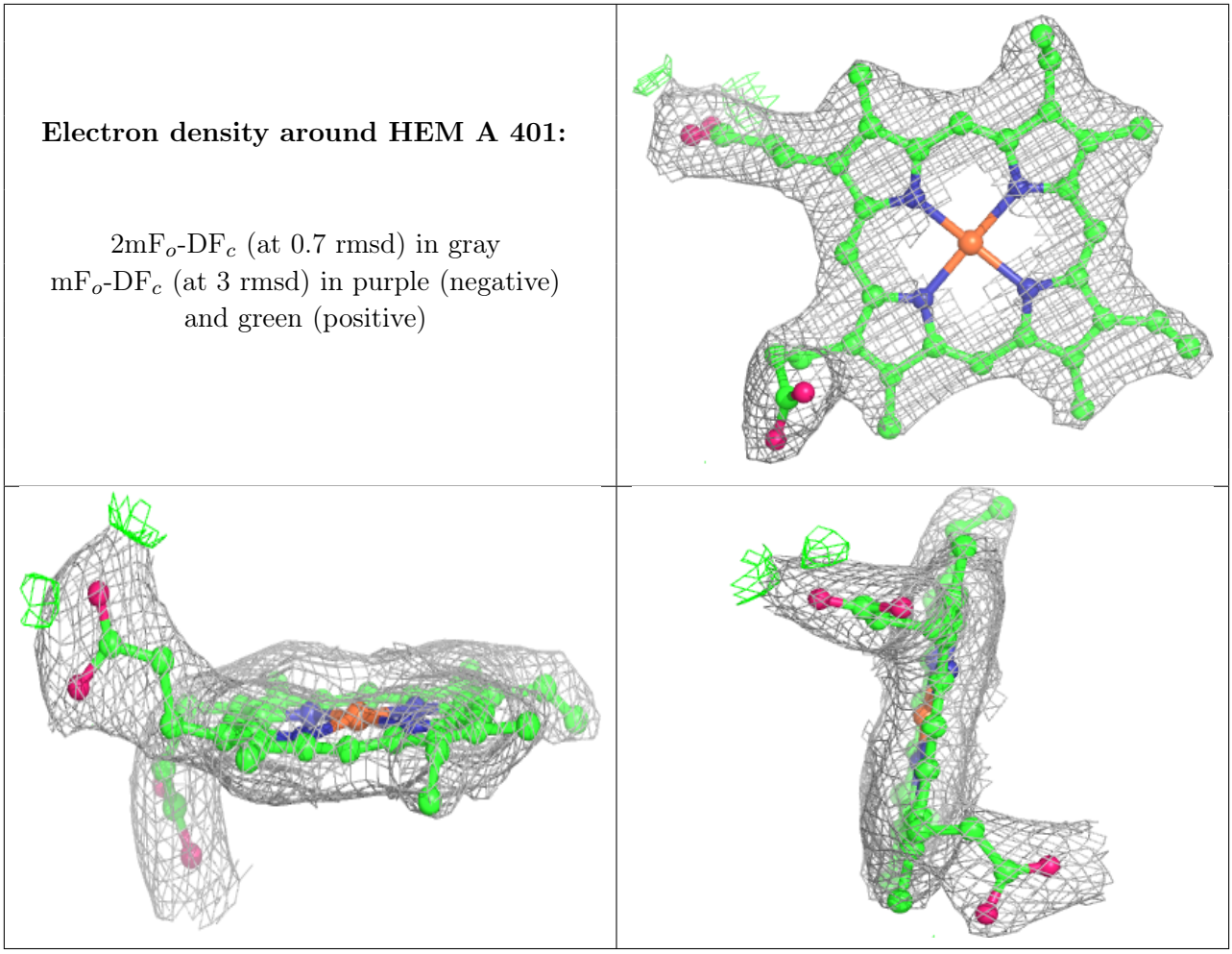
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.