



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:40 PM UTC

PDB ID : 9B1Q / pdb_00009b1q
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

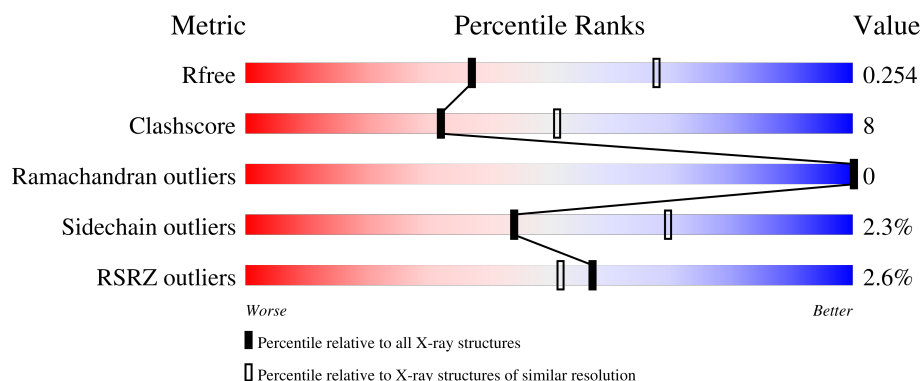
1 Overall quality at a glance

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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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	0% 72% 17% • 9%
1	B	380	3% 72% 17% • 9%
1	C	380	4% 67% 19% • 13%
1	D	380	2% 74% 16% • 10%

2 Entry composition

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
1	A	345	Total	C	N	O	S	0	0	0
			2932	1884	514	523	11			
1	B	345	Total	C	N	O	S	0	0	0
			2932	1884	514	523	11			
1	C	331	Total	C	N	O	S	0	0	0
			2819	1817	491	500	11			
1	D	343	Total	C	N	O	S	0	0	0
			2913	1873	510	519	11			

There are 32 discrepancies between the modelled and reference sequences:

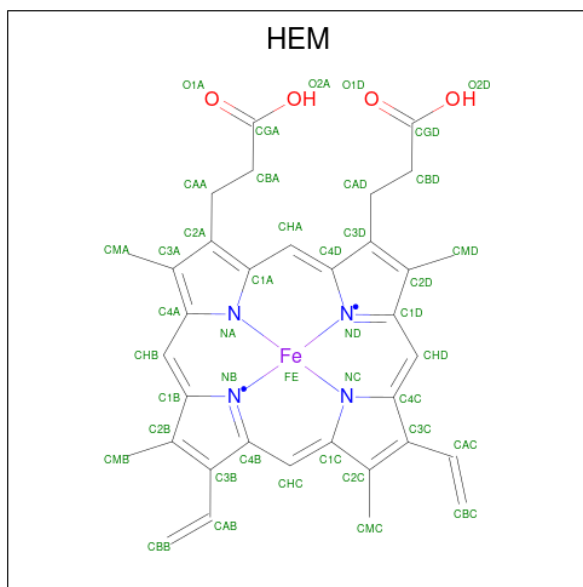
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression 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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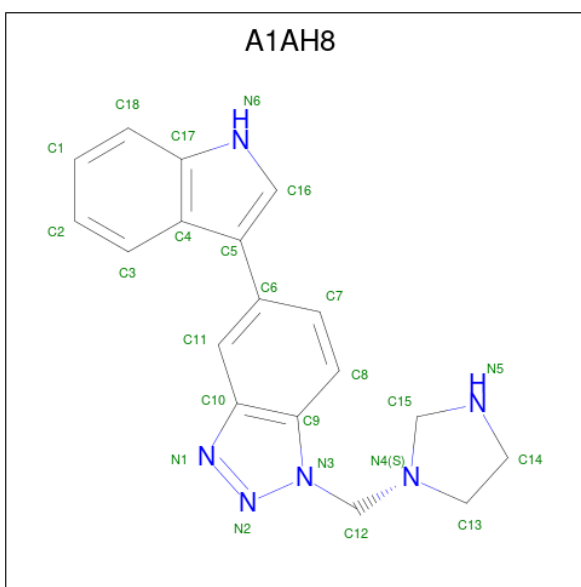
Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression 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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



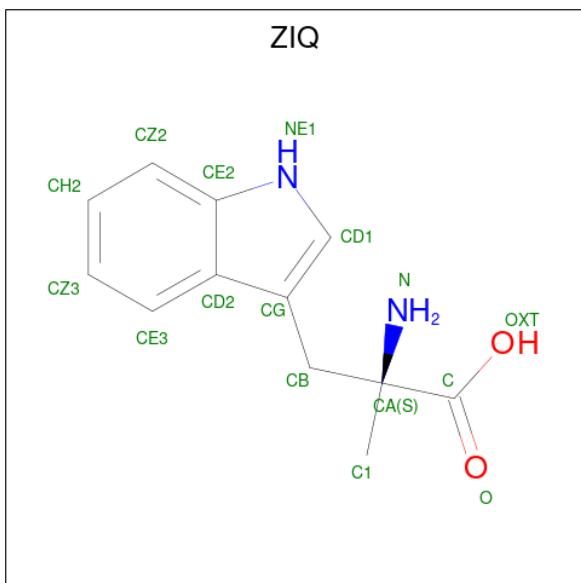
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (5P)-1-[(imidazolidin-1-yl)methyl]-5-(1H-indol-3-yl)-1H-1,2,3-benzotriazole (CCD ID: 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	0	0
			24	18	6		
3	B	1	Total	C	N	0	0
			24	18	6		
3	C	1	Total	C	N	0	0
			24	18	6		
3	D	1	Total	C	N	0	0
			24	18	6		

- Molecule 4 is alpha-methyl-L-tryptophan (CCD ID: 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		

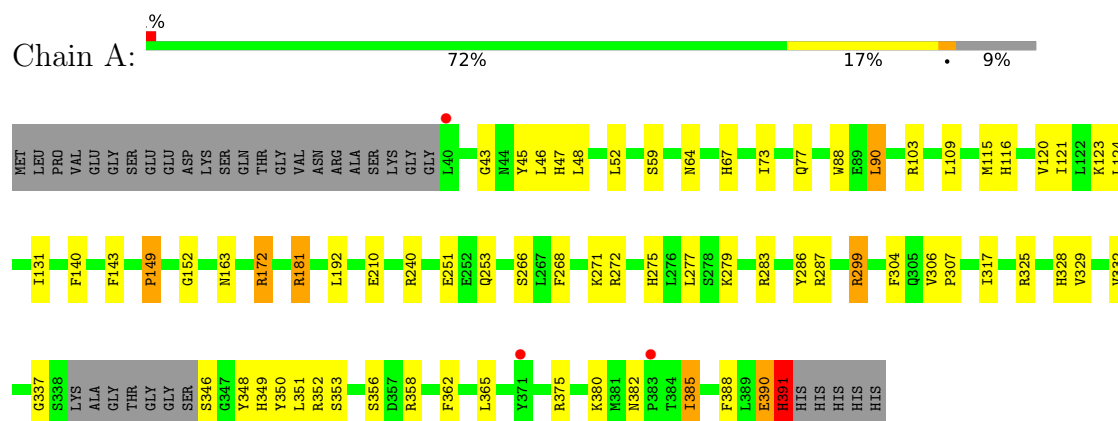
- Molecule 5 is water.

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		

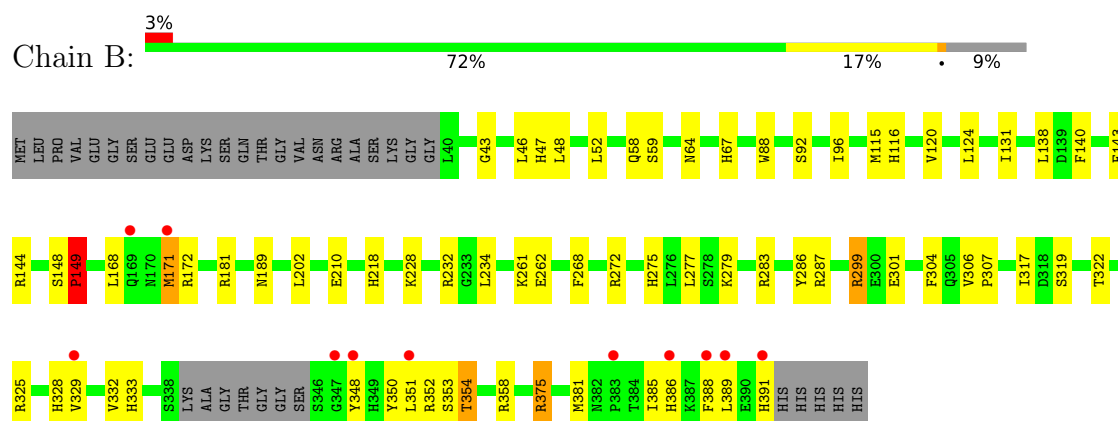
3 Residue-property plots [i](#)

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.

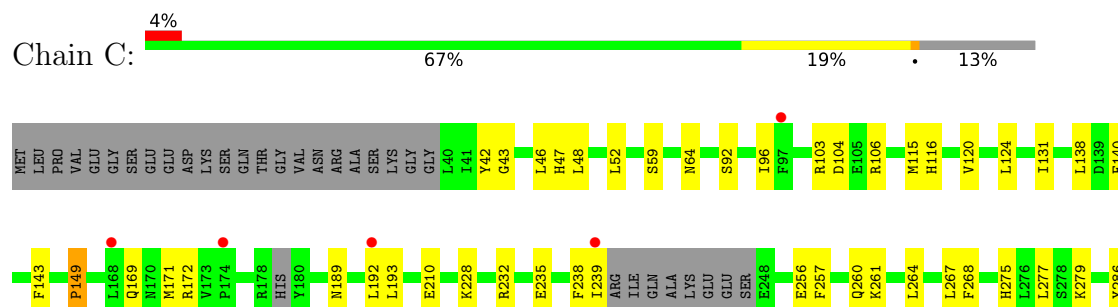
• Molecule 1: Tryptophan 2,3-dioxygenase

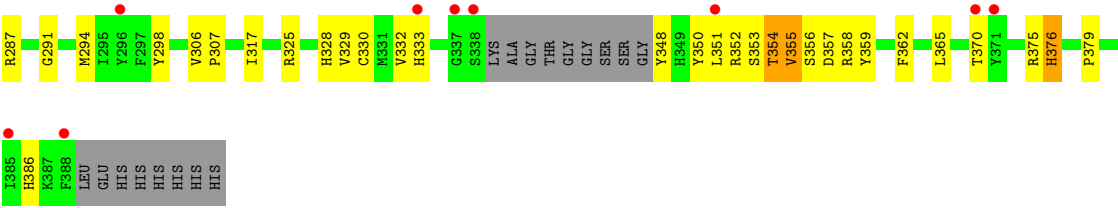


• Molecule 1: Tryptophan 2,3-dioxygenase

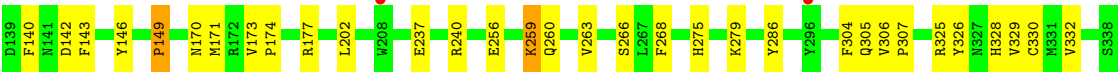
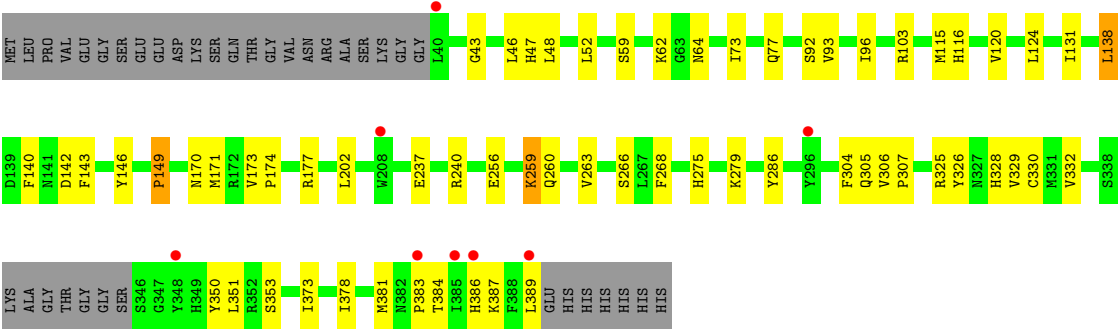


• Molecule 1: Tryptophan 2,3-dioxygenase





● Molecule 1: Tryptophan 2,3-dioxygenase



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)	Xtriage
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 (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZIQ, A1AH8

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	0.58	0/3001	1.10	2/4039 (0.0%)
1	B	0.57	0/3001	1.10	3/4039 (0.1%)
1	C	0.53	0/2884	1.06	2/3880 (0.1%)
1	D	0.56	0/2981	1.09	1/4012 (0.0%)
All	All	0.56	0/11867	1.09	8/15970 (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 (8) 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	388	PHE	CB-CA-C	6.21	121.40	110.85
1	B	149	PRO	N-CA-CB	-5.93	96.08	102.60
1	A	391	HIS	CA-CB-CG	5.43	119.23	113.80
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	5.11	120.60	110.17
1	C	42	TYR	N-CA-CB	-5.06	101.93	110.49

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

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	49	0
1	B	2932	0	2914	51	0
1	C	2819	0	2806	51	0
1	D	2913	0	2901	41	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	4	0	0	0	0
All	All	11940	0	11655	188	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 (188) 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:D:93:VAL:HG21	1:D:115:MET:HE3	1.51	0.93
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
1:D:381:MET:HE3	1:D:386:HIS:HA	1.66	0.76
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:D:115:MET:HA	1:D:115:MET:HE2	1.74	0.69
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:B:115:MET:HE3	1:B:317:ILE:CD1	2.25	0.67
1:A:275:HIS:CE1	1:A:279:LYS:HD2	2.31	0.66
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.26	0.66
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.26	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HH2	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: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
1:D:381:MET:HE1	1:D:389:LEU:HB2	1.89	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: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: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
1:C:325:ARG:HD3	1:C:354:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:381:MET:HE3	1:B:386:HIS:HA	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: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:375:ARG:HE	1:D:142:ASP:CG	2.22	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
2:C:401:HEM:HBB2	2:C:401:HEM:CMB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:390:GLU:O	1:A:391:HIS:C	2.60	0.43
1:D:259:LYS:HZ3	1:D:260:GLN:HB2	1.83	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:C:115:MET:HE3	1:C:317:ILE:HD13	1.98	0.43
1:D:46:LEU:O	1:D:47:HIS:C	2.62	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:C:356:SER:C	1:C:358:ARG:H	2.25	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:46:LEU:O	1:B:47:HIS:C	2.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:202:LEU:C	1:D:202:LEU:HD13	2.45	0.41
1:A:46:LEU:O	1:A:47:HIS:C	2.62	0.41
1:A:73:ILE:O	1:A:77:GLN:HG3	2.21	0.41
1:C:46:LEU:O	1:C:47:HIS:C	2.62	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:B:381:MET:HE1	1:B:389:LEU:HD22	2.02	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
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: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: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:115:MET:HE3	1:A:317:ILE:HD13	2.03	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%)	313 (97%)	9 (3%)	38	64
1	B	322/348 (92%)	316 (98%)	6 (2%)	50	74
1	C	310/348 (89%)	302 (97%)	8 (3%)	40	66
1	D	320/348 (92%)	314 (98%)	6 (2%)	50	74
All	All	1274/1392 (92%)	1245 (98%)	29 (2%)	44	69

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	123	LYS

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Mol	Chain	Res	Type
1	A	149	PRO
1	A	251	GLU
1	A	266	SER
1	A	277	LEU
1	A	385	ILE
1	A	390	GLU
1	A	391	HIS
1	B	138	LEU
1	B	149	PRO
1	B	171	MET
1	B	262	GLU
1	B	354	THR
1	B	391	HIS
1	C	138	LEU
1	C	149	PRO
1	C	277	LEU
1	C	330	CYS
1	C	354	THR
1	C	355	VAL
1	C	376	HIS
1	C	386	HIS
1	D	138	LEU
1	D	149	PRO
1	D	170	ASN
1	D	171	MET
1	D	259	LYS
1	D	330	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	183	ASN
1	A	309	GLN
1	B	98	GLN
1	B	176	ASN
1	B	309	GLN
1	B	327	ASN
1	B	391	HIS
1	C	141	ASN
1	C	154	GLN
1	C	176	ASN

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Mol	Chain	Res	Type
1	C	197	GLN
1	C	290	GLN
1	C	309	GLN
1	C	376	HIS
1	D	101	HIS
1	D	189	ASN
1	D	197	GLN
1	D	309	GLN
1	D	327	ASN

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 oligosaccharides 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	$\# Z > 2$
3	A1AH8	D	402	-	27,28,28	0.74	0	38,40,40	0.77	0
4	ZIQ	B	403	-	14,17,17	0.64	0	20,25,25	1.28	3 (15%)
3	A1AH8	A	402	-	27,28,28	0.75	1 (3%)	38,40,40	0.69	0
3	A1AH8	C	402	-	27,28,28	0.69	0	38,40,40	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	401	1	50,50,50	1.75	10 (20%)	67,82,82	1.83	18 (26%)
2	HEM	C	401	1	50,50,50	1.61	6 (12%)	67,82,82	1.68	15 (22%)
4	ZIQ	A	403	-	14,17,17	0.75	0	20,25,25	1.19	2 (10%)
4	ZIQ	D	403	-	14,17,17	0.76	0	20,25,25	0.89	1 (5%)
3	A1AH8	B	402	-	27,28,28	0.81	1 (3%)	38,40,40	0.99	2 (5%)
2	HEM	A	401	1	50,50,50	1.65	10 (20%)	67,82,82	1.82	18 (26%)
4	ZIQ	C	403	-	14,17,17	0.62	0	20,25,25	1.04	1 (5%)
2	HEM	B	401	1	50,50,50	1.60	6 (12%)	67,82,82	1.68	15 (22%)

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	A1AH8	D	402	-	-	3/8/15/15	0/5/5/5
4	ZIQ	B	403	-	-	2/11/11/11	0/2/2/2
3	A1AH8	A	402	-	-	2/8/15/15	0/5/5/5
3	A1AH8	C	402	-	-	5/8/15/15	0/5/5/5
2	HEM	D	401	1	-	2/14/54/54	-
2	HEM	C	401	1	-	4/14/54/54	-
4	ZIQ	A	403	-	-	7/11/11/11	0/2/2/2
4	ZIQ	D	403	-	-	7/11/11/11	0/2/2/2
3	A1AH8	B	402	-	-	2/8/15/15	0/5/5/5
2	HEM	A	401	1	-	2/14/54/54	-
4	ZIQ	C	403	-	-	3/11/11/11	0/2/2/2
2	HEM	B	401	1	-	3/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	FE-NB	6.18	2.13	1.94
2	B	401	HEM	FE-NB	5.73	2.12	1.94
2	C	401	HEM	FE-NC	4.81	2.11	1.95
2	A	401	HEM	FE-NB	4.66	2.09	1.94
2	D	401	HEM	C1B-NB	-4.62	1.32	1.40
2	D	401	HEM	FE-NB	4.56	2.08	1.94
2	B	401	HEM	FE-NC	4.56	2.10	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C1B-NB	-3.88	1.33	1.40
2	D	401	HEM	C4B-NB	-3.71	1.31	1.38
2	A	401	HEM	C3C-C4C	-3.56	1.39	1.46
2	A	401	HEM	C4B-NB	-3.17	1.32	1.38
2	A	401	HEM	C1B-NB	-3.08	1.34	1.40
2	A	401	HEM	C1D-ND	-3.06	1.32	1.38
2	D	401	HEM	FE-NC	3.01	2.05	1.95
2	C	401	HEM	C1C-C2C	-2.96	1.39	1.45
2	D	401	HEM	C3C-C4C	-2.95	1.40	1.46
2	D	401	HEM	C1D-ND	-2.85	1.33	1.38
2	C	401	HEM	C1B-NB	-2.85	1.35	1.40
2	D	401	HEM	C4D-ND	-2.84	1.35	1.40
2	B	401	HEM	C1C-C2C	-2.76	1.39	1.45
2	A	401	HEM	C4D-ND	-2.68	1.35	1.40
2	D	401	HEM	C1C-C2C	-2.66	1.40	1.45
2	A	401	HEM	C1C-NC	-2.62	1.34	1.39
2	A	401	HEM	C3B-C4B	2.52	1.49	1.44
2	A	401	HEM	FE-ND	-2.38	1.87	1.94
2	B	401	HEM	C4D-ND	-2.27	1.36	1.40
2	C	401	HEM	C4D-ND	-2.24	1.36	1.40
2	C	401	HEM	C4B-NB	-2.19	1.34	1.38
2	D	401	HEM	FE-ND	-2.18	1.88	1.94
2	A	401	HEM	FE-NC	2.17	2.02	1.95
2	D	401	HEM	C4A-NA	-2.10	1.35	1.39
3	B	402	A1AH8	C11-C6	-2.09	1.36	1.39
3	A	402	A1AH8	C7-C6	2.09	1.42	1.39
2	B	401	HEM	C3C-C4C	-2.03	1.42	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CHA-C4D-ND	5.23	130.83	124.37
2	A	401	HEM	CHD-C4C-NC	4.83	129.71	124.45
2	D	401	HEM	CHD-C1D-ND	4.66	129.44	124.42
2	D	401	HEM	CHC-C4B-NB	4.50	129.27	124.42
2	C	401	HEM	CHC-C4B-NB	4.50	129.26	124.42
2	D	401	HEM	O2D-CGD-CBD	4.43	128.00	114.00
2	C	401	HEM	CHA-C4D-ND	4.31	129.70	124.37
2	A	401	HEM	O2D-CGD-CBD	3.98	126.58	114.00
2	B	401	HEM	CHC-C4B-NB	3.94	128.66	124.42
2	A	401	HEM	CHD-C1D-ND	3.93	128.65	124.42
2	B	401	HEM	CHA-C4D-ND	3.71	128.96	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CHB-C1B-NB	3.64	128.87	124.37
2	C	401	HEM	CHD-C1D-ND	3.62	128.32	124.42
4	C	403	ZIQ	O-C-CA	-3.61	116.31	122.78
4	B	403	ZIQ	C1-CA-CB	-3.57	105.81	110.82
2	D	401	HEM	CHA-C4D-ND	3.49	128.68	124.37
2	A	401	HEM	O2A-CGA-O1A	-3.43	114.51	123.33
2	B	401	HEM	C3B-C4B-NB	-3.40	107.02	109.47
2	B	401	HEM	C1B-NB-C4B	3.40	109.23	105.21
2	B	401	HEM	CHD-C1D-ND	3.34	128.01	124.42
2	A	401	HEM	CHD-C1D-C2D	-3.33	119.77	125.03
2	D	401	HEM	CBD-CAD-C3D	-3.32	103.35	112.53
2	A	401	HEM	CHA-C4D-C3D	-3.28	119.19	125.23
2	D	401	HEM	C1B-NB-C4B	3.23	109.03	105.21
2	B	401	HEM	C4C-NC-C1C	3.11	110.89	105.82
2	B	401	HEM	O2A-CGA-CBA	3.07	123.71	114.00
2	B	401	HEM	O2D-CGD-CBD	3.06	123.66	114.00
2	C	401	HEM	C4D-ND-C1D	3.05	108.82	105.21
4	A	403	ZIQ	O-C-CA	-3.02	117.36	122.78
2	B	401	HEM	CHD-C4C-NC	2.92	127.63	124.45
2	A	401	HEM	C1A-CHA-C4D	-2.91	119.40	126.25
2	D	401	HEM	O2D-CGD-O1D	-2.89	115.91	123.33
3	B	402	A1AH8	N4-C12-N3	2.88	121.27	114.97
4	A	403	ZIQ	C1-CA-CB	-2.85	106.83	110.82
2	A	401	HEM	C1B-NB-C4B	2.84	108.58	105.21
4	D	403	ZIQ	O-C-CA	-2.83	117.71	122.78
2	A	401	HEM	C4C-NC-C1C	2.74	110.28	105.82
2	B	401	HEM	O2A-CGA-O1A	-2.67	116.47	123.33
2	D	401	HEM	C4C-NC-C1C	2.66	110.16	105.82
2	C	401	HEM	C1B-NB-C4B	2.64	108.33	105.21
2	C	401	HEM	C2A-C1A-NA	-2.62	107.24	110.15
4	B	403	ZIQ	O-C-CA	-2.60	118.12	122.78
2	A	401	HEM	C4C-CHD-C1D	-2.58	120.55	126.02
2	A	401	HEM	CBD-CAD-C3D	-2.55	105.48	112.53
4	B	403	ZIQ	CB-CA-C	2.55	112.61	109.10
2	D	401	HEM	CHD-C1D-C2D	-2.54	121.02	125.03
2	C	401	HEM	C4C-C3C-C2C	2.53	109.00	106.81
2	D	401	HEM	C1A-CHA-C4D	-2.51	120.35	126.25
2	C	401	HEM	CBD-CAD-C3D	-2.50	105.62	112.53
2	C	401	HEM	C1A-CHA-C4D	-2.50	120.38	126.25
2	B	401	HEM	C1A-CHA-C4D	-2.45	120.49	126.25
2	C	401	HEM	O2A-CGA-CBA	2.44	121.71	114.00
2	B	401	HEM	CHB-C1B-NB	2.42	127.37	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	O2D-CGD-O1D	-2.38	117.21	123.33
2	A	401	HEM	O2A-CGA-CBA	2.32	121.34	114.00
2	C	401	HEM	CHB-C1B-NB	2.31	127.22	124.37
2	D	401	HEM	CHB-C1B-C2B	-2.26	120.52	126.95
2	D	401	HEM	CHD-C4C-NC	2.26	126.91	124.45
3	B	402	A1AH8	C12-N3-N2	2.26	121.55	119.35
2	D	401	HEM	CAD-C3D-C4D	2.25	128.62	124.70
2	D	401	HEM	O1D-CGD-CBD	-2.21	116.09	123.09
2	C	401	HEM	O2A-CGA-O1A	-2.19	117.69	123.33
2	D	401	HEM	CHC-C1C-NC	2.19	126.83	124.45
2	A	401	HEM	C4B-C3B-C2B	-2.18	105.28	107.28
2	B	401	HEM	CHA-C4D-C3D	-2.18	121.21	125.23
2	A	401	HEM	O1D-CGD-CBD	-2.17	116.21	123.09
2	D	401	HEM	CHA-C4D-C3D	-2.17	121.23	125.23
2	C	401	HEM	CHD-C4C-NC	2.16	126.81	124.45
2	B	401	HEM	CHD-C1D-C2D	-2.16	121.62	125.03
2	C	401	HEM	C4C-NC-C1C	2.12	109.28	105.82
2	A	401	HEM	CHC-C4B-NB	2.09	126.67	124.42
2	D	401	HEM	C4C-CHD-C1D	-2.08	121.59	126.02
2	A	401	HEM	CHB-C1B-NB	2.08	126.94	124.37
2	C	401	HEM	CHB-C4A-NA	2.03	127.55	123.86
2	B	401	HEM	CHA-C1A-NA	2.02	127.52	123.86

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1AH8	N4-C12-N3-C9
3	A	402	A1AH8	N4-C12-N3-N2
3	B	402	A1AH8	N3-C12-N4-C13
3	B	402	A1AH8	N3-C12-N4-C15
3	C	402	A1AH8	N4-C12-N3-C9
3	C	402	A1AH8	N4-C12-N3-N2
3	D	402	A1AH8	N4-C12-N3-C9
3	D	402	A1AH8	N4-C12-N3-N2
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	C1-CA-CB-CG
4	D	403	ZIQ	O-C-CA-C1

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Mol	Chain	Res	Type	Atoms
4	A	403	ZIQ	N-CA-CB-CG
4	A	403	ZIQ	OXT-C-CA-CB
4	A	403	ZIQ	O-C-CA-C1
4	D	403	ZIQ	N-CA-CB-CG
4	C	403	ZIQ	O-C-CA-C1
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
3	C	402	A1AH8	C4-C5-C6-C7
2	B	401	HEM	CAA-CBA-CGA-O2A
2	A	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	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	C4C-C3C-CAC-CBC
3	C	402	A1AH8	C16-C5-C6-C7
3	D	402	A1AH8	C16-C5-C6-C7
4	C	403	ZIQ	OXT-C-CA-C1
3	C	402	A1AH8	C4-C5-C6-C11
4	C	403	ZIQ	C-CA-CB-CG

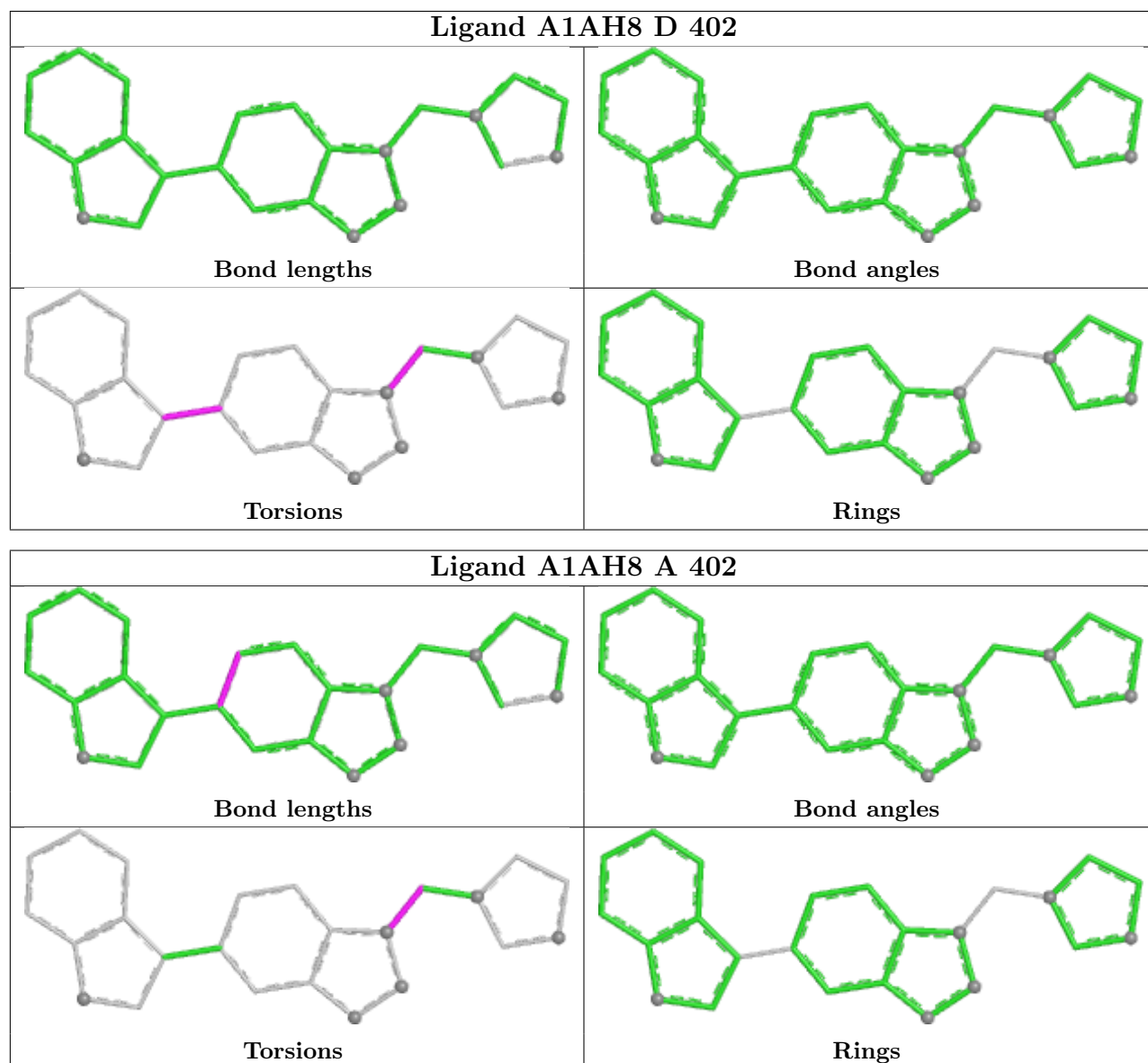
There are no ring outliers.

6 monomers are involved in 19 short contacts:

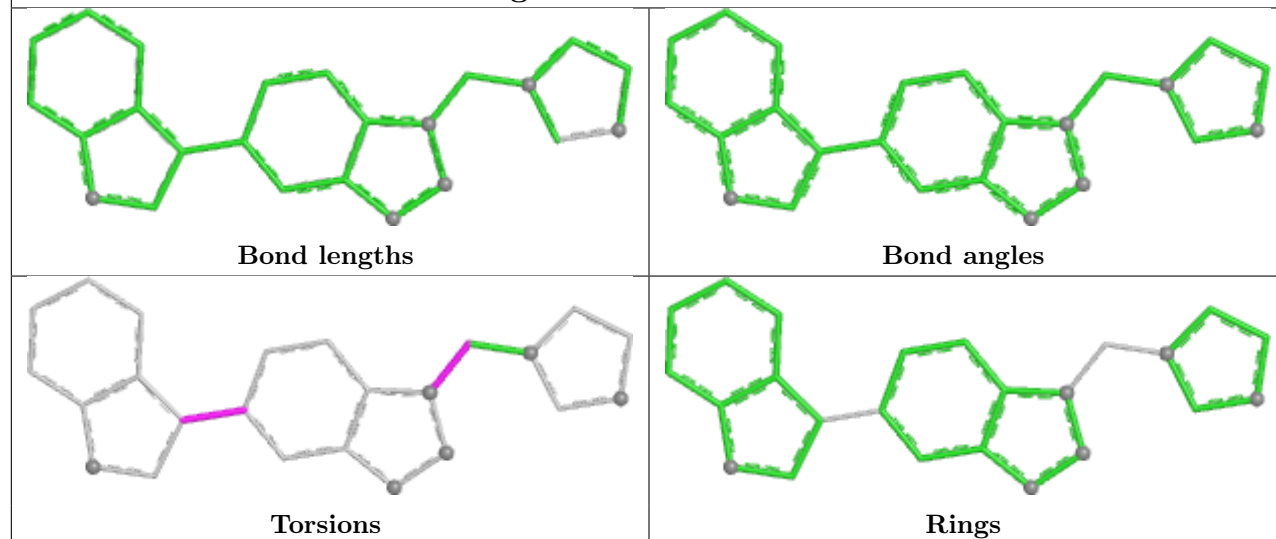
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	4	0
2	C	401	HEM	3	0
4	A	403	ZIQ	1	0
2	A	401	HEM	5	0
4	C	403	ZIQ	1	0
2	B	401	HEM	5	0

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

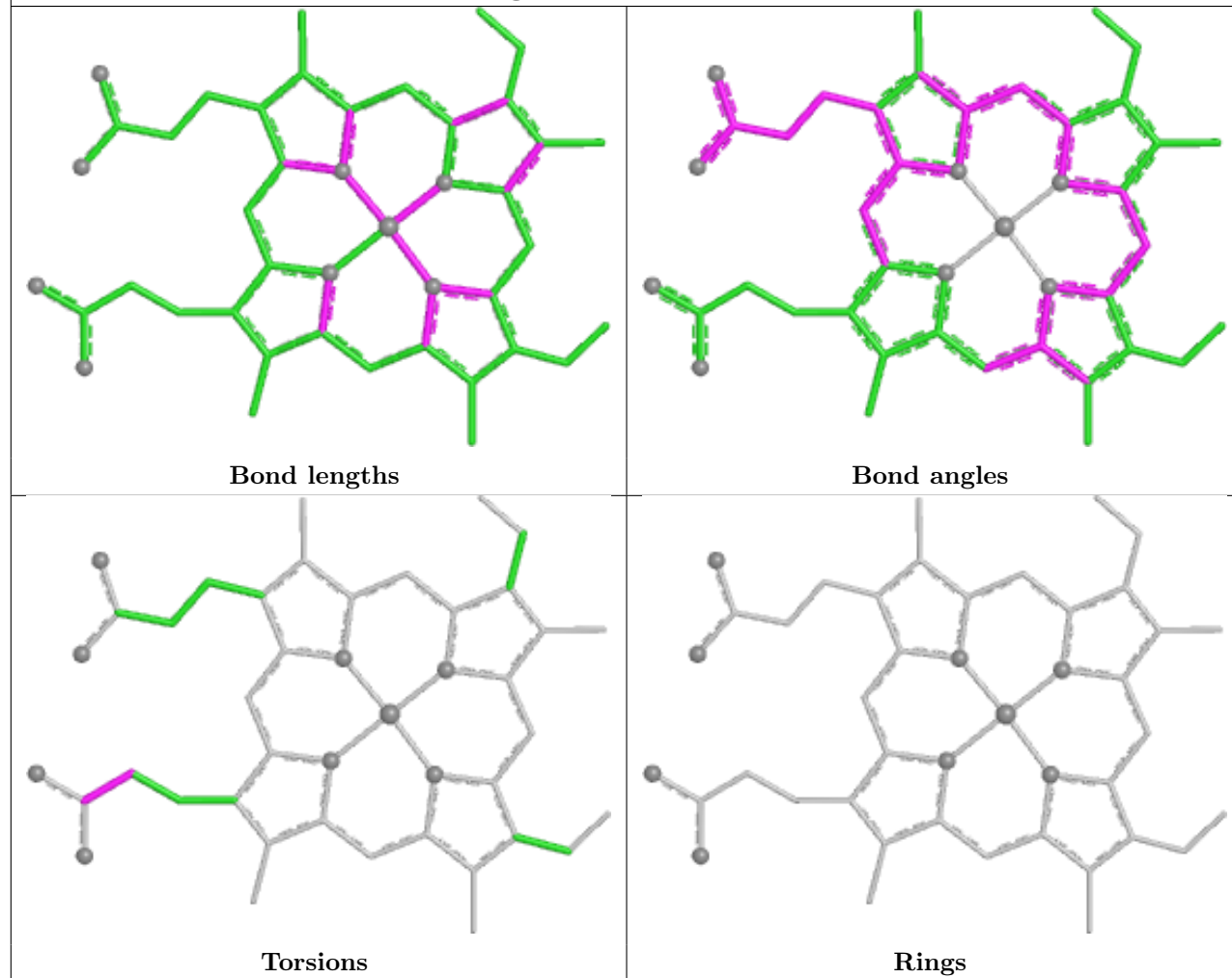
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



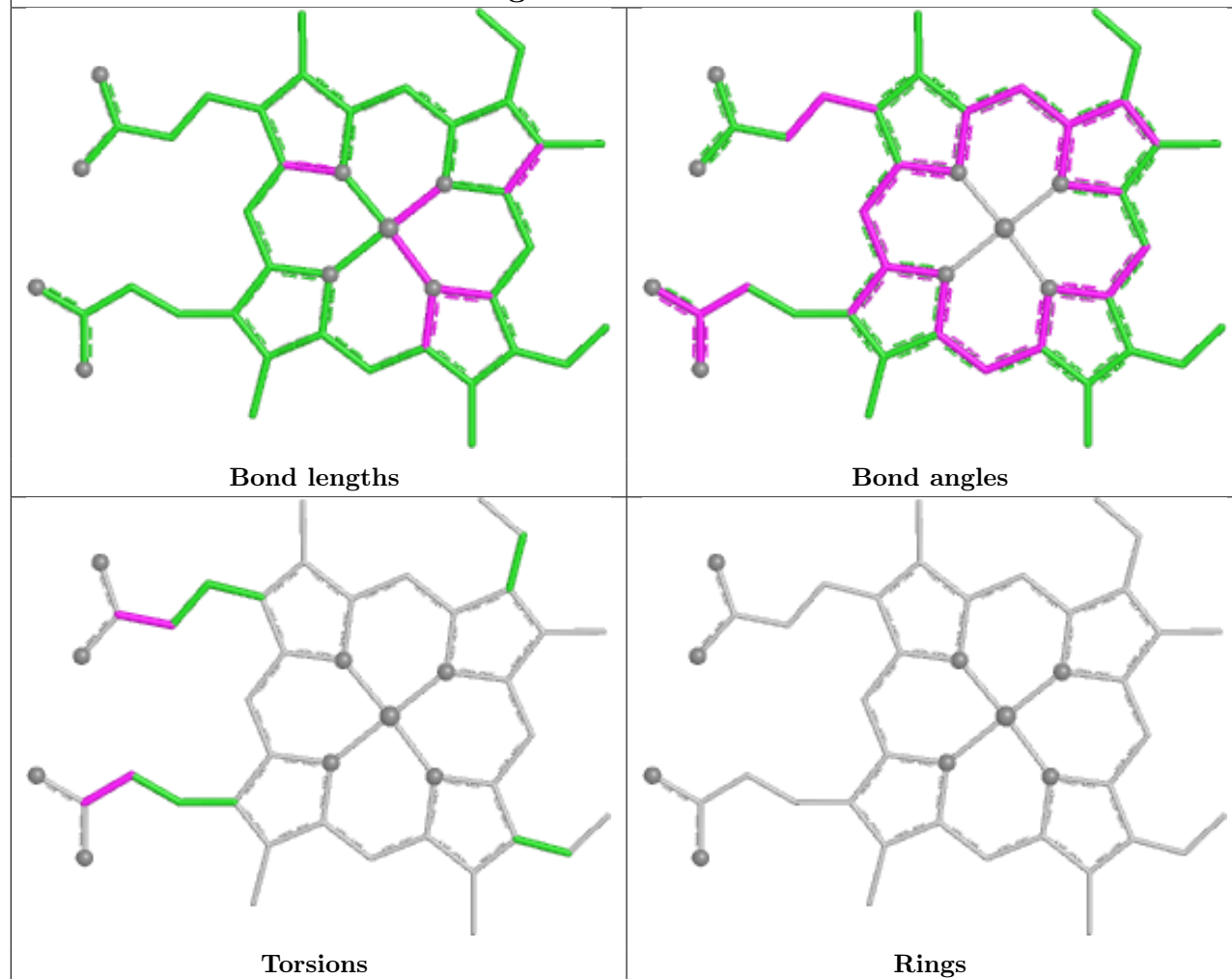
Ligand A1AH8 C 402



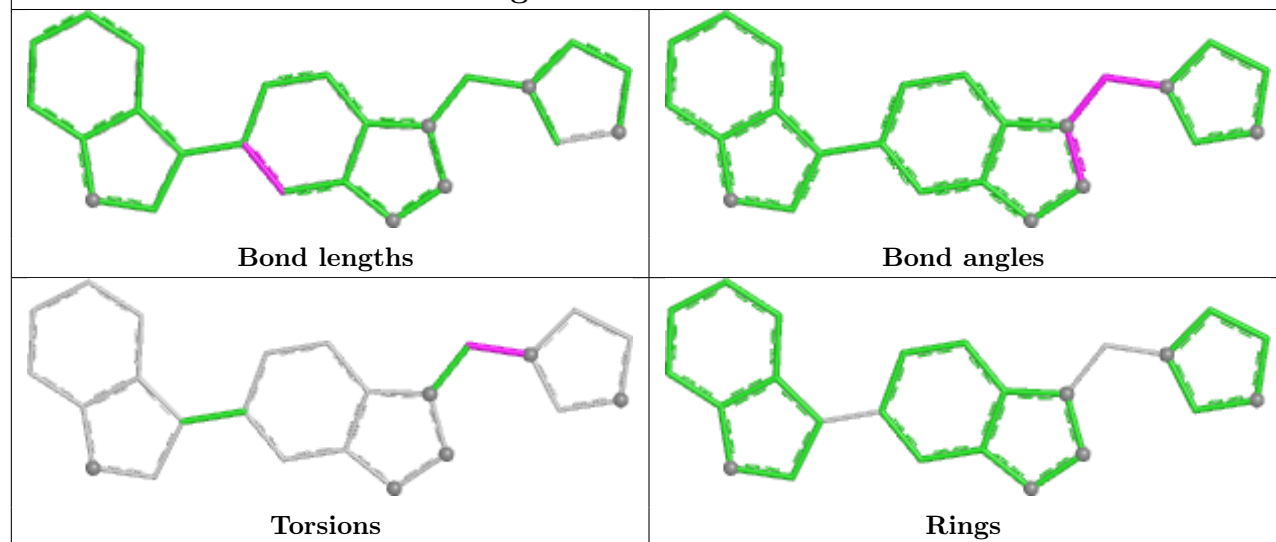
Ligand HEM D 401

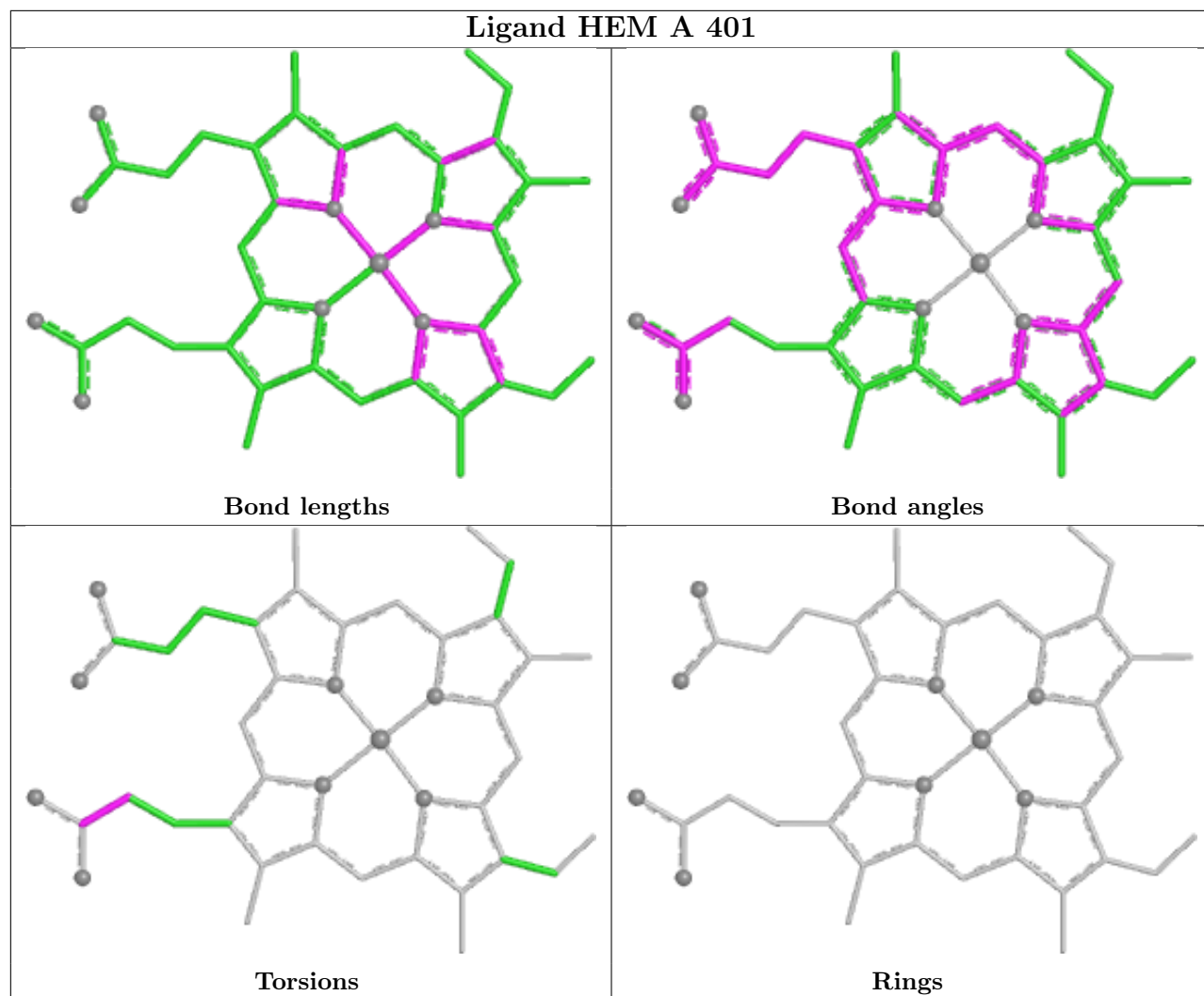


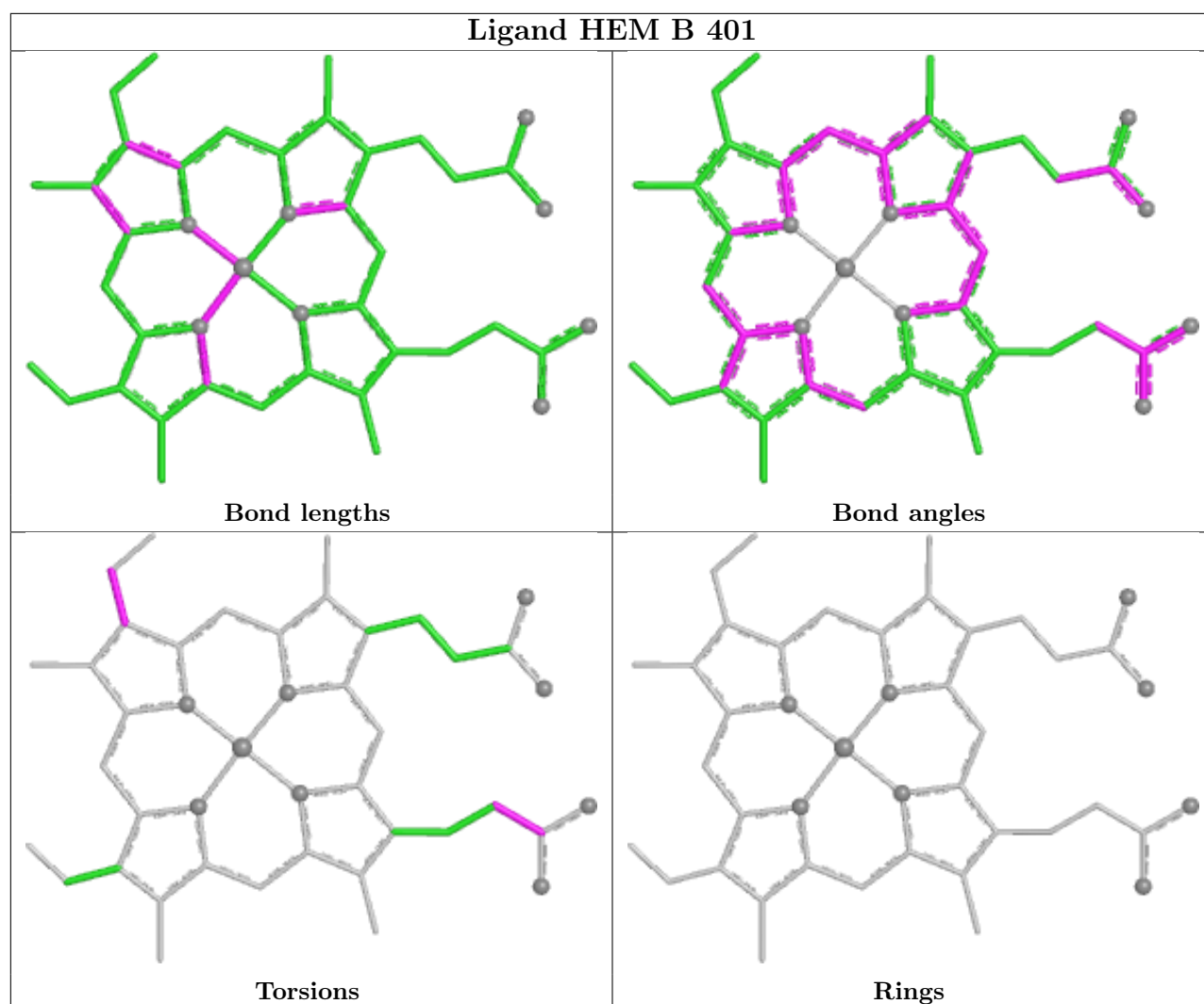
Ligand HEM C 401



Ligand A1AH8 B 402







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%)	-0.06	3 (0%) 81 78	28, 59, 119, 180	0
1	B	345/380 (90%)	0.07	11 (3%) 50 45	26, 64, 133, 181	0
1	C	331/380 (87%)	0.25	14 (4%) 40 35	37, 88, 167, 225	0
1	D	343/380 (90%)	0.02	8 (2%) 61 56	29, 67, 138, 209	0
All	All	1364/1520 (89%)	0.07	36 (2%) 57 52	26, 68, 143, 225	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	389	LEU	3.4
1	D	389	LEU	3.3
1	C	97	PHE	3.3
1	C	385	ILE	3.3
1	C	338	SER	3.1
1	B	171	MET	3.0
1	D	348	TYR	2.9
1	C	351	LEU	2.9
1	D	386	HIS	2.8
1	B	351	LEU	2.7
1	B	386	HIS	2.7
1	C	388	PHE	2.6
1	D	40	LEU	2.6
1	B	348	TYR	2.6
1	B	391	HIS	2.5
1	A	383	PRO	2.5
1	A	40	LEU	2.5
1	D	383	PRO	2.4
1	B	383	PRO	2.4
1	D	385	ILE	2.3
1	B	169	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	168	LEU	2.3
1	C	174	PRO	2.3
1	C	192	LEU	2.3
1	C	371	TYR	2.3
1	D	208	TRP	2.3
1	C	239	ILE	2.2
1	B	347	GLY	2.2
1	B	388	PHE	2.1
1	C	296	TYR	2.1
1	C	370	THR	2.1
1	C	333	HIS	2.1
1	C	337	GLY	2.1
1	A	371	TYR	2.1
1	B	329	VAL	2.0
1	D	296	TYR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	A1AH8	A	402	24/24	0.84	0.15	61,77,133,135	0
4	ZIQ	D	403	16/16	0.86	0.13	71,83,130,136	0
4	ZIQ	C	403	16/16	0.87	0.11	78,85,96,102	0
3	A1AH8	C	402	24/24	0.89	0.12	77,101,148,149	0
3	A1AH8	B	402	24/24	0.90	0.12	55,68,102,106	0
4	ZIQ	A	403	16/16	0.91	0.10	34,38,54,62	0
3	A1AH8	D	402	24/24	0.92	0.10	46,52,90,92	0
2	HEM	C	401	43/43	0.93	0.13	79,110,129,136	0

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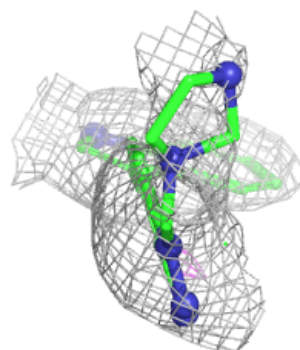
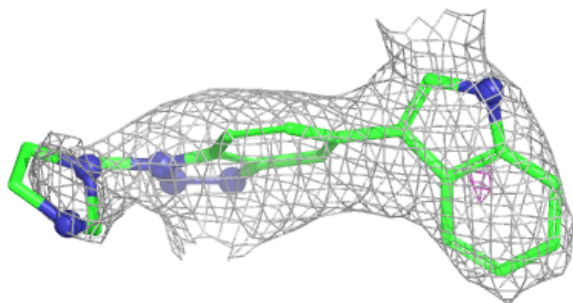
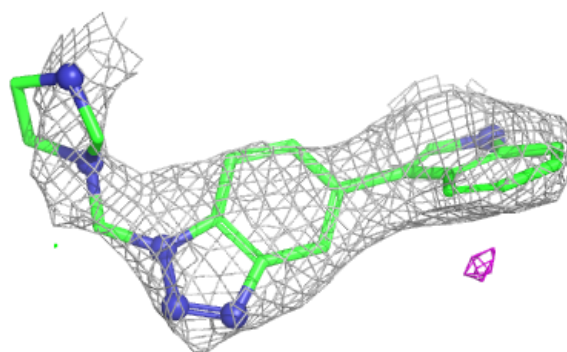
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	401	43/43	0.93	0.12	73,94,105,110	0
4	ZIQ	B	403	16/16	0.95	0.07	52,57,63,68	0
2	HEM	A	401	43/43	0.96	0.08	54,64,77,82	0
2	HEM	D	401	43/43	0.98	0.07	38,46,61,75	0

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.

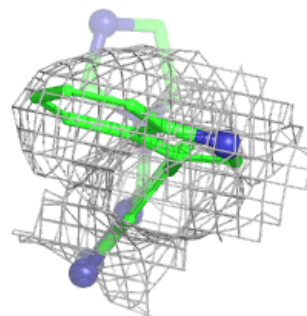
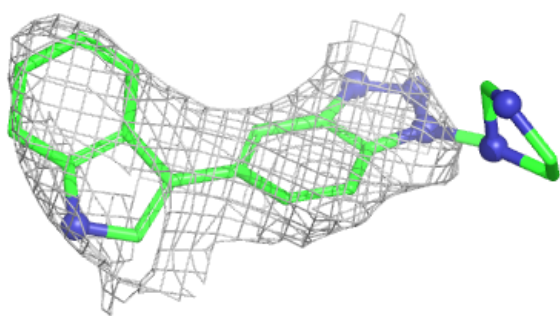
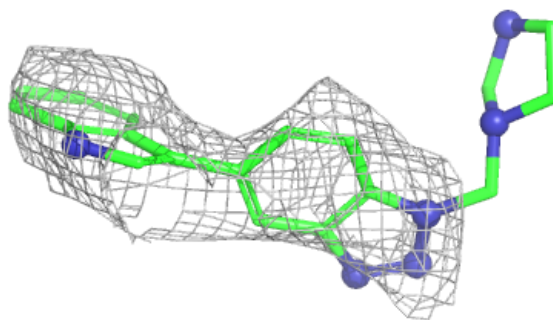
Electron density around A1AH8 A 402:

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

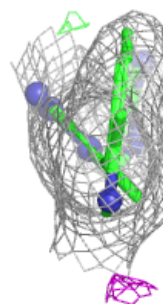
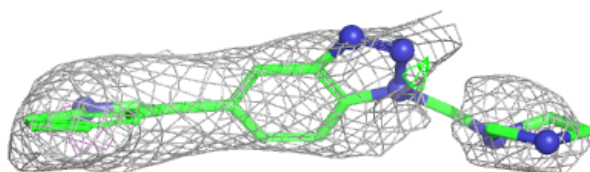
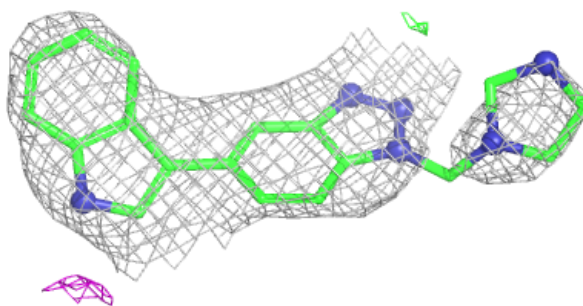


Electron density around A1AH8 C 402:

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

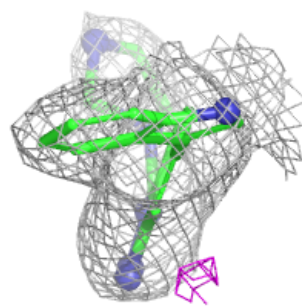
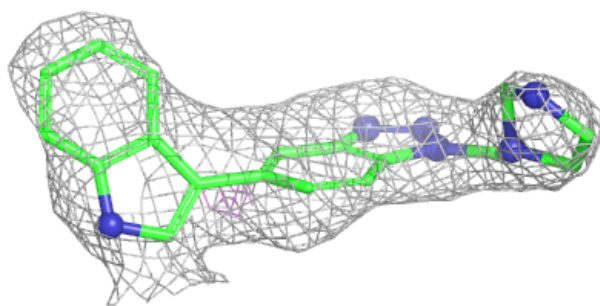
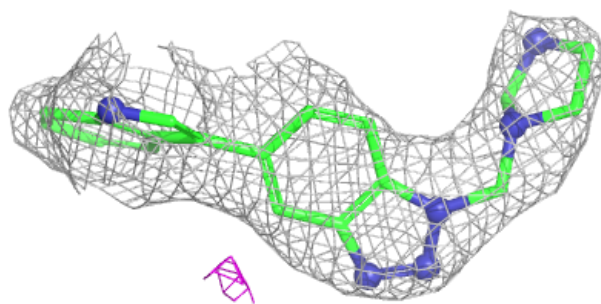
**Electron density around A1AH8 B 402:**

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



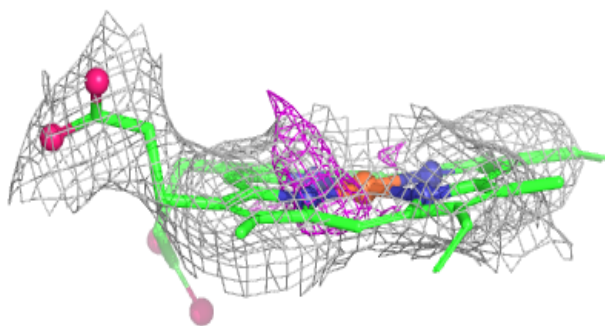
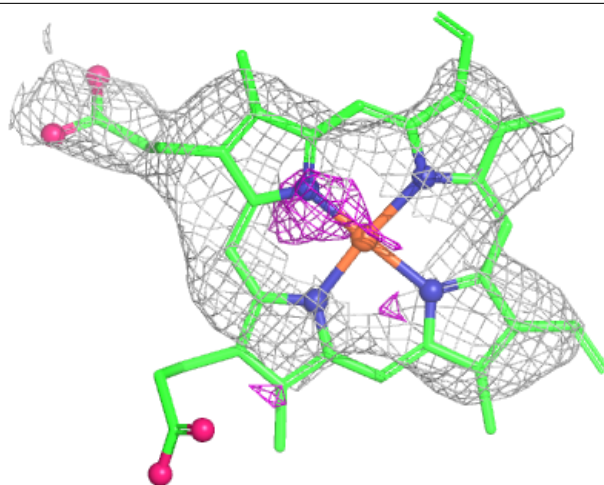
Electron density around A1AH8 D 402:

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



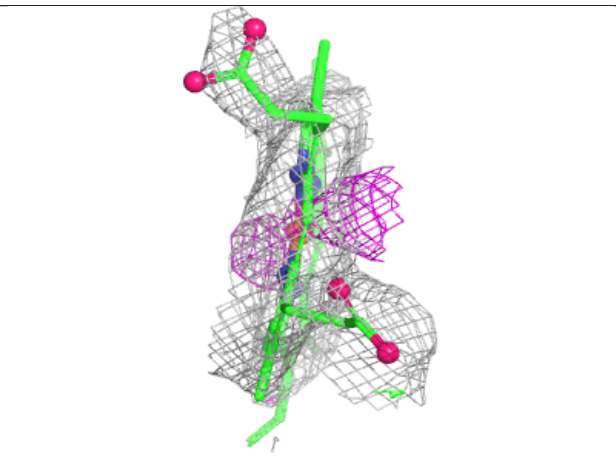
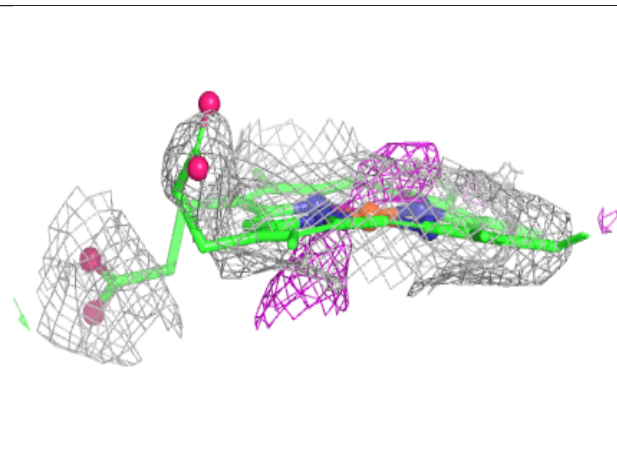
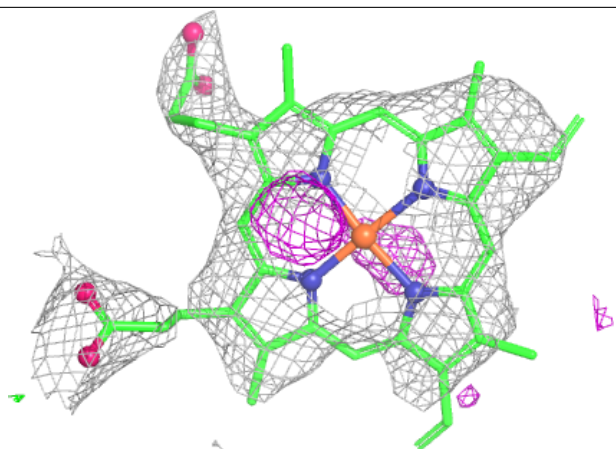
Electron density around HEM C 401:

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



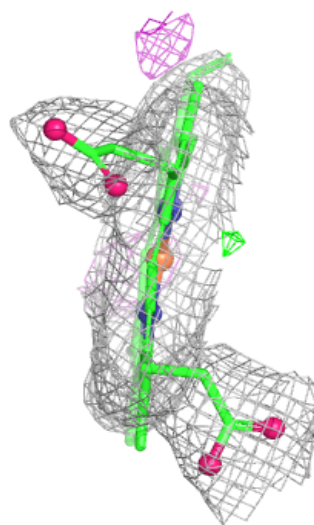
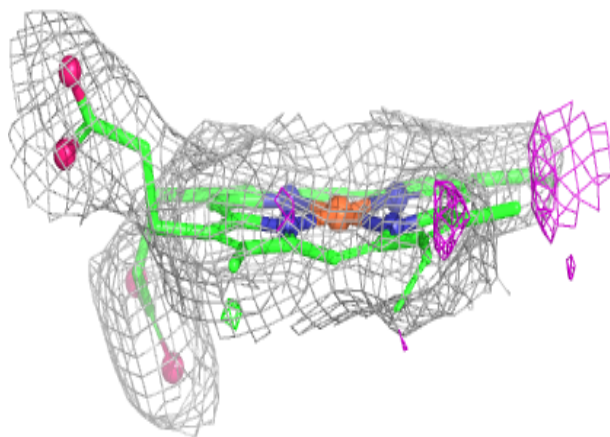
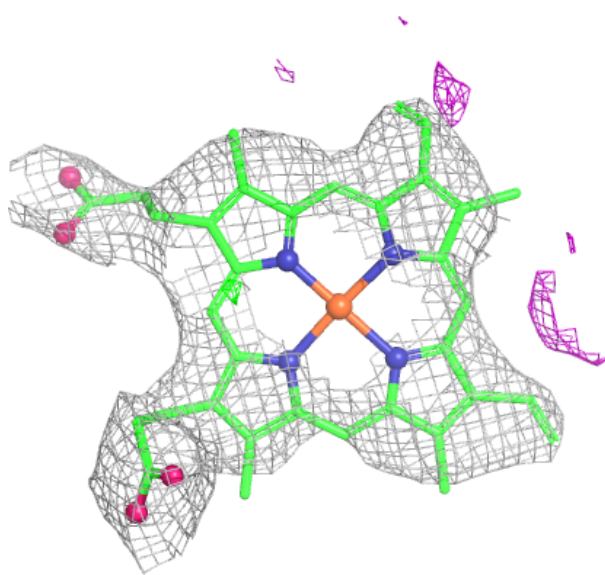
Electron density around HEM B 401:

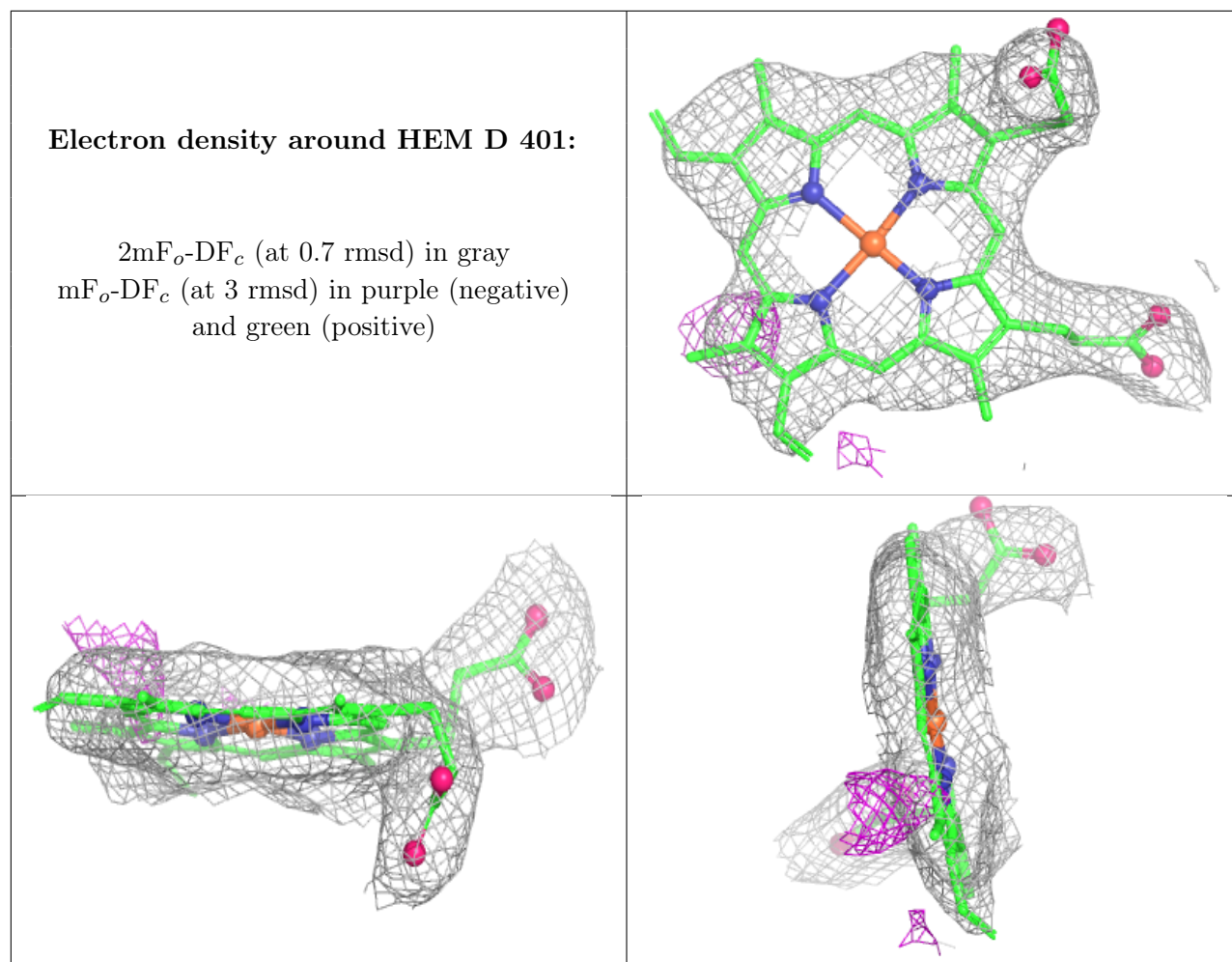
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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 ⓘ

There are no such residues in this entry.