



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2024 – 09:28 PM EDT

PDB ID : 9B1Q
Title : Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PYN1 inhibitor
Authors : Geeraerts, Z.; Yeh, S.-R.
Deposited on : 2024-03-13
Resolution : 2.62 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

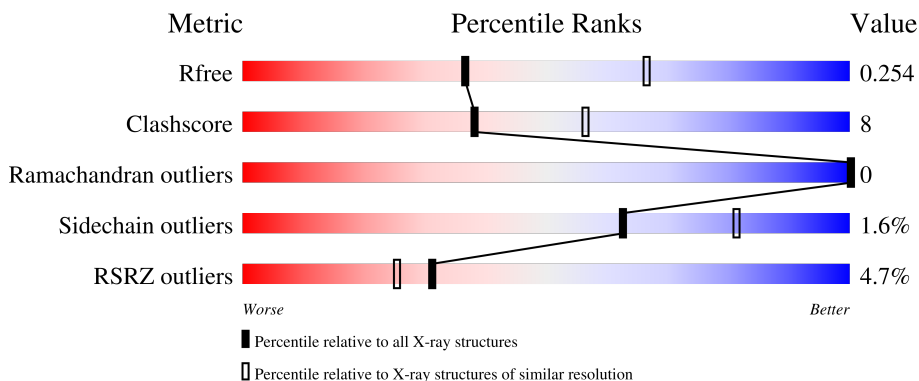
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 $\leq 5\%$. 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	 3% 73% 17% • 9%
1	B	380	 5% 73% 16% • 9%
1	C	380	 7% 68% 18% • 13%
1	D	380	 3% 75% 14% • 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11940 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	345	2932	1884	514	523	11	0	0	0
1	B	345	2932	1884	514	523	11	0	0	0
1	C	331	2819	1817	491	500	11	0	0	0
1	D	343	2913	1873	510	519	11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

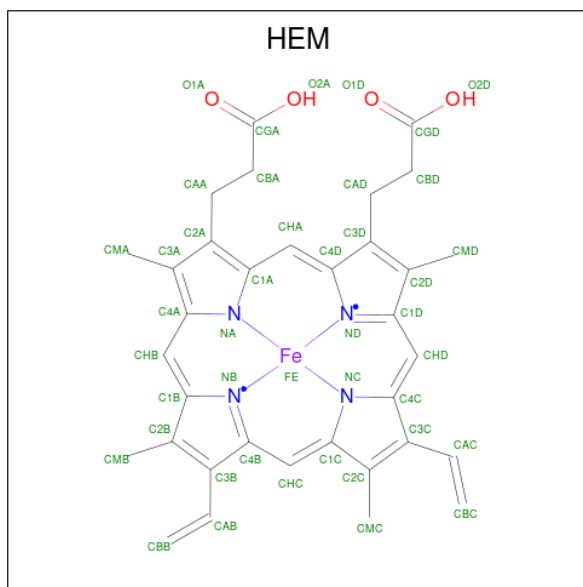
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression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

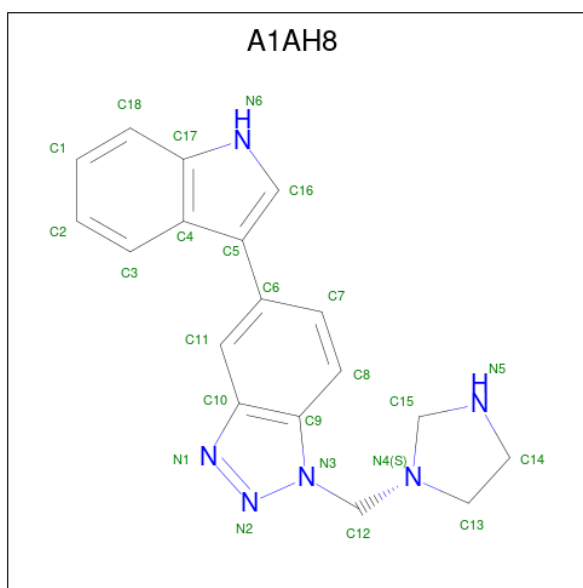
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

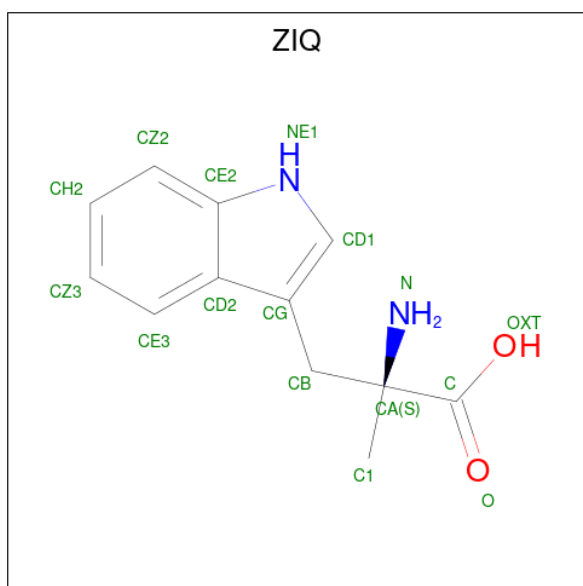
- Molecule 3 is (5P)-1-[(imidazolidin-1-yl)methyl]-5-(1H-indol-3-yl)-1H-1,2,3-benzotriazole (three-letter code: A1AH8) (formula: $C_{18}H_{18}N_6$) (labeled as "Ligand of Interest" by

depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 24 18 6	0	0
3	B	1	Total C N 24 18 6	0	0
3	C	1	Total C N 24 18 6	0	0
3	D	1	Total C N 24 18 6	0	0

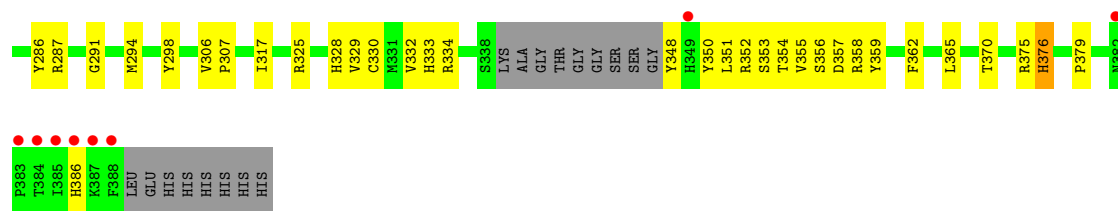
- Molecule 4 is alpha-methyl-L-tryptophan (three-letter code: ZIQ) (formula: $C_{12}H_{14}N_2O_2$).



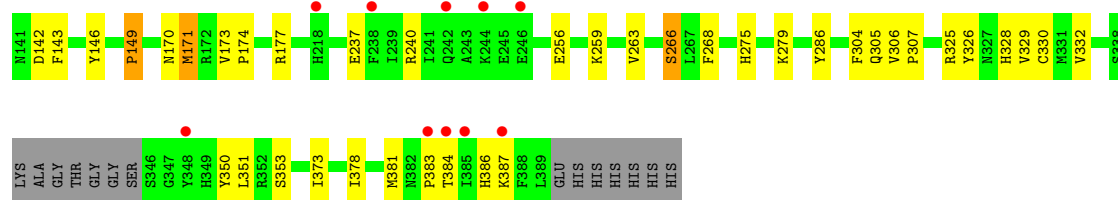
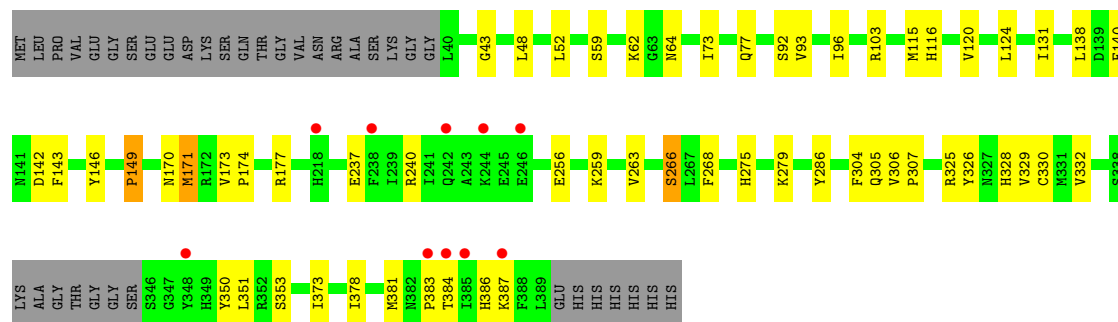
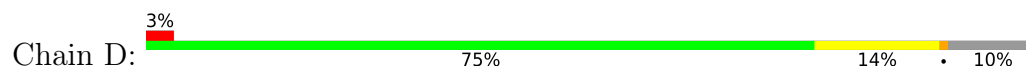
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	12	2	2		
4	B	1	Total	C	N	O	0	0
			16	12	2	2		
4	C	1	Total	C	N	O	0	0
			16	12	2	2		
4	D	1	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 5 is water.

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



● Molecule 1: Tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.96Å 154.17Å 88.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.29 – 2.62 34.29 – 2.62	Depositor EDS
% Data completeness (in resolution range)	53.8 (34.29-2.62) 53.8 (34.29-2.62)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.202 , 0.258 0.204 , 0.254	Depositor DCC
R_{free} test set	1625 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtrriage
Anisotropy	0.209	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11940	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: A1AH8, ZIQ, HEM

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	0.43	0/3001	0.81	1/4039 (0.0%)
1	B	0.42	0/3001	0.81	4/4039 (0.1%)
1	C	0.40	0/2884	0.77	2/3880 (0.1%)
1	D	0.42	0/2981	0.80	2/4012 (0.0%)
All	All	0.42	0/11867	0.80	9/15970 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	1
1	D	0	2
All	All	0	12

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	PRO	N-CA-CB	-6.32	95.64	102.60
1	B	149	PRO	N-CA-CB	-5.93	96.08	102.60
1	B	388	PHE	CB-CA-C	5.50	121.40	110.40
1	C	334	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	149	PRO	N-CA-CB	-5.30	96.77	102.60
1	C	149	PRO	N-CA-CB	-5.25	96.83	102.60
1	B	218	HIS	CB-CA-C	5.10	120.60	110.40
1	B	336	LEU	CB-CG-CD1	5.04	119.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	MET	CG-SD-CE	5.02	108.23	100.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	ARG	Sidechain
1	A	181	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	299	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	172	ARG	Sidechain
1	B	299	ARG	Sidechain
1	B	375	ARG	Sidechain
1	C	375	ARG	Sidechain
1	D	103	ARG	Sidechain
1	D	177	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2932	0	2914	47	0
1	B	2932	0	2914	49	0
1	C	2819	0	2806	49	0
1	D	2913	0	2901	39	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
3	A	24	0	0	0	0
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
4	A	16	0	0	1	0
4	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	16	0	0	1	0
4	D	16	0	0	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	D	4	0	0	0	0
All	All	11940	0	11655	180	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 8.

All (180) 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:B:304:PHE:HA	1:B:307:PRO:HG2	1.39	1.05
1:A:304:PHE:HA	1:A:307:PRO:HG2	1.38	1.03
1:D:304:PHE:HA	1:D:307:PRO:HG2	1.37	1.02
1:C:329:VAL:HG22	1:C:351:LEU:HB3	1.51	0.92
1:B:329:VAL:HG22	1:B:351:LEU:HB3	1.58	0.86
1:A:382:ASN:HB2	1:A:385:ILE:HB	1.56	0.85
2:A:401:HEM:HBC2	2:A:401:HEM:HHD	1.68	0.74
2:B:401:HEM:HBC2	2:B:401:HEM:HHD	1.71	0.71
1:B:272:ARG:HH21	1:B:272:ARG:HG2	1.56	0.71
1:A:329:VAL:HG22	1:A:351:LEU:HB3	1.73	0.70
1:A:304:PHE:CA	1:A:307:PRO:HG2	2.21	0.69
1:C:124:LEU:HD22	1:D:131:ILE:HD11	1.75	0.69
1:C:238:PHE:HE1	1:C:257:PHE:HB3	1.57	0.68
2:A:401:HEM:HHD	2:A:401:HEM:CBC	2.24	0.68
1:D:329:VAL:HG22	1:D:351:LEU:HB3	1.75	0.67
1:B:381:MET:HA	1:B:385:ILE:HD11	1.75	0.67
1:A:275:HIS:CE1	1:A:279:LYS:HD2	2.31	0.66
1:B:304:PHE:CA	1:B:307:PRO:HG2	2.21	0.64
1:B:325:ARG:HD3	1:B:354:THR:HG23	1.80	0.64
1:C:325:ARG:O	1:C:329:VAL:HG23	1.98	0.64
1:B:325:ARG:O	1:B:329:VAL:HG23	1.99	0.63
1:C:351:LEU:O	1:C:354:THR:HG22	1.98	0.63
1:D:304:PHE:CA	1:D:307:PRO:HG2	2.20	0.61
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	1.82	0.61
1:C:131:ILE:HD11	1:D:124:LEU:HD22	1.81	0.61
1:C:131:ILE:CD1	1:D:124:LEU:HD22	2.30	0.61
1:C:238:PHE:HZ	1:C:261:LYS:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:VAL:N	1:D:307:PRO:HD2	2.17	0.59
1:A:306:VAL:N	1:A:307:PRO:HD2	2.18	0.59
1:B:306:VAL:N	1:B:307:PRO:HD2	2.19	0.58
1:C:268:PHE:HA	1:C:286:TYR:OH	2.04	0.57
1:A:385:ILE:HG13	1:A:388:PHE:HE2	1.69	0.57
1:C:124:LEU:HD22	1:D:131:ILE:CD1	2.34	0.57
2:C:401:HEM:HBC2	2:C:401:HEM:HHD	1.86	0.57
1:B:301:GLU:OE1	1:C:106:ARG:NH2	2.38	0.56
1:D:268:PHE:HA	1:D:286:TYR:OH	2.05	0.56
2:D:401:HEM:CMB	2:D:401:HEM:HBB2	2.35	0.56
1:C:169:GLN:HA	1:C:172:ARG:HD2	1.87	0.56
1:D:268:PHE:HA	1:D:286:TYR:HH	1.70	0.56
1:B:268:PHE:HA	1:B:286:TYR:HH	1.71	0.55
1:B:268:PHE:HA	1:B:286:TYR:OH	2.05	0.55
1:A:268:PHE:HA	1:A:286:TYR:OH	2.06	0.55
2:D:401:HEM:HBB2	2:D:401:HEM:HMB1	1.90	0.53
1:A:43:GLY:HA2	1:A:48:LEU:HD12	1.91	0.52
1:A:268:PHE:HA	1:A:286:TYR:HH	1.74	0.52
1:B:351:LEU:O	1:B:354:THR:HG22	2.10	0.51
1:A:382:ASN:CB	1:A:385:ILE:HB	2.34	0.51
1:A:181:ARG:HG2	1:A:192:LEU:HD23	1.92	0.51
1:B:181:ARG:HG2	1:B:189:ASN:OD1	2.10	0.51
1:A:240:ARG:NH2	1:A:253:GLN:OE1	2.44	0.51
1:B:333:HIS:HB2	1:B:348:TYR:CE1	2.46	0.51
1:B:43:GLY:HA2	1:B:48:LEU:HD12	1.93	0.51
1:D:275:HIS:CE1	1:D:279:LYS:HD2	2.47	0.50
1:A:337:GLY:HA3	1:C:370:THR:CG2	2.41	0.50
1:A:325:ARG:O	1:A:329:VAL:HG23	2.12	0.50
1:C:350:TYR:O	1:C:353:SER:HB3	2.12	0.50
1:D:43:GLY:HA2	1:D:48:LEU:HD12	1.92	0.50
2:A:401:HEM:HBC2	2:A:401:HEM:CHD	2.35	0.49
1:D:256:GLU:O	1:D:259:LYS:HG3	2.13	0.49
1:C:268:PHE:HA	1:C:286:TYR:HH	1.76	0.49
1:B:272:ARG:HH21	1:B:272:ARG:CG	2.25	0.48
1:C:355:VAL:HG22	1:C:355:VAL:O	2.12	0.48
1:B:319:SER:O	1:B:322:THR:HG22	2.13	0.48
2:C:401:HEM:HMB1	2:C:401:HEM:HBB2	1.95	0.48
1:A:131:ILE:HD11	1:B:124:LEU:HD22	1.94	0.48
1:B:171:MET:HB3	1:B:358:ARG:HG2	1.95	0.48
1:A:356:SER:HB3	1:A:358:ARG:HG2	1.94	0.48
1:A:362:PHE:HB3	1:A:365:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ARG:HD3	1:C:354:THR:HG23	1.95	0.48
1:C:43:GLY:HA2	1:C:48:LEU:HD12	1.96	0.48
1:A:350:TYR:O	1:A:353:SER:HB3	2.13	0.47
1:C:235:GLU:O	1:C:239:ILE:HG12	2.14	0.47
1:D:383:PRO:HA	1:D:386:HIS:HB3	1.97	0.47
1:C:228:LYS:HG2	1:C:232:ARG:HD3	1.96	0.47
1:A:121:ILE:HG12	1:B:131:ILE:HD13	1.97	0.47
1:B:348:TYR:CZ	1:B:352:ARG:HD2	2.49	0.47
1:C:328:HIS:O	1:C:332:VAL:HG23	2.15	0.47
1:A:48:LEU:HB3	1:A:52:LEU:HD12	1.97	0.47
1:D:93:VAL:HG21	1:D:115:MET:CE	2.45	0.47
1:A:152:GLY:HA3	2:A:401:HEM:C1D	2.50	0.47
1:A:328:HIS:O	1:A:332:VAL:HG23	2.15	0.47
2:B:401:HEM:CMB	2:B:401:HEM:HBB2	2.45	0.47
1:B:202:LEU:CD2	1:B:283:ARG:NH1	2.78	0.46
1:A:299:ARG:HH12	1:A:375:ARG:HH12	1.61	0.46
1:A:348:TYR:CZ	1:A:352:ARG:HD2	2.50	0.46
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.45	0.46
1:A:124:LEU:HD22	1:B:131:ILE:CD1	2.46	0.46
2:B:401:HEM:HBB2	2:B:401:HEM:HMB1	1.98	0.46
1:C:333:HIS:HB2	1:C:348:TYR:CD1	2.50	0.46
1:A:45:TYR:CE1	1:B:58:GLN:HG2	2.51	0.46
1:A:116:HIS:O	1:A:120:VAL:HG23	2.16	0.46
1:A:131:ILE:CD1	1:B:124:LEU:HD22	2.46	0.45
1:A:163:ASN:OD1	1:A:172:ARG:NH2	2.49	0.45
1:C:275:HIS:CE1	1:C:279:LYS:HD2	2.50	0.45
1:D:116:HIS:O	1:D:120:VAL:HG23	2.16	0.45
1:B:234:LEU:HD13	1:B:261:LYS:HG3	1.98	0.45
1:C:362:PHE:HB3	1:C:365:LEU:HD12	1.98	0.45
1:A:337:GLY:HA3	1:C:370:THR:HG22	1.97	0.45
1:B:328:HIS:O	1:B:332:VAL:HG23	2.16	0.45
1:C:116:HIS:O	1:C:120:VAL:HG23	2.16	0.45
1:D:237:GLU:O	1:D:240:ARG:HB3	2.16	0.45
1:D:328:HIS:O	1:D:332:VAL:HG23	2.17	0.45
1:D:387:LYS:HB3	1:D:387:LYS:HE2	1.86	0.44
1:A:59:SER:HB2	1:A:64:ASN:O	2.17	0.44
1:C:256:GLU:O	1:C:260:GLN:HG3	2.17	0.44
1:D:350:TYR:O	1:D:353:SER:HB3	2.18	0.44
1:B:116:HIS:O	1:B:120:VAL:HG23	2.16	0.44
1:D:373:ILE:HD11	1:D:378:ILE:HG12	2.00	0.44
1:C:59:SER:HB2	1:C:64:ASN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:HEM:HBB2	2:C:401:HEM:CMB	2.48	0.44
1:B:322:THR:HG23	1:D:326:TYR:OH	2.17	0.44
1:A:210:GLU:HG2	1:A:287:ARG:HB3	1.99	0.44
1:B:59:SER:HB2	1:B:64:ASN:O	2.18	0.44
1:C:104:ASP:OD2	1:C:106:ARG:HD2	2.18	0.43
1:C:306:VAL:N	1:C:307:PRO:CD	2.82	0.43
1:C:48:LEU:HB3	1:C:52:LEU:HD12	2.00	0.43
1:C:352:ARG:HD2	1:C:352:ARG:HA	1.82	0.43
1:D:59:SER:HB2	1:D:64:ASN:O	2.17	0.43
1:A:109:LEU:HD22	1:D:305:GLN:HG2	2.00	0.43
1:B:140:PHE:HA	1:B:143:PHE:CE2	2.54	0.43
1:B:228:LYS:HE2	1:B:232:ARG:HH11	1.82	0.43
1:C:210:GLU:HG2	1:C:287:ARG:HB3	1.99	0.43
1:A:88:TRP:CD1	1:B:67:HIS:CE1	3.07	0.43
1:C:376:HIS:CD2	1:C:376:HIS:H	2.37	0.43
1:D:62:LYS:HD3	1:D:146:TYR:HD1	1.84	0.43
1:C:264:LEU:O	1:C:267:LEU:HB2	2.19	0.42
1:B:210:GLU:HG2	1:B:287:ARG:HB3	2.02	0.42
1:B:168:LEU:HB2	1:B:171:MET:SD	2.59	0.42
1:B:350:TYR:O	1:B:353:SER:HB3	2.19	0.42
1:D:263:VAL:O	1:D:266:SER:HB3	2.20	0.42
1:B:381:MET:CA	1:B:385:ILE:HD11	2.47	0.42
1:B:92:SER:O	1:B:96:ILE:HG13	2.20	0.42
1:B:306:VAL:N	1:B:307:PRO:CD	2.83	0.42
1:D:173:VAL:HA	1:D:174:PRO:HD3	1.88	0.42
1:D:325:ARG:O	1:D:329:VAL:HG23	2.20	0.42
1:C:140:PHE:HA	1:C:143:PHE:CE2	2.55	0.42
1:C:298:TYR:OH	1:C:379:PRO:HB2	2.20	0.42
1:B:48:LEU:HB3	1:B:52:LEU:HD12	2.01	0.42
1:C:356:SER:O	1:C:357:ASP:HB2	2.19	0.42
1:D:48:LEU:HB3	1:D:52:LEU:HD12	2.01	0.42
1:D:92:SER:O	1:D:96:ILE:HG13	2.19	0.42
1:D:115:MET:CE	1:D:115:MET:HA	2.50	0.42
1:D:140:PHE:HA	1:D:143:PHE:CE2	2.55	0.42
1:D:306:VAL:N	1:D:307:PRO:CD	2.82	0.42
1:A:271:LYS:HD2	1:A:271:LYS:H	1.84	0.42
1:C:192:LEU:HD23	1:C:192:LEU:HA	1.93	0.42
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.86	0.41
1:A:140:PHE:HA	1:A:143:PHE:CE2	2.54	0.41
1:B:148:SER:HA	1:B:149:PRO:HA	1.86	0.41
1:C:189:ASN:O	1:C:193:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:PHE:CZ	1:C:261:LYS:HB2	2.52	0.41
1:B:332:VAL:HG22	2:B:401:HEM:C1B	2.56	0.41
1:B:375:ARG:HE	1:D:142:ASP:CG	2.22	0.41
1:A:73:ILE:O	1:A:77:GLN:HG3	2.21	0.41
1:B:275:HIS:NE2	1:B:279:LYS:HD2	2.35	0.41
2:D:401:HEM:HHD	2:D:401:HEM:CBC	2.48	0.41
1:B:333:HIS:HB2	1:B:348:TYR:CD1	2.55	0.41
1:A:67:HIS:CE1	1:B:88:TRP:CD1	3.09	0.41
1:A:192:LEU:HD12	1:A:192:LEU:HA	1.86	0.41
1:A:306:VAL:N	1:A:307:PRO:CD	2.82	0.41
1:A:380:LYS:HA	1:A:380:LYS:HD3	1.86	0.41
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.51	0.41
1:C:171:MET:O	1:C:358:ARG:NH2	2.54	0.41
1:C:291:GLY:O	1:C:294:MET:HB3	2.21	0.41
1:D:381:MET:CE	1:D:386:HIS:HA	2.51	0.41
2:B:401:HEM:HHD	2:B:401:HEM:CBC	2.48	0.41
1:A:332:VAL:HG22	2:A:401:HEM:C1B	2.56	0.40
1:A:346:SER:HB3	1:A:349:HIS:ND1	2.36	0.40
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.92	0.40
1:C:354:THR:HA	1:C:359:TYR:CE1	2.56	0.40
1:D:73:ILE:O	1:D:77:GLN:HG3	2.21	0.40
1:A:115:MET:HE2	1:A:201:LEU:HD21	2.03	0.40
1:B:299:ARG:CZ	1:D:138:LEU:HD13	2.51	0.40
1:C:92:SER:O	1:C:96:ILE:HG13	2.22	0.40
1:D:93:VAL:HG21	1:D:115:MET:HE2	2.02	0.40
1:C:103:ARG:HA	4:C:403:ZIQ:O	2.22	0.40
1:C:228:LYS:HG2	1:C:232:ARG:CD	2.52	0.40
1:A:103:ARG:HA	4:A:403:ZIQ:OXT	2.21	0.40
1:C:329:VAL:HG22	1:C:351:LEU:CB	2.37	0.40
1:D:384:THR:O	1:D:387:LYS:HB2	2.22	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	341/380 (90%)	333 (98%)	8 (2%)	0	100	100
1	B	341/380 (90%)	332 (97%)	9 (3%)	0	100	100
1	C	323/380 (85%)	313 (97%)	10 (3%)	0	100	100
1	D	339/380 (89%)	331 (98%)	8 (2%)	0	100	100
All	All	1344/1520 (88%)	1309 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	322/348 (92%)	316 (98%)	6 (2%)	57	78
1	B	322/348 (92%)	317 (98%)	5 (2%)	62	81
1	C	310/348 (89%)	305 (98%)	5 (2%)	62	81
1	D	320/348 (92%)	315 (98%)	5 (2%)	62	81
All	All	1274/1392 (92%)	1253 (98%)	21 (2%)	62	81

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

Mol	Chain	Res	Type
1	A	149	PRO
1	A	251	GLU
1	A	266	SER
1	A	330	CYS
1	A	390	GLU
1	A	391	HIS
1	B	149	PRO
1	B	171	MET
1	B	262	GLU
1	B	354	THR

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Mol	Chain	Res	Type
1	B	391	HIS
1	C	106	ARG
1	C	149	PRO
1	C	330	CYS
1	C	376	HIS
1	C	386	HIS
1	D	149	PRO
1	D	170	ASN
1	D	171	MET
1	D	266	SER
1	D	330	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	GLN
1	C	376	HIS
1	D	101	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
2	HEM	A	401	1	41,50,50	1.48	7 (17%)	45,82,82	1.96	14 (31%)
2	HEM	B	401	1	41,50,50	1.33	3 (7%)	45,82,82	1.76	14 (31%)
4	ZIQ	A	403	-	13,17,17	0.91	0	14,25,25	1.38	2 (14%)
3	A1AH8	A	402	-	23,28,28	0.82	1 (4%)	27,40,40	1.05	1 (3%)
2	HEM	D	401	1	41,50,50	1.56	5 (12%)	45,82,82	2.06	16 (35%)
4	ZIQ	D	403	-	13,17,17	0.92	0	14,25,25	0.84	0
2	HEM	C	401	1	41,50,50	1.34	6 (14%)	45,82,82	1.87	13 (28%)
3	A1AH8	D	402	-	23,28,28	0.77	0	27,40,40	1.07	1 (3%)
4	ZIQ	B	403	-	13,17,17	0.79	0	14,25,25	1.51	3 (21%)
4	ZIQ	C	403	-	13,17,17	0.79	0	14,25,25	0.89	1 (7%)
3	A1AH8	B	402	-	23,28,28	0.88	0	27,40,40	1.31	3 (11%)
3	A1AH8	C	402	-	23,28,28	0.77	0	27,40,40	1.15	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	401	1	-	2/12/54/54	-
2	HEM	B	401	1	-	2/12/54/54	-
4	ZIQ	A	403	-	-	7/9/11/11	0/2/2/2
3	A1AH8	A	402	-	-	0/6/15/15	0/5/5/5
2	HEM	D	401	1	-	2/12/54/54	-
4	ZIQ	D	403	-	-	7/9/11/11	0/2/2/2
2	HEM	C	401	1	-	4/12/54/54	-
3	A1AH8	D	402	-	-	0/6/15/15	0/5/5/5
4	ZIQ	B	403	-	-	2/9/11/11	0/2/2/2
4	ZIQ	C	403	-	-	3/9/11/11	0/2/2/2
3	A1AH8	B	402	-	-	2/6/15/15	0/5/5/5
3	A1AH8	C	402	-	-	3/6/15/15	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEM	C1B-NB	-4.67	1.32	1.40
2	B	401	HEM	C1B-NB	-3.93	1.33	1.40
2	D	401	HEM	C4B-NB	-3.51	1.31	1.38
2	C	401	HEM	FE-NB	3.45	2.13	1.96
2	B	401	HEM	FE-NB	3.17	2.12	1.96
2	A	401	HEM	C1B-NB	-3.13	1.34	1.40
2	A	401	HEM	C4B-NB	-3.00	1.32	1.38
2	A	401	HEM	C1D-ND	-2.90	1.32	1.38
2	C	401	HEM	C1B-NB	-2.90	1.35	1.40
2	D	401	HEM	C4D-ND	-2.89	1.35	1.40
2	A	401	HEM	C4D-ND	-2.73	1.35	1.40
2	D	401	HEM	C1D-ND	-2.69	1.33	1.38
2	A	401	HEM	CHB-C1B	2.55	1.41	1.35
2	C	401	HEM	CHB-C1B	2.54	1.41	1.35
2	A	401	HEM	FE-NB	2.50	2.09	1.96
2	A	401	HEM	C3B-C4B	2.48	1.49	1.44
2	D	401	HEM	FE-NB	2.44	2.08	1.96
2	B	401	HEM	C4D-ND	-2.32	1.36	1.40
2	C	401	HEM	C4D-ND	-2.29	1.36	1.40
2	C	401	HEM	C4B-NB	-2.06	1.34	1.38
2	C	401	HEM	CHA-C4D	2.05	1.40	1.35
3	A	402	A1AH8	N1-N2	-2.02	1.30	1.34

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CHA-C4D-ND	5.22	130.83	124.38
2	D	401	HEM	CHD-C1D-ND	4.61	129.44	124.43
2	D	401	HEM	CHC-C4B-NB	4.45	129.27	124.43
2	C	401	HEM	CHC-C4B-NB	4.45	129.26	124.43
2	D	401	HEM	O2D-CGD-CBD	4.35	128.00	114.03
2	C	401	HEM	CHA-C4D-ND	4.31	129.70	124.38
2	B	401	HEM	C1B-NB-C4B	4.02	109.23	105.07
2	A	401	HEM	O2D-CGD-CBD	3.91	126.58	114.03
2	B	401	HEM	CHC-C4B-NB	3.89	128.66	124.43
2	A	401	HEM	CHD-C1D-ND	3.88	128.65	124.43
2	D	401	HEM	C1B-NB-C4B	3.83	109.03	105.07
4	B	403	ZIQ	C1-CA-CB	-3.78	105.81	110.94
2	B	401	HEM	CHA-C4D-ND	3.70	128.96	124.38
2	C	401	HEM	C4D-ND-C1D	3.63	108.82	105.07
2	D	401	HEM	CHB-C1B-NB	3.63	128.87	124.38
2	C	401	HEM	CHD-C1D-ND	3.58	128.32	124.43
2	A	401	HEM	O2A-CGA-O1A	-3.53	114.51	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CHA-C4D-ND	3.48	128.68	124.38
2	A	401	HEM	C1B-NB-C4B	3.39	108.58	105.07
2	D	401	HEM	CBD-CAD-C3D	-3.34	103.35	112.63
2	A	401	HEM	CHD-C1D-C2D	-3.34	119.77	124.98
2	B	401	HEM	CHD-C1D-ND	3.30	128.01	124.43
2	A	401	HEM	CHA-C4D-C3D	-3.27	119.19	125.33
2	C	401	HEM	C1B-NB-C4B	3.15	108.33	105.07
4	A	403	ZIQ	C1-CA-CB	-3.04	106.83	110.94
2	C	401	HEM	C2C-C3C-C4C	3.02	109.00	106.90
2	B	401	HEM	O2A-CGA-CBA	3.01	123.71	114.03
2	B	401	HEM	O2D-CGD-CBD	3.00	123.66	114.03
3	B	402	A1AH8	N3-C12-N4	2.97	121.27	114.99
2	D	401	HEM	O2D-CGD-O1D	-2.97	115.91	123.30
3	B	402	A1AH8	C12-N3-N2	2.89	121.55	116.94
2	B	401	HEM	O2A-CGA-O1A	-2.74	116.47	123.30
2	C	401	HEM	C3C-C4C-NC	-2.74	105.78	110.94
2	B	401	HEM	C3C-C4C-NC	-2.73	105.78	110.94
2	C	401	HEM	CBA-CAA-C2A	-2.68	108.05	112.62
2	A	401	HEM	CBD-CAD-C3D	-2.57	105.48	112.63
4	B	403	ZIQ	CB-CA-C	2.54	112.61	109.02
3	A	402	A1AH8	C6-C11-C10	-2.54	119.22	121.44
2	D	401	HEM	CHD-C1D-C2D	-2.53	121.02	124.98
2	C	401	HEM	CBD-CAD-C3D	-2.52	105.62	112.63
3	C	402	A1AH8	C6-C11-C10	-2.51	119.24	121.44
2	A	401	HEM	O2D-CGD-O1D	-2.44	117.21	123.30
4	A	403	ZIQ	CH2-CZ2-CE2	-2.44	116.57	120.08
2	D	401	HEM	CBA-CAA-C2A	-2.42	108.49	112.62
2	B	401	HEM	CHB-C1B-NB	2.42	127.37	124.38
2	C	401	HEM	O2A-CGA-CBA	2.39	121.71	114.03
2	A	401	HEM	C4B-C3B-C2B	-2.31	105.28	107.11
2	C	401	HEM	CHB-C1B-NB	2.30	127.22	124.38
2	A	401	HEM	O2A-CGA-CBA	2.27	121.34	114.03
2	D	401	HEM	CAD-C3D-C4D	2.27	128.62	124.66
2	C	401	HEM	O2A-CGA-O1A	-2.25	117.69	123.30
2	D	401	HEM	CHB-C1B-C2B	-2.24	120.52	126.72
2	C	401	HEM	CMA-C3A-C4A	-2.24	125.02	128.46
3	B	402	A1AH8	C1-C18-C17	-2.22	116.89	120.08
2	D	401	HEM	C3C-C4C-NC	-2.20	106.79	110.94
2	B	401	HEM	CHA-C4D-C3D	-2.19	121.21	125.33
2	D	401	HEM	CHA-C4D-C3D	-2.18	121.23	125.33
2	D	401	HEM	O1D-CGD-CBD	-2.17	116.09	123.08
4	B	403	ZIQ	CH2-CZ2-CE2	-2.15	116.99	120.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	CHD-C1D-C2D	-2.15	121.62	124.98
2	B	401	HEM	C4D-ND-C1D	2.15	107.29	105.07
2	A	401	HEM	O1D-CGD-CBD	-2.14	116.21	123.08
4	C	403	ZIQ	CH2-CZ2-CE2	-2.13	117.02	120.08
3	C	402	A1AH8	C1-C18-C17	-2.13	117.02	120.08
3	D	402	A1AH8	C6-C11-C10	-2.12	119.58	121.44
3	C	402	A1AH8	C12-N3-N2	2.09	120.27	116.94
2	B	401	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
2	A	401	HEM	CHB-C1B-NB	2.07	126.94	124.38
2	A	401	HEM	CHC-C4B-NB	2.06	126.67	124.43
2	B	401	HEM	O2D-CGD-O1D	-2.03	118.24	123.30
2	D	401	HEM	C4D-ND-C1D	2.02	107.16	105.07

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	A1AH8	N3-C12-N4-C13
3	B	402	A1AH8	N3-C12-N4-C15
3	C	402	A1AH8	C4-C5-C6-C7
4	A	403	ZIQ	C1-CA-CB-CG
4	A	403	ZIQ	C-CA-CB-CG
4	D	403	ZIQ	C-CA-CB-CG
4	D	403	ZIQ	OXT-C-CA-C1
4	A	403	ZIQ	OXT-C-CA-C1
4	D	403	ZIQ	O-C-CA-C1
4	D	403	ZIQ	C1-CA-CB-CG
4	A	403	ZIQ	OXT-C-CA-CB
4	A	403	ZIQ	N-CA-CB-CG
4	A	403	ZIQ	O-C-CA-C1
3	C	402	A1AH8	C4-C5-C6-C11
4	D	403	ZIQ	N-CA-CB-CG
4	A	403	ZIQ	O-C-CA-CB
4	D	403	ZIQ	O-C-CA-CB
4	D	403	ZIQ	OXT-C-CA-CB
2	C	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O1A
4	C	403	ZIQ	O-C-CA-C1
2	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O2A

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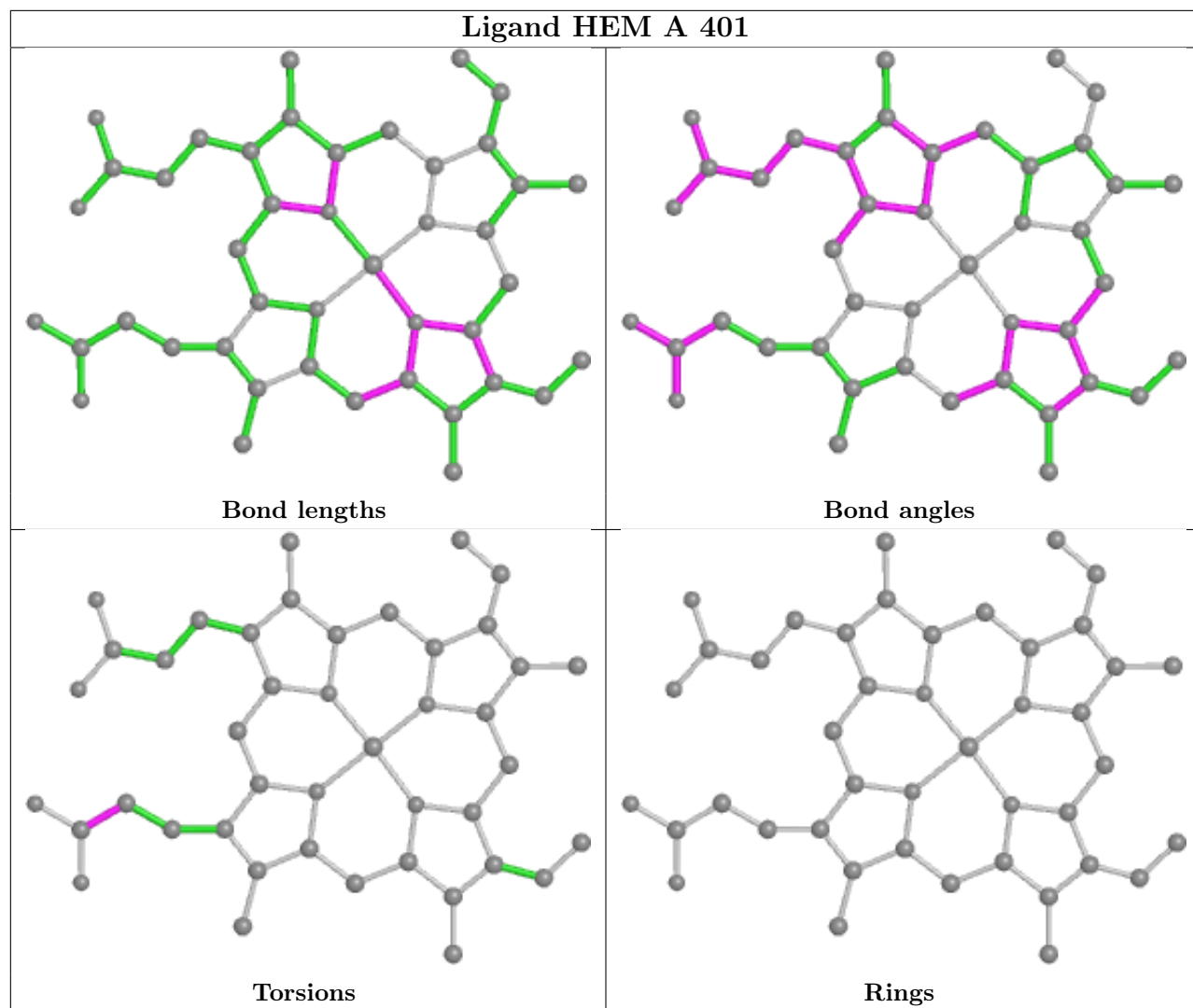
Mol	Chain	Res	Type	Atoms
2	D	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
4	B	403	ZIQ	O-C-CA-C1
4	B	403	ZIQ	OXT-C-CA-C1
2	C	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D
3	C	402	A1AH8	C16-C5-C6-C7
4	C	403	ZIQ	C-CA-CB-CG
4	C	403	ZIQ	OXT-C-CA-C1

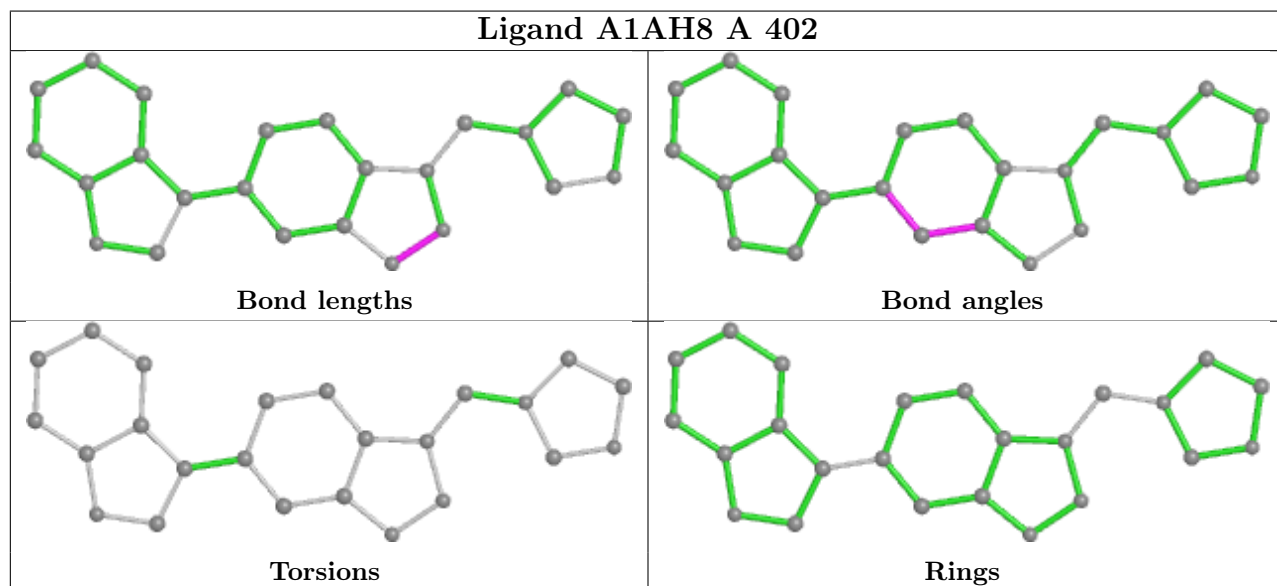
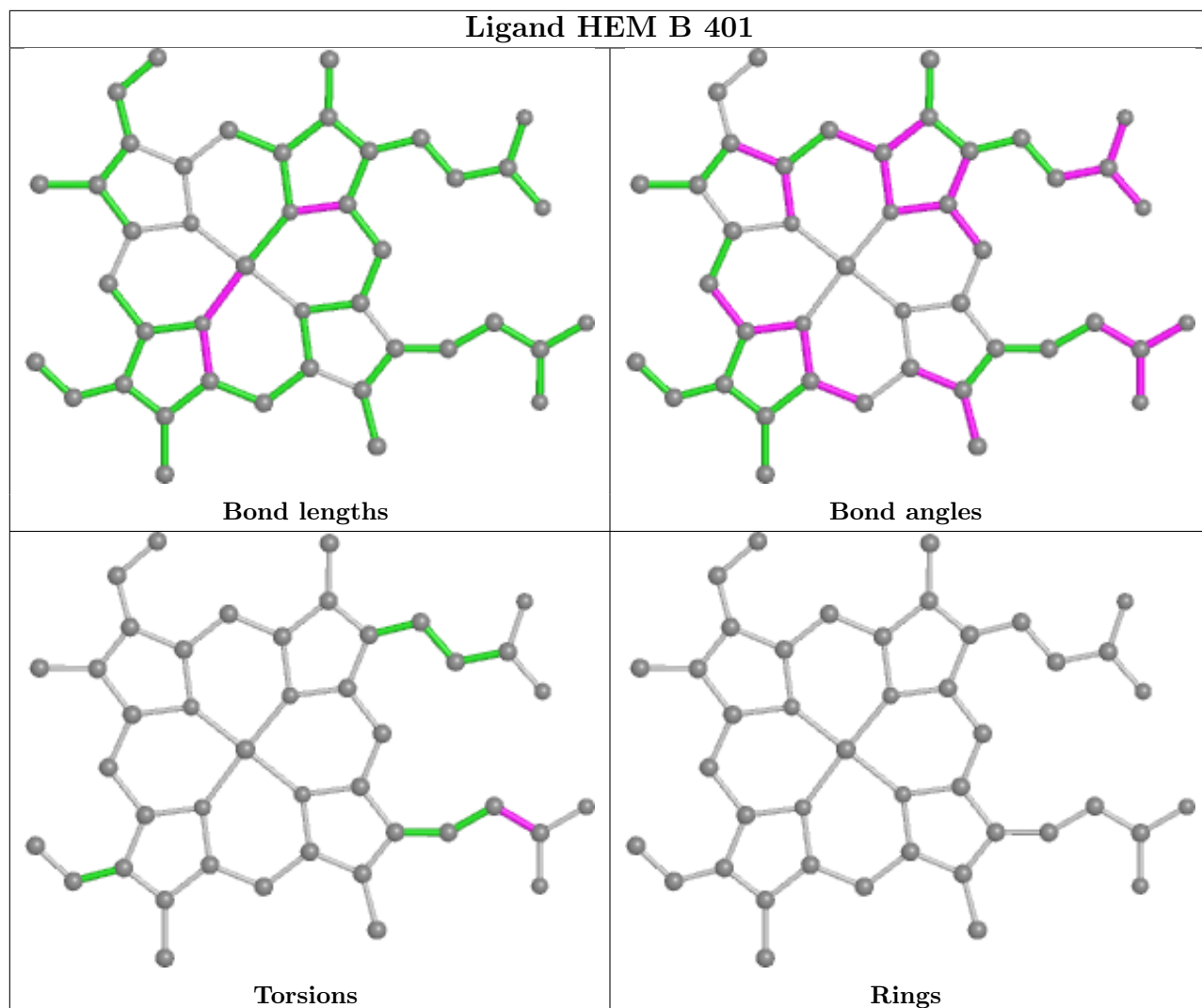
There are no ring outliers.

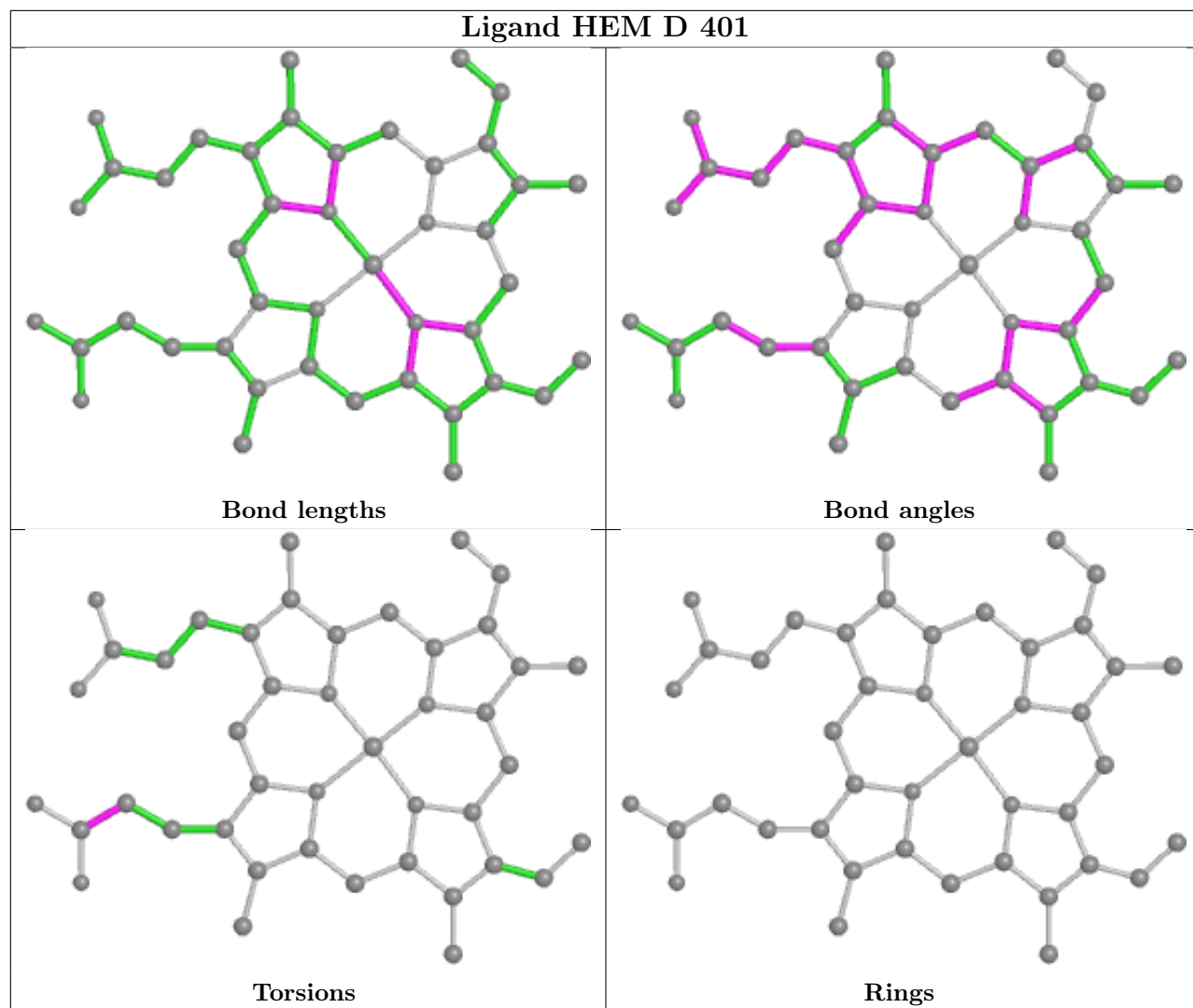
6 monomers are involved in 19 short contacts:

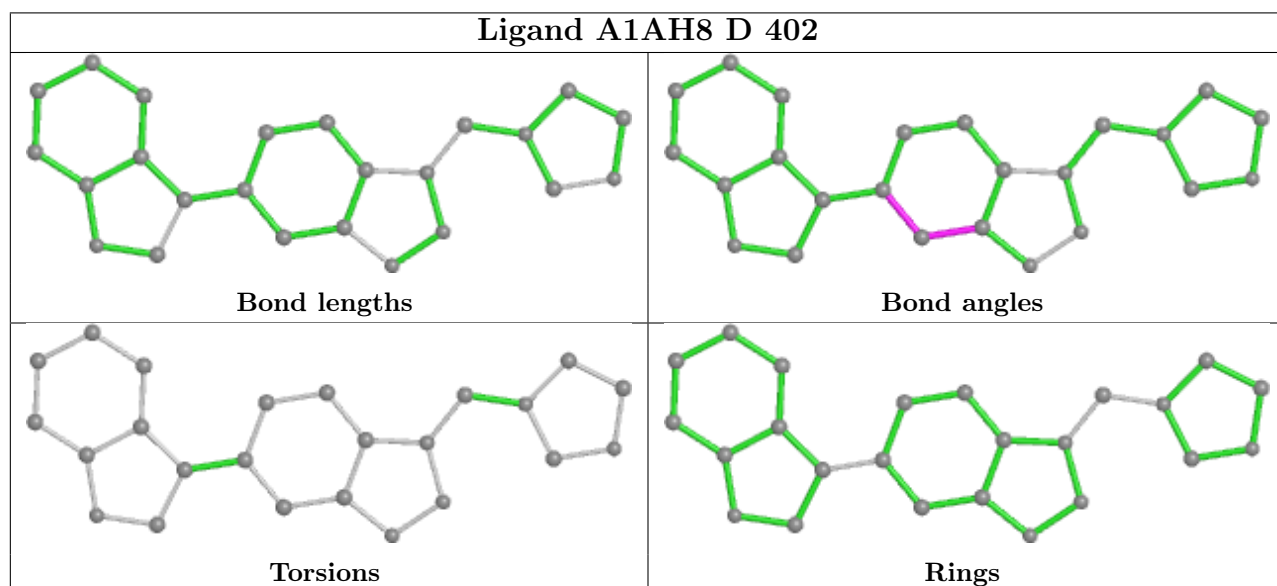
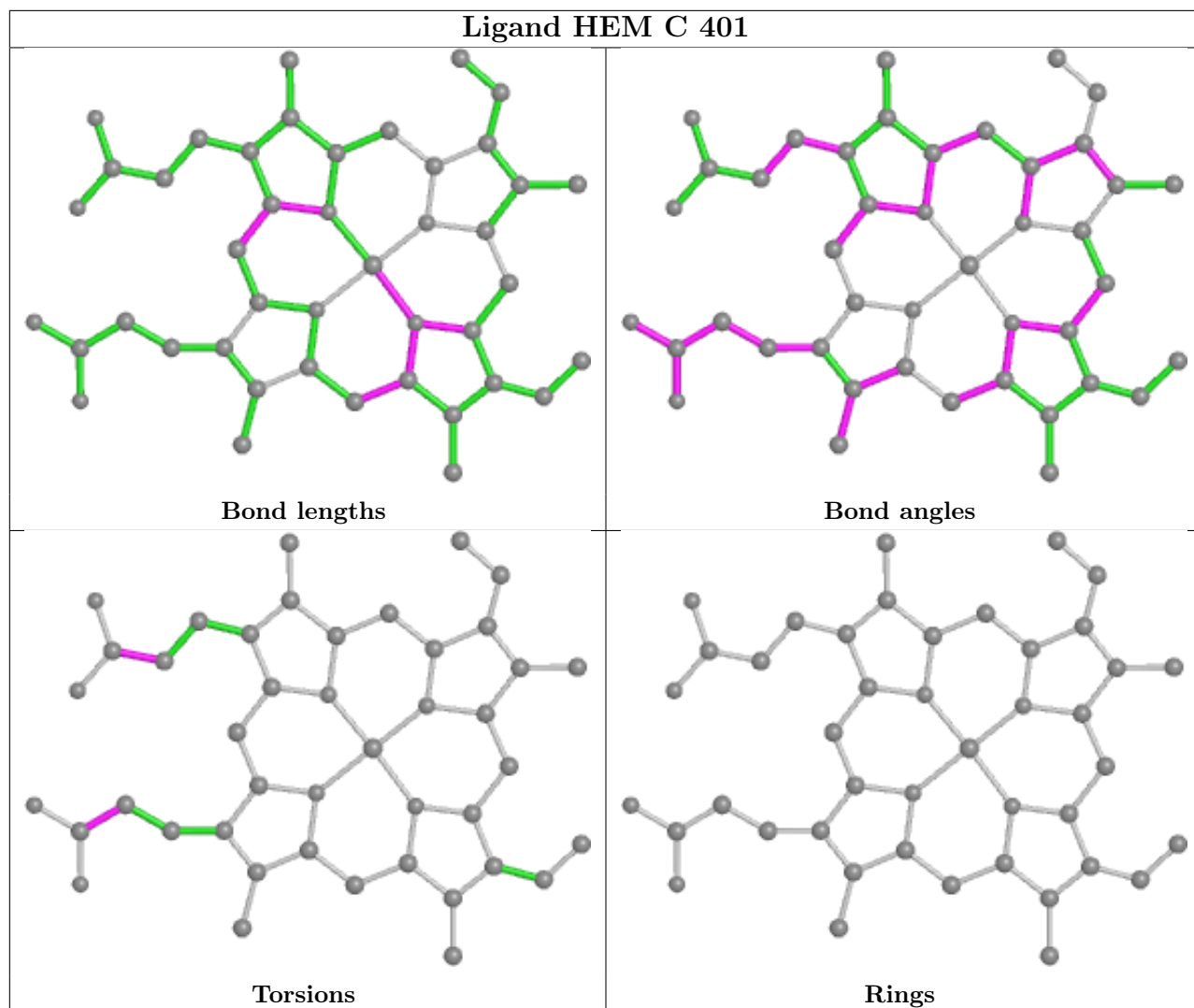
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	5	0
2	B	401	HEM	5	0
4	A	403	ZIQ	1	0
2	D	401	HEM	4	0
2	C	401	HEM	3	0
4	C	403	ZIQ	1	0

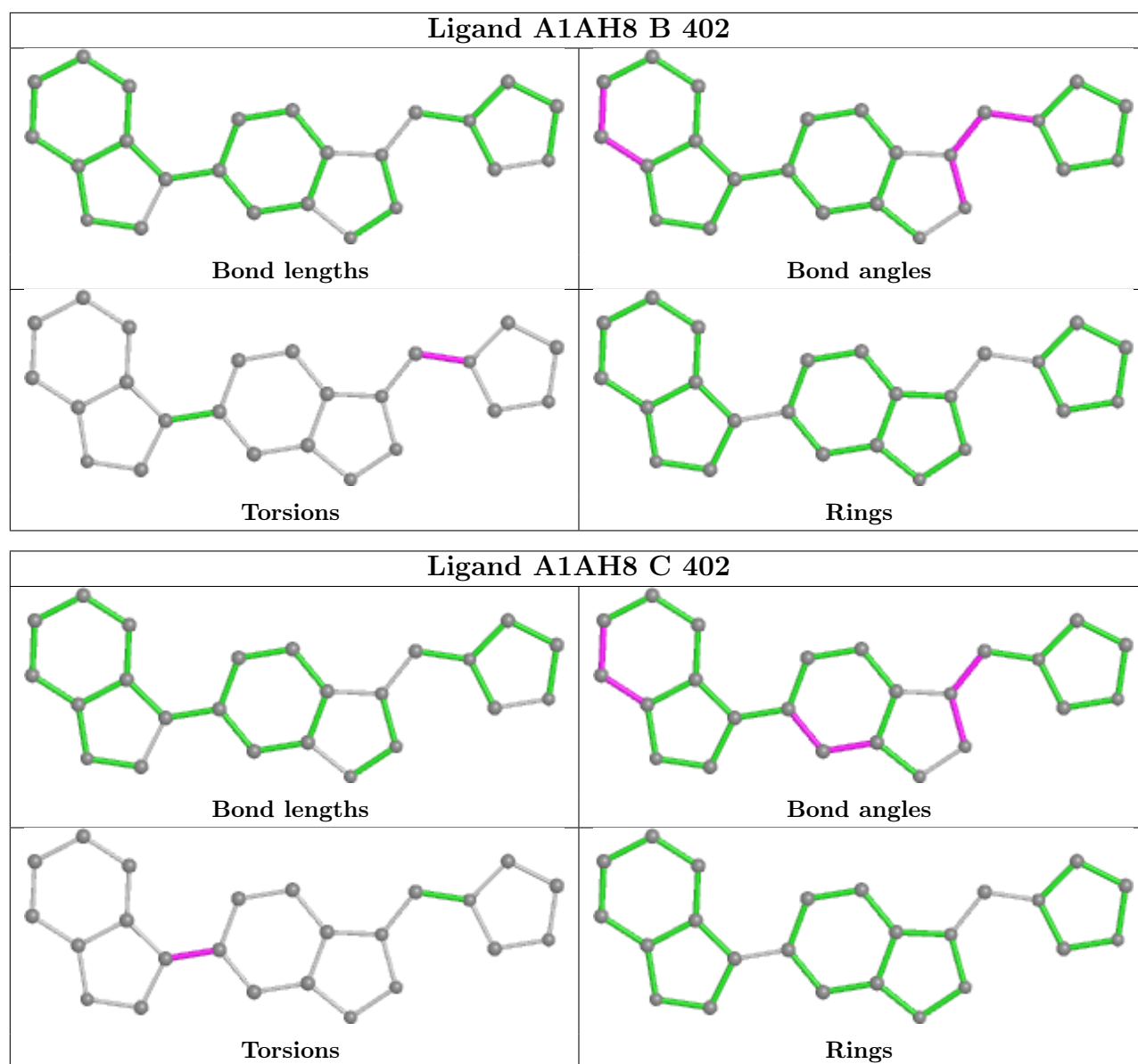
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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, 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	345/380 (90%)	-0.26	10 (2%) 51 45	28, 59, 119, 180	0
1	B	345/380 (90%)	-0.11	19 (5%) 25 20	26, 64, 133, 181	0
1	C	331/380 (87%)	0.12	25 (7%) 13 10	37, 88, 167, 225	0
1	D	343/380 (90%)	-0.23	10 (2%) 51 45	29, 67, 138, 209	0
All	All	1364/1520 (89%)	-0.12	64 (4%) 31 25	26, 68, 143, 225	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	HIS	6.1
1	C	385	ILE	5.8
1	B	386	HIS	5.6
1	C	387	LYS	5.2
1	C	384	THR	5.2
1	B	384	THR	4.5
1	D	387	LYS	4.4
1	C	176	ASN	4.3
1	A	382	ASN	4.2
1	C	349	HIS	4.1
1	D	384	THR	4.1
1	B	385	ILE	4.1
1	A	246	GLU	3.9
1	A	247	SER	3.8
1	B	178	ARG	3.7
1	B	387	LYS	3.6
1	B	171	MET	3.6
1	A	178	ARG	3.6
1	C	178	ARG	3.6
1	C	238	PHE	3.5
1	C	175	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	383	PRO	3.4
1	C	218	HIS	3.3
1	C	383	PRO	3.3
1	B	348	TYR	3.2
1	B	239	ILE	3.2
1	C	182	ASP	3.1
1	C	191	LEU	3.0
1	C	177	ARG	3.0
1	B	240	ARG	3.0
1	B	382	ASN	3.0
1	C	388	PHE	2.9
1	B	245	GLU	2.9
1	A	177	ARG	2.9
1	C	382	ASN	2.9
1	B	179	HIS	2.8
1	C	248	GLU	2.8
1	B	182	ASP	2.8
1	C	257	PHE	2.7
1	B	390	GLU	2.7
1	B	383	PRO	2.6
1	D	218	HIS	2.6
1	C	193	LEU	2.6
1	D	238	PHE	2.5
1	B	177	ARG	2.4
1	D	246	GLU	2.4
1	A	255	ALA	2.4
1	A	389	LEU	2.4
1	C	190	GLU	2.4
1	C	254	VAL	2.4
1	D	385	ILE	2.3
1	C	251	GLU	2.3
1	B	347	GLY	2.3
1	B	349	HIS	2.3
1	C	253	GLN	2.3
1	A	384	THR	2.2
1	D	348	TYR	2.2
1	D	383	PRO	2.2
1	D	244	LYS	2.1
1	A	386	HIS	2.1
1	B	244	LYS	2.1
1	C	192	LEU	2.1
1	C	239	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	242	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](#)

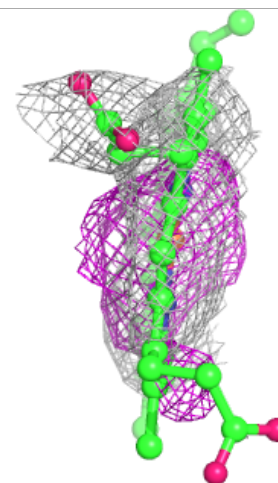
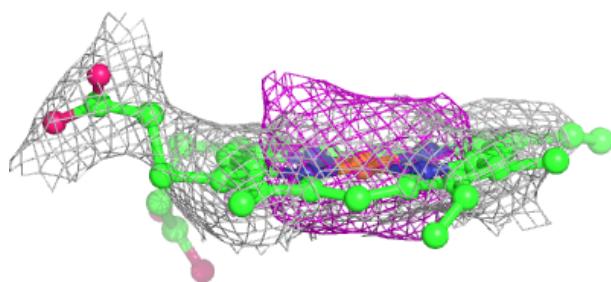
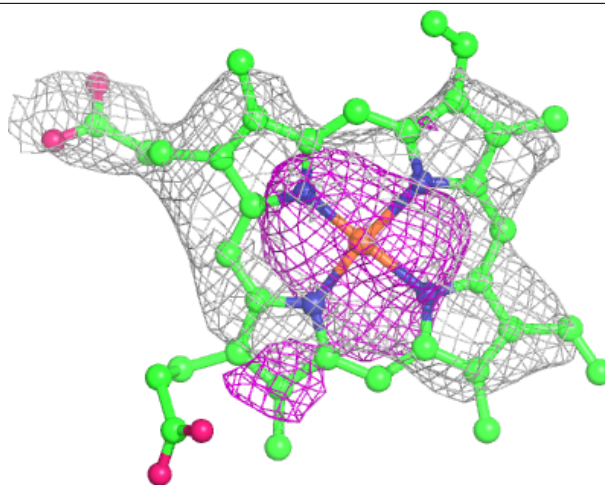
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	C	401	43/43	0.91	0.24	79,110,129,136	0
3	A1AH8	B	402	24/24	0.93	0.19	55,68,102,106	0
3	A1AH8	C	402	24/24	0.93	0.21	77,101,148,149	0
4	ZIQ	C	403	16/16	0.93	0.21	78,85,96,102	0
3	A1AH8	A	402	24/24	0.94	0.19	61,77,133,135	0
2	HEM	B	401	43/43	0.94	0.19	73,94,105,110	0
4	ZIQ	D	403	16/16	0.94	0.21	71,83,130,136	0
3	A1AH8	D	402	24/24	0.96	0.16	46,52,90,92	0
4	ZIQ	A	403	16/16	0.96	0.13	34,38,54,62	0
2	HEM	A	401	43/43	0.97	0.13	54,64,77,82	0
4	ZIQ	B	403	16/16	0.97	0.11	52,57,63,68	0
2	HEM	D	401	43/43	0.98	0.13	38,46,61,75	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.

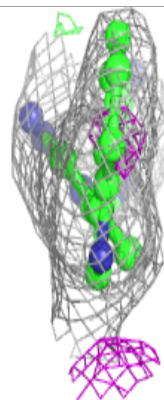
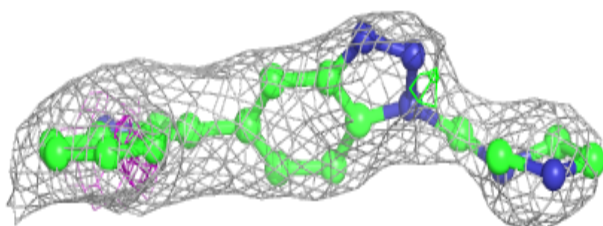
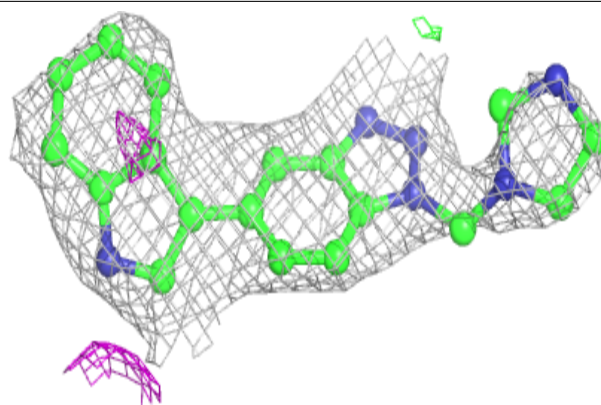
Electron density around HEM C 401:

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

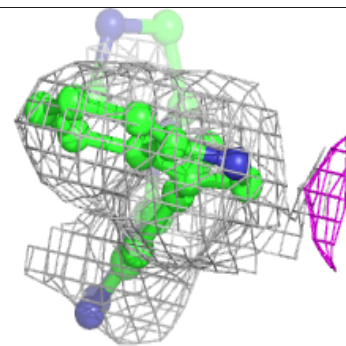
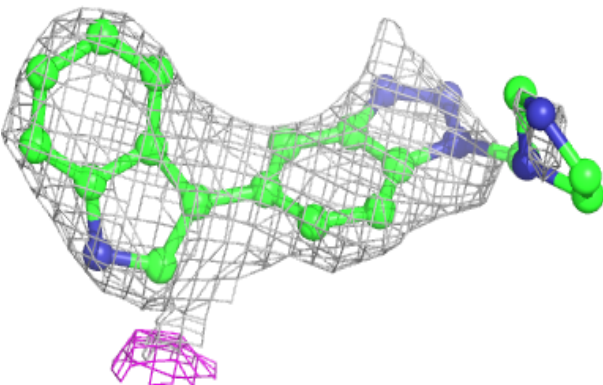
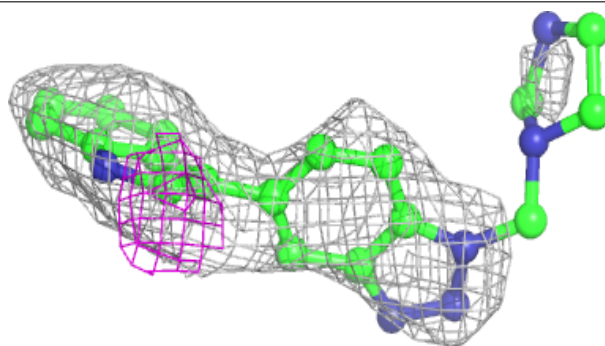


Electron density around A1AH8 B 402:

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

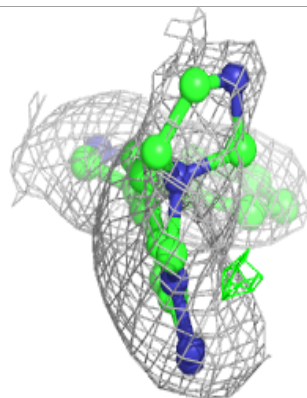
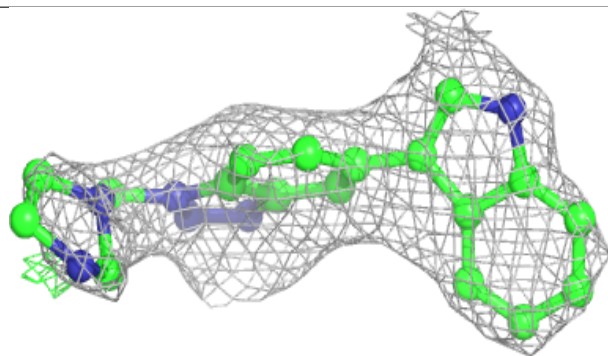
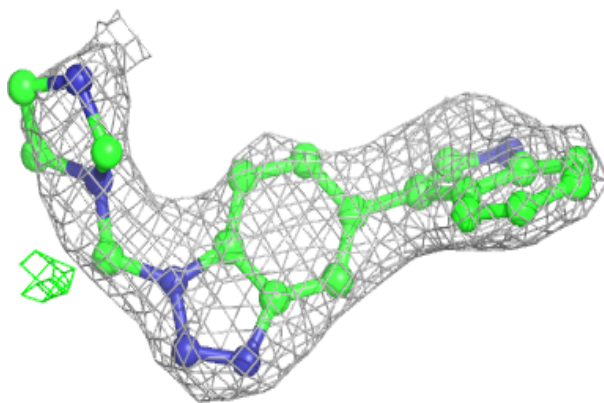
**Electron density around A1AH8 C 402:**

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



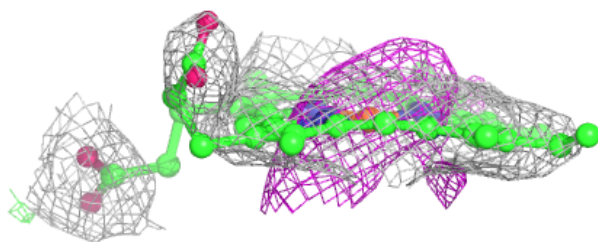
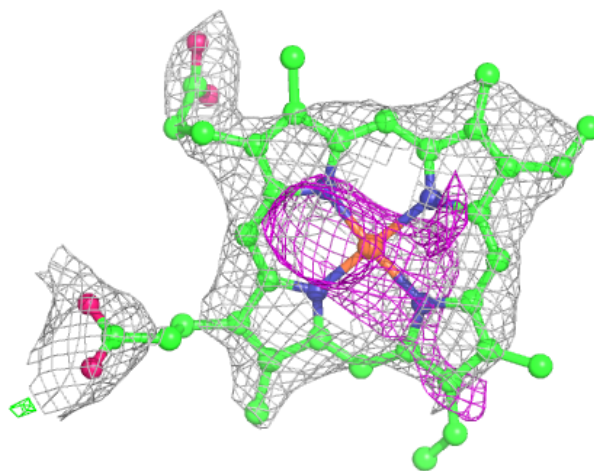
Electron density around A1AH8 A 402:

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



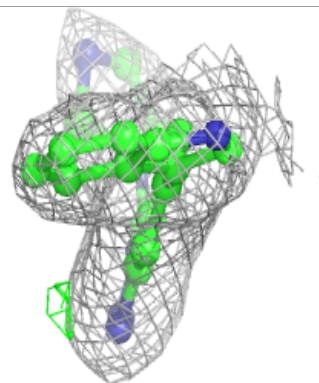
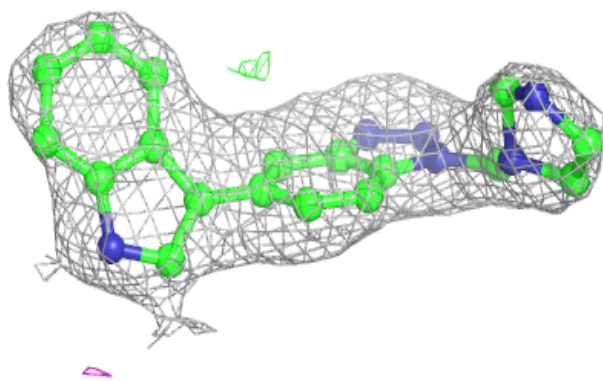
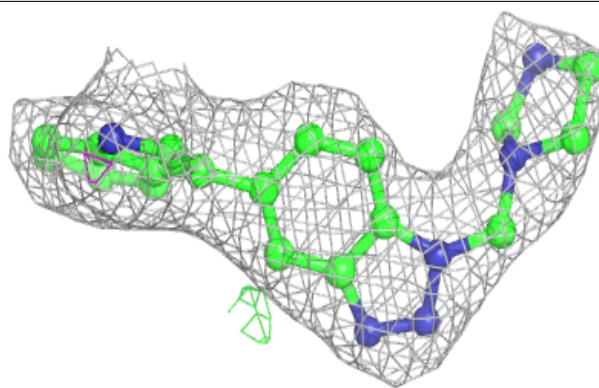
Electron density around HEM B 401:

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



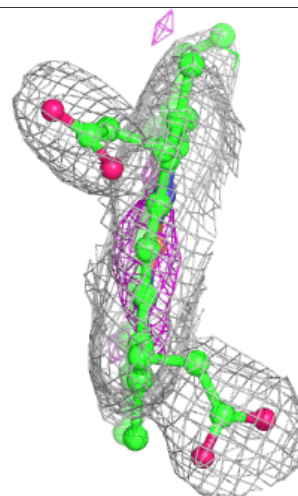
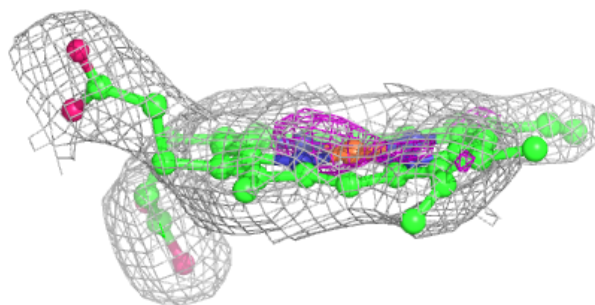
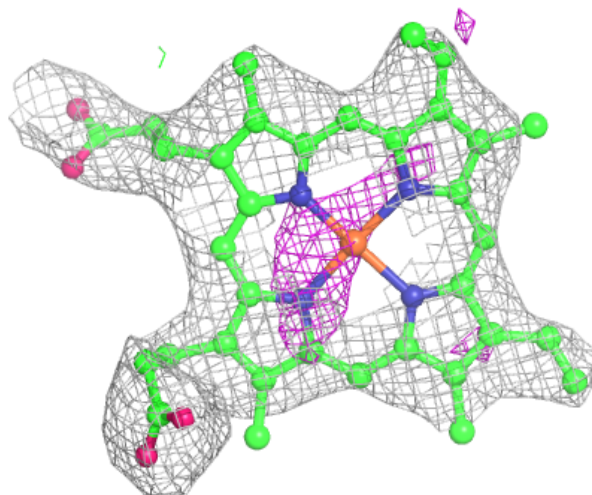
Electron density around A1AH8 D 402:

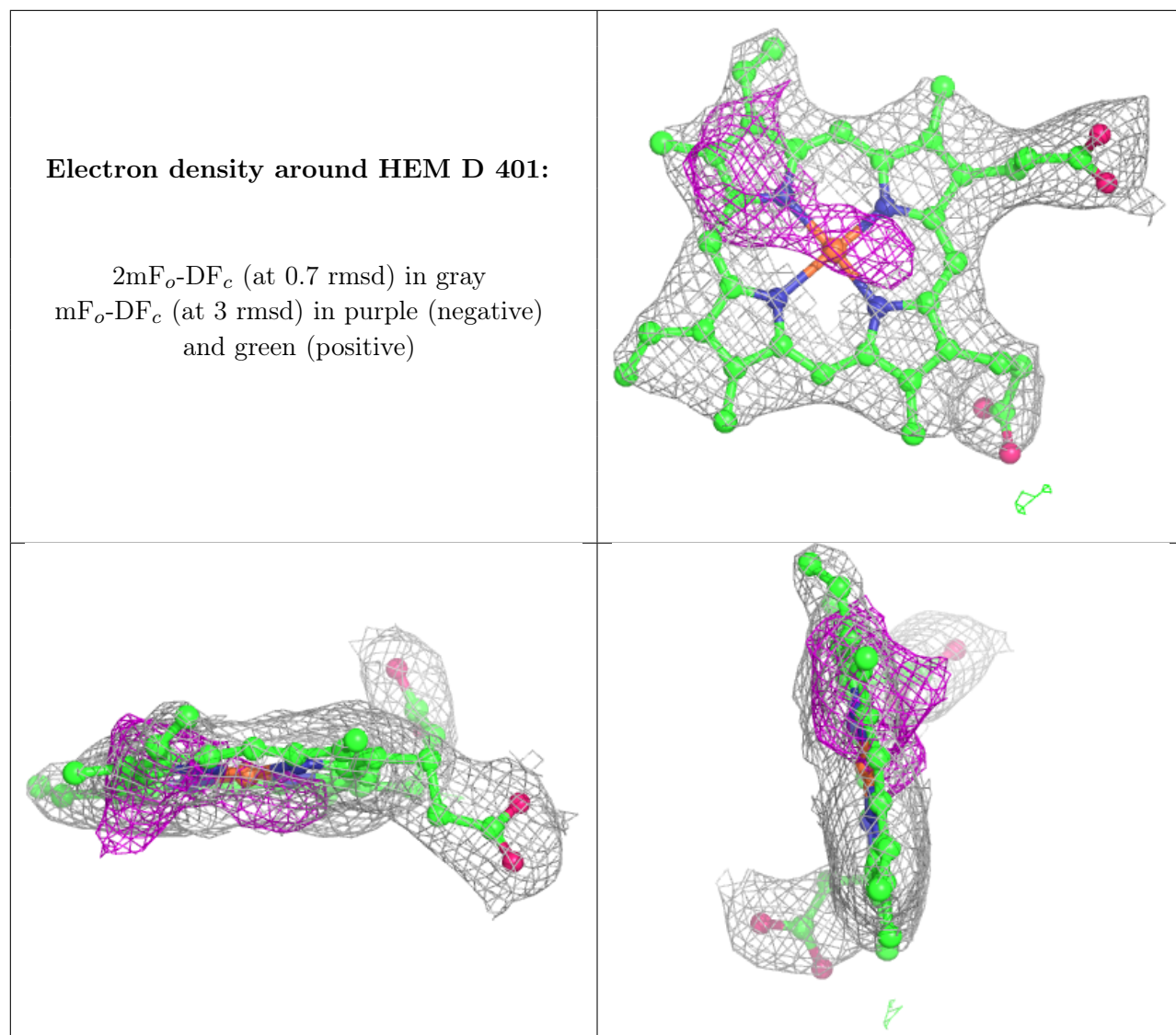
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.