



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:57 AM UTC

PDB ID : 8W1H / pdb_00008w1h
Title : Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PYN3 inhibitor
Authors : Geeraerts, Z.; Yeh, S.-R.
Deposited on : 2024-02-15
Resolution : 2.10 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

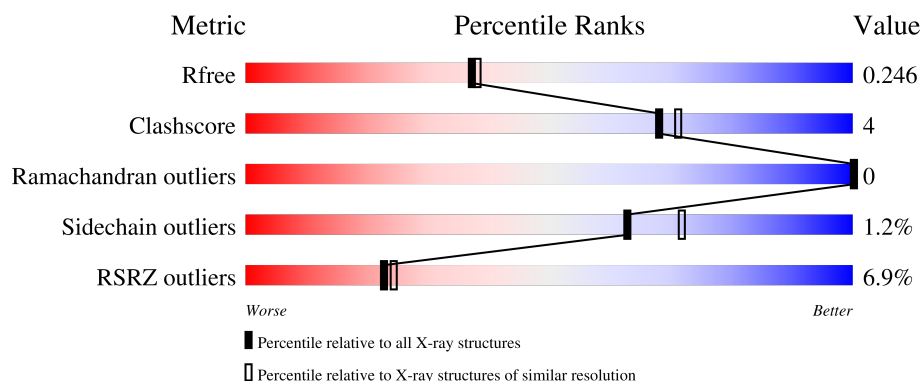
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	4% 83% 8% 9%
1	B	380	7% 82% 8% 10%
1	C	380	8% 78% 8% 12%
1	D	380	5% 82% 7% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12063 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	346	Total	C	N	O	S	0	0	0
			2941	1890	516	524	11			
1	B	343	Total	C	N	O	S	0	0	0
			2916	1877	509	519	11			
1	C	335	Total	C	N	O	S	0	0	0
			2848	1835	501	501	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

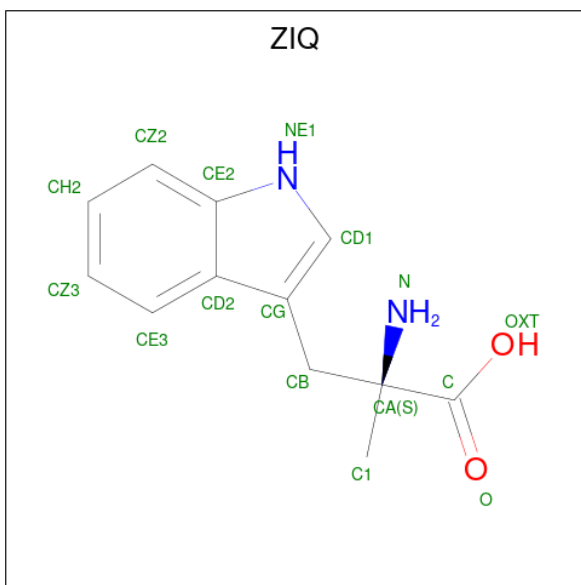
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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391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

- # HEM

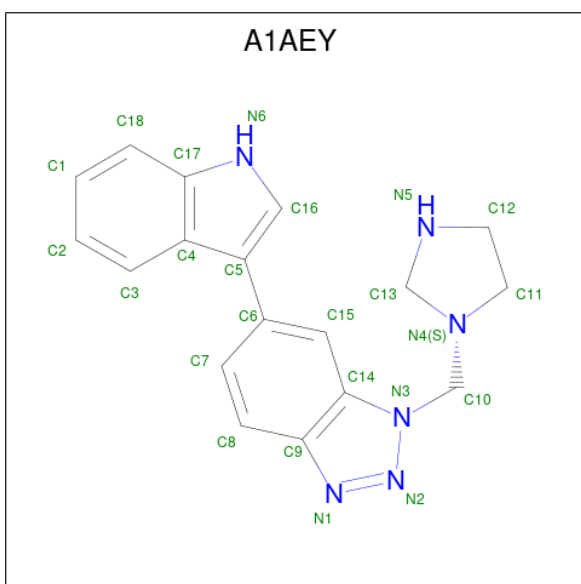
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



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

- Molecule 4 is (6M)-1-[(imidazolidin-1-yl)methyl]-6-(1H-indol-3-yl)-1H-benzotriazole (CCD ID: A1AEY) (formula: $C_{18}H_{18}N_6$) (labeled as "Ligand of Interest" by depositor).



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

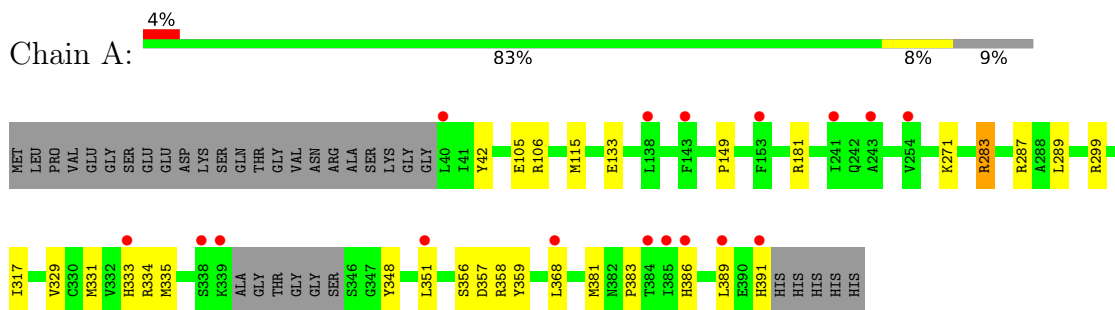
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total	O	0	0
			42	42		
5	B	35	Total	O	0	0
			35	35		
5	C	13	Total	O	0	0
			13	13		
5	D	23	Total	O	0	0
			23	23		

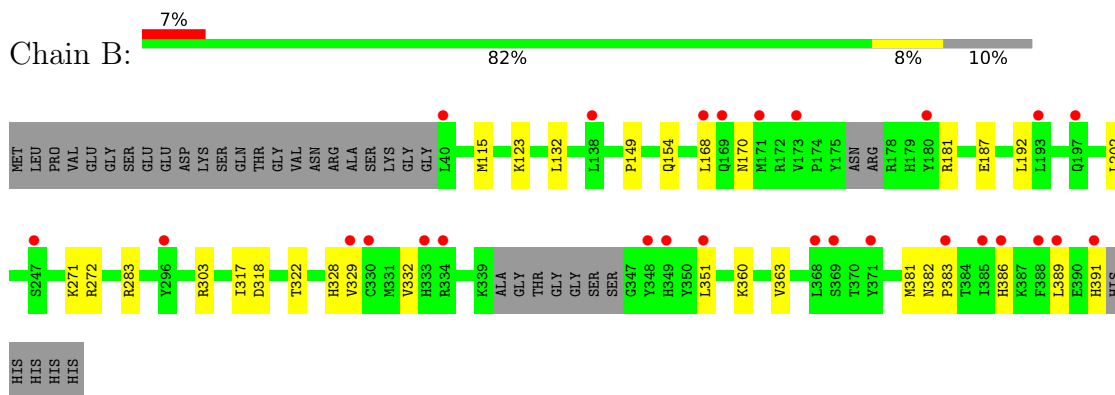
3 Residue-property plots [i](#)

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.

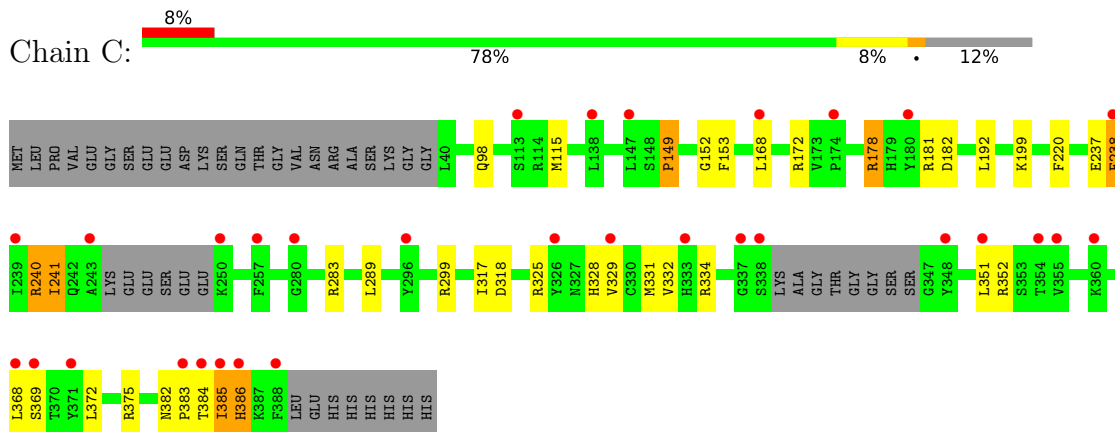
- Molecule 1: Tryptophan 2,3-dioxygenase



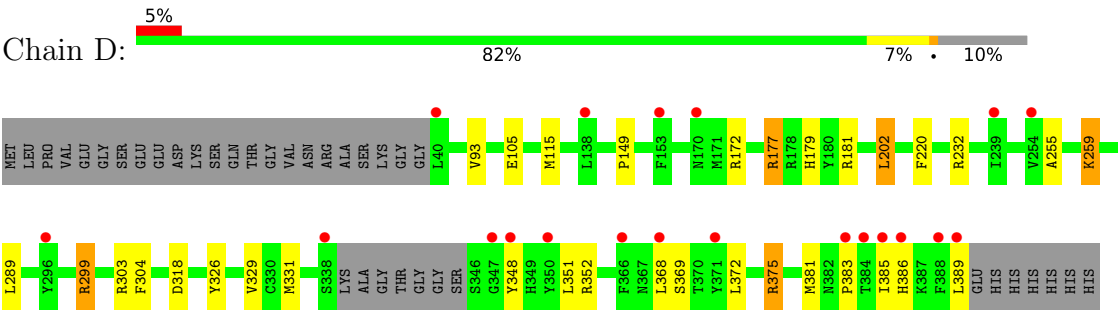
- Molecule 1: Tryptophan 2,3-dioxygenase



- 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	143.80Å 154.75Å 88.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.41 – 2.10 88.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (88.41-2.10) 99.8 (88.41-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.203 , 0.234 (Not available) , 0.246	Depositor DCC
R_{free} test set	5857 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12063	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: A1AEY, HEM, ZIQ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/3010	0.98	1/4050 (0.0%)
1	B	0.57	0/2984	0.99	1/4014 (0.0%)
1	C	0.54	0/2915	0.98	3/3923 (0.1%)
1	D	0.58	0/2981	0.99	3/4012 (0.1%)
All	All	0.57	0/11890	0.98	8/15999 (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	4
1	C	0	4
1	D	0	5
All	All	0	13

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	ARG	NE-CZ-NH2	8.73	127.06	119.20
1	B	318	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	318	ASP	CA-CB-CG	6.31	118.91	112.60
1	D	318	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	238	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	105	GLU	CB-CG-CD	5.44	121.84	112.60
1	D	105	GLU	CB-CG-CD	5.43	121.83	112.60
1	C	149	PRO	N-CA-CB	-5.07	97.02	102.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	287	ARG	Sidechain
1	A	299	ARG	Sidechain
1	C	172	ARG	Sidechain
1	C	178	ARG	Sidechain
1	C	240	ARG	Sidechain
1	C	334	ARG	Sidechain
1	D	172	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	232	ARG	Sidechain
1	D	299	ARG	Sidechain
1	D	375	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	2941	0	2927	18	0
1	B	2916	0	2902	22	0
1	C	2848	0	2842	28	0
1	D	2913	0	2901	18	0
2	A	43	0	30	0	0
2	B	43	0	30	3	0
2	C	43	0	30	6	0
2	D	43	0	30	2	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
4	A	24	0	0	0	0
4	B	24	0	0	0	0
4	C	24	0	0	0	0
4	D	24	0	0	0	0
5	A	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	35	0	0	0	0
5	C	13	0	0	0	0
5	D	23	0	0	0	0
All	All	12063	0	11692	84	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 (84) 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:348:TYR:O	1:D:352:ARG:HG3	1.72	0.89
1:D:93:VAL:HG21	1:D:115:MET:HE3	1.58	0.85
1:C:329:VAL:HG22	1:C:351:LEU:HB3	1.58	0.83
1:B:329:VAL:HG22	1:B:351:LEU:HB3	1.70	0.74
1:D:299:ARG:HH12	1:D:375:ARG:HH12	1.38	0.72
1:A:383:PRO:HA	1:A:386:HIS:HB3	1.73	0.70
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.21	0.70
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.23	0.69
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.26	0.65
1:D:381:MET:SD	1:D:389:LEU:HD12	2.39	0.63
1:A:381:MET:SD	1:A:389:LEU:HD12	2.42	0.58
1:C:299:ARG:HH22	1:C:375:ARG:HH22	1.51	0.58
1:C:178:ARG:HH11	1:C:182:ASP:HB3	1.69	0.58
1:D:329:VAL:HG22	1:D:351:LEU:HB3	1.85	0.57
1:A:283:ARG:HH21	1:A:283:ARG:HG3	1.70	0.57
1:C:220:PHE:CE1	1:C:385:ILE:HG13	2.41	0.55
1:B:383:PRO:HA	1:B:386:HIS:HB3	1.88	0.55
1:B:381:MET:SD	1:B:389:LEU:HD12	2.46	0.55
1:D:383:PRO:HA	1:D:386:HIS:HB3	1.88	0.55
1:C:237:GLU:O	1:C:241:ILE:HG12	2.08	0.54
1:D:202:LEU:C	1:D:202:LEU:HD13	2.33	0.54
1:C:329:VAL:HG22	1:C:351:LEU:CB	2.34	0.54
1:A:329:VAL:HG22	1:A:351:LEU:HB3	1.90	0.53
1:A:106:ARG:HD2	1:D:386:HIS:NE2	2.23	0.53
1:B:329:VAL:HG22	1:B:351:LEU:CB	2.38	0.51
1:C:152:GLY:HA3	2:C:401:HEM:C1D	2.45	0.51
1:B:272:ARG:HH21	1:B:272:ARG:HG2	1.76	0.51
1:D:303:ARG:HD3	1:D:389:LEU:HA	1.93	0.51
1:B:168:LEU:HB3	1:B:170:ASN:OD1	2.12	0.50
1:C:383:PRO:HA	1:C:386:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:PHE:CE2	1:D:389:LEU:HD13	2.46	0.50
1:C:98:GLN:OE1	1:C:199:LYS:HD3	2.13	0.49
1:B:383:PRO:HA	1:B:386:HIS:CB	2.42	0.49
1:A:383:PRO:CA	1:A:386:HIS:HB3	2.42	0.49
1:C:168:LEU:HG	1:C:283:ARG:NH2	2.28	0.49
1:B:303:ARG:HD3	1:B:389:LEU:HA	1.95	0.48
1:B:332:VAL:HG22	2:B:401:HEM:C1B	2.48	0.48
1:A:358:ARG:HG3	1:A:359:TYR:CD1	2.48	0.48
1:D:179:HIS:HE1	1:D:181:ARG:NH2	2.13	0.47
1:B:328:HIS:CE1	2:B:401:HEM:C4D	3.03	0.47
1:B:332:VAL:HG22	2:B:401:HEM:CHB	2.44	0.47
1:A:333:HIS:HB2	1:A:348:TYR:CE1	2.51	0.46
1:D:115:MET:HA	1:D:115:MET:HE2	1.98	0.45
1:C:328:HIS:CE1	2:C:401:HEM:C4D	3.05	0.45
1:A:283:ARG:NH1	1:A:357:ASP:O	2.50	0.45
1:B:382:ASN:N	1:B:382:ASN:OD1	2.50	0.45
1:D:289:LEU:HD11	1:D:368:LEU:HD21	1.98	0.45
1:C:332:VAL:HG22	2:C:401:HEM:C1B	2.53	0.44
1:A:331:MET:HE2	1:A:331:MET:HB2	1.87	0.44
1:A:356:SER:OG	1:A:358:ARG:HG2	2.17	0.44
1:B:181:ARG:HG2	1:B:192:LEU:HD13	1.99	0.44
1:C:331:MET:HE2	1:C:331:MET:HB2	1.91	0.44
1:D:220:PHE:HD1	1:D:385:ILE:HG12	1.81	0.44
1:C:352:ARG:HD3	1:C:352:ARG:HA	1.91	0.44
1:B:187:GLU:H	1:B:187:GLU:CD	2.26	0.44
1:A:42:TYR:CB	1:B:154:GLN:HB2	2.48	0.43
1:C:153:PHE:CD1	2:C:401:HEM:HAD2	2.52	0.43
1:C:240:ARG:HH22	1:C:241:ILE:HG23	1.83	0.43
1:D:331:MET:HE3	2:D:401:HEM:HAB	2.00	0.43
1:A:334:ARG:NH1	1:A:335:MET:HE2	2.33	0.43
1:B:272:ARG:HG2	1:B:272:ARG:NH2	2.34	0.43
1:C:369:SER:O	1:C:372:LEU:HG	2.19	0.43
1:A:133:GLU:HA	1:A:334:ARG:NH1	2.33	0.43
1:C:153:PHE:HD1	2:C:401:HEM:HAD2	1.83	0.42
1:C:220:PHE:CD1	1:C:385:ILE:HG13	2.54	0.42
1:A:106:ARG:HB2	1:A:106:ARG:HH21	1.85	0.42
1:B:322:THR:HG22	1:D:326:TYR:OH	2.19	0.42
1:C:289:LEU:HD11	1:C:368:LEU:HD21	2.02	0.42
1:C:181:ARG:HG2	1:C:192:LEU:HD13	2.01	0.42
1:B:115:MET:HE3	1:B:317:ILE:HD12	2.00	0.42
1:B:360:LYS:O	1:B:363:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:VAL:HG22	2:C:401:HEM:CHB	2.50	0.41
1:B:202:LEU:CD2	1:B:283:ARG:NH1	2.84	0.41
1:D:255:ALA:O	1:D:259:LYS:HG2	2.20	0.41
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.91	0.41
1:A:289:LEU:HD11	1:A:368:LEU:HD21	2.02	0.41
1:C:115:MET:HE3	1:C:317:ILE:HD12	2.00	0.41
1:C:240:ARG:HH12	1:C:241:ILE:HG23	1.85	0.41
1:C:325:ARG:O	1:C:329:VAL:HG23	2.19	0.41
1:D:369:SER:O	1:D:372:LEU:HG	2.21	0.41
1:B:132:LEU:HD12	1:B:132:LEU:HA	2.00	0.40
1:C:238:PHE:O	1:C:241:ILE:HG13	2.22	0.40
1:C:383:PRO:O	1:C:384:THR:C	2.65	0.40
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	2.03	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	342/380 (90%)	333 (97%)	9 (3%)	0	100	100
1	B	337/380 (89%)	331 (98%)	6 (2%)	0	100	100
1	C	329/380 (87%)	323 (98%)	6 (2%)	0	100	100
1	D	339/380 (89%)	329 (97%)	10 (3%)	0	100	100
All	All	1347/1520 (89%)	1316 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	323/348 (93%)	320 (99%)	3 (1%)	70	78
1	B	320/348 (92%)	316 (99%)	4 (1%)	61	69
1	C	312/348 (90%)	307 (98%)	5 (2%)	55	64
1	D	320/348 (92%)	317 (99%)	3 (1%)	70	78
All	All	1275/1392 (92%)	1260 (99%)	15 (1%)	63	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	271	LYS
1	A	391	HIS
1	B	123	LYS
1	B	149	PRO
1	B	271	LYS
1	B	391	HIS
1	C	149	PRO
1	C	241	ILE
1	C	382	ASN
1	C	385	ILE
1	C	386	HIS
1	D	149	PRO
1	D	202	LEU
1	D	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	309	GLN
1	A	376	HIS
1	B	183	ASN

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Mol	Chain	Res	Type
1	B	309	GLN
1	B	376	HIS
1	C	183	ASN
1	C	189	ASN
1	C	290	GLN
1	C	309	GLN
1	C	376	HIS
1	D	44	ASN
1	D	169	GLN
1	D	179	HIS
1	D	183	ASN
1	D	197	GLN
1	D	290	GLN
1	D	309	GLN

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
4	A1AEY	C	403	-	27,28,28	0.65	0	38,40,40	0.81	1 (2%)
2	HEM	A	401	1	50,50,50	1.55	8 (16%)	67,82,82	1.67	15 (22%)
4	A1AEY	A	403	-	27,28,28	0.82	1 (3%)	38,40,40	0.82	1 (2%)
4	A1AEY	D	403	-	27,28,28	0.75	1 (3%)	38,40,40	0.82	1 (2%)
2	HEM	B	401	1	50,50,50	1.49	6 (12%)	67,82,82	1.67	13 (19%)
3	ZIQ	B	402	-	14,17,17	0.62	0	20,25,25	0.96	1 (5%)
3	ZIQ	C	402	-	14,17,17	0.63	0	20,25,25	0.90	1 (5%)
4	A1AEY	B	403	-	27,28,28	0.73	1 (3%)	38,40,40	0.85	1 (2%)
3	ZIQ	A	402	-	14,17,17	0.61	0	20,25,25	1.19	1 (5%)
3	ZIQ	D	402	-	14,17,17	0.63	0	20,25,25	1.06	1 (5%)
2	HEM	C	401	1	50,50,50	1.58	7 (14%)	67,82,82	1.69	15 (22%)
2	HEM	D	401	1	50,50,50	1.63	12 (24%)	67,82,82	1.73	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
4	A1AEY	C	403	-	-	1/8/15/15	0/5/5/5
2	HEM	A	401	1	-	2/14/54/54	-
4	A1AEY	A	403	-	-	2/8/15/15	0/5/5/5
4	A1AEY	D	403	-	-	1/8/15/15	0/5/5/5
2	HEM	B	401	1	-	3/14/54/54	-
3	ZIQ	B	402	-	-	1/11/11/11	0/2/2/2
3	ZIQ	C	402	-	-	2/11/11/11	0/2/2/2
4	A1AEY	B	403	-	-	1/8/15/15	0/5/5/5
3	ZIQ	A	402	-	-	4/11/11/11	0/2/2/2
3	ZIQ	D	402	-	-	4/11/11/11	0/2/2/2
2	HEM	C	401	1	-	3/14/54/54	-
2	HEM	D	401	1	-	2/14/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	FE-NB	5.32	2.11	1.94
2	A	401	HEM	FE-NB	5.27	2.11	1.94
2	B	401	HEM	FE-NB	4.82	2.09	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEM	FE-NB	4.46	2.08	1.94
2	C	401	HEM	FE-NC	4.09	2.08	1.95
2	B	401	HEM	FE-NC	3.92	2.08	1.95
2	B	401	HEM	C1B-NB	-3.63	1.34	1.40
2	D	401	HEM	C4B-NB	-3.57	1.31	1.38
2	D	401	HEM	C1B-NB	-3.48	1.34	1.40
2	C	401	HEM	C1B-NB	-3.48	1.34	1.40
2	D	401	HEM	FE-NC	3.48	2.06	1.95
2	A	401	HEM	C1B-NB	-3.45	1.34	1.40
2	A	401	HEM	C1D-ND	-3.34	1.32	1.38
2	C	401	HEM	C4D-ND	-3.03	1.35	1.40
2	A	401	HEM	FE-NC	2.91	2.04	1.95
2	C	401	HEM	C4B-NB	-2.83	1.33	1.38
2	C	401	HEM	C1C-C2C	-2.80	1.39	1.45
4	A	403	A1AEY	C15-C6	-2.70	1.35	1.39
2	A	401	HEM	C1C-C2C	-2.66	1.40	1.45
2	D	401	HEM	FE-NA	2.65	2.03	1.95
2	D	401	HEM	C1C-C2C	-2.65	1.40	1.45
2	A	401	HEM	C4B-NB	-2.63	1.33	1.38
2	A	401	HEM	C4D-ND	-2.63	1.35	1.40
2	B	401	HEM	C4D-ND	-2.57	1.35	1.40
2	B	401	HEM	C1C-C2C	-2.57	1.40	1.45
4	D	403	A1AEY	C15-C6	-2.36	1.36	1.39
2	C	401	HEM	C3C-C4C	-2.33	1.42	1.46
2	D	401	HEM	C4A-NA	-2.31	1.35	1.39
2	D	401	HEM	O2D-CGD	-2.29	1.23	1.30
2	B	401	HEM	C4B-NB	-2.27	1.34	1.38
2	D	401	HEM	C4D-ND	-2.14	1.36	1.40
4	B	403	A1AEY	C15-C6	-2.10	1.36	1.39
2	D	401	HEM	C1C-NC	-2.09	1.35	1.39
2	A	401	HEM	C3C-C4C	-2.09	1.42	1.46
2	D	401	HEM	C1D-ND	-2.08	1.34	1.38
2	D	401	HEM	O1D-CGD	2.04	1.28	1.22

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CHC-C4B-NB	4.73	129.51	124.42
2	C	401	HEM	CHC-C4B-NB	4.71	129.49	124.42
2	B	401	HEM	CHC-C4B-NB	4.51	129.28	124.42
2	A	401	HEM	CHC-C4B-NB	4.37	129.12	124.42
2	B	401	HEM	C1B-NB-C4B	4.18	110.16	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	HEM	CHD-C1D-ND	4.15	128.88	124.42
2	D	401	HEM	C1B-NB-C4B	4.10	110.06	105.21
2	D	401	HEM	CHA-C4D-ND	4.03	129.36	124.37
3	D	402	ZIQ	O-C-CA	-3.85	115.88	122.78
2	A	401	HEM	CHA-C4D-ND	3.83	129.10	124.37
2	D	401	HEM	CHB-C1B-NB	3.79	129.06	124.37
2	C	401	HEM	C1B-NB-C4B	3.75	109.64	105.21
3	A	402	ZIQ	O-C-CA	-3.73	116.09	122.78
2	A	401	HEM	CHD-C4C-NC	3.68	128.46	124.45
2	A	401	HEM	C1B-NB-C4B	3.66	109.54	105.21
2	B	401	HEM	CHD-C1D-ND	3.64	128.34	124.42
2	D	401	HEM	CHD-C1D-ND	3.52	128.22	124.42
2	D	401	HEM	CBD-CAD-C3D	-3.50	102.86	112.53
2	B	401	HEM	CHA-C4D-ND	3.33	128.49	124.37
2	A	401	HEM	CHD-C1D-ND	3.33	128.01	124.42
2	C	401	HEM	CBD-CAD-C3D	-3.33	103.33	112.53
2	B	401	HEM	CBD-CAD-C3D	-3.29	103.44	112.53
2	A	401	HEM	CBD-CAD-C3D	-3.19	103.71	112.53
3	B	402	ZIQ	O-C-CA	-3.18	117.08	122.78
2	D	401	HEM	CHD-C4C-NC	3.16	127.89	124.45
2	C	401	HEM	CHA-C4D-ND	3.14	128.26	124.37
2	B	401	HEM	CHB-C1B-NB	3.14	128.25	124.37
4	C	403	A1AEY	C15-C14-N3	3.11	134.68	131.30
2	C	401	HEM	CHB-C1B-NB	3.11	128.21	124.37
2	B	401	HEM	CHD-C4C-NC	3.03	127.76	124.45
2	A	401	HEM	CHB-C1B-NB	2.97	128.04	124.37
2	D	401	HEM	C4C-NC-C1C	2.91	110.57	105.82
3	C	402	ZIQ	O-C-CA	-2.84	117.69	122.78
4	B	403	A1AEY	C15-C14-N3	2.82	134.36	131.30
2	C	401	HEM	CHD-C4C-NC	2.78	127.48	124.45
4	D	403	A1AEY	C15-C14-N3	2.71	134.24	131.30
4	A	403	A1AEY	C15-C14-N3	2.60	134.13	131.30
2	A	401	HEM	C4C-NC-C1C	2.52	109.94	105.82
2	B	401	HEM	CHD-C1D-C2D	-2.46	121.14	125.03
2	D	401	HEM	C3B-C4B-NB	-2.46	107.70	109.47
2	B	401	HEM	C3B-C4B-NB	-2.46	107.70	109.47
2	D	401	HEM	CMD-C2D-C1D	2.44	128.85	125.03
2	C	401	HEM	CHD-C1D-C2D	-2.31	121.38	125.03
2	C	401	HEM	C4D-ND-C1D	2.30	107.93	105.21
2	A	401	HEM	O2A-CGA-CBA	2.30	121.27	114.00
2	C	401	HEM	C4C-NC-C1C	2.26	109.51	105.82
2	C	401	HEM	CAC-C3C-C4C	2.24	130.17	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CAC-C3C-C4C	2.23	130.14	124.82
2	B	401	HEM	O2A-CGA-CBA	2.18	120.90	114.00
2	B	401	HEM	O2A-CGA-O1A	-2.16	117.78	123.33
2	B	401	HEM	C4C-NC-C1C	2.16	109.34	105.82
2	D	401	HEM	CHA-C4D-C3D	-2.16	121.25	125.23
2	C	401	HEM	C2A-C1A-NA	-2.15	107.76	110.15
2	A	401	HEM	CHD-C1D-C2D	-2.15	121.63	125.03
2	A	401	HEM	C4D-ND-C1D	2.14	107.74	105.21
2	C	401	HEM	CAC-C3C-C2C	-2.12	121.53	128.43
2	A	401	HEM	C3B-C4B-NB	-2.12	107.95	109.47
2	D	401	HEM	CHD-C1D-C2D	-2.11	121.69	125.03
2	C	401	HEM	C1A-CHA-C4D	-2.10	121.31	126.25
2	C	401	HEM	C4B-C3B-C2B	-2.09	105.36	107.28
2	B	401	HEM	CAC-C3C-C4C	2.08	129.80	124.82
2	A	401	HEM	CAC-C3C-C4C	2.08	129.79	124.82
2	A	401	HEM	CHA-C4D-C3D	-2.08	121.39	125.23
2	A	401	HEM	O2A-CGA-O1A	-2.07	118.01	123.33
2	D	401	HEM	CAD-C3D-C4D	2.06	128.28	124.70
2	D	401	HEM	CHB-C1B-C2B	-2.00	121.26	126.95

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	ZIQ	OXT-C-CA-C1
3	D	402	ZIQ	OXT-C-CA-C1
4	A	403	A1AEY	N3-C10-N4-C11
4	B	403	A1AEY	N3-C10-N4-C11
3	A	402	ZIQ	O-C-CA-C1
4	C	403	A1AEY	N3-C10-N4-C11
4	D	403	A1AEY	N3-C10-N4-C11
3	D	402	ZIQ	O-C-CA-C1
3	A	402	ZIQ	OXT-C-CA-CB
2	B	401	HEM	C2C-C3C-CAC-CBC
2	C	401	HEM	C2C-C3C-CAC-CBC
4	A	403	A1AEY	N3-C10-N4-C13
3	A	402	ZIQ	O-C-CA-CB
3	D	402	ZIQ	O-C-CA-CB
3	D	402	ZIQ	OXT-C-CA-CB
2	D	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A

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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	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
3	B	402	ZIQ	O-C-CA-C1
3	C	402	ZIQ	O-C-CA-C1
3	C	402	ZIQ	OXT-C-CA-C1

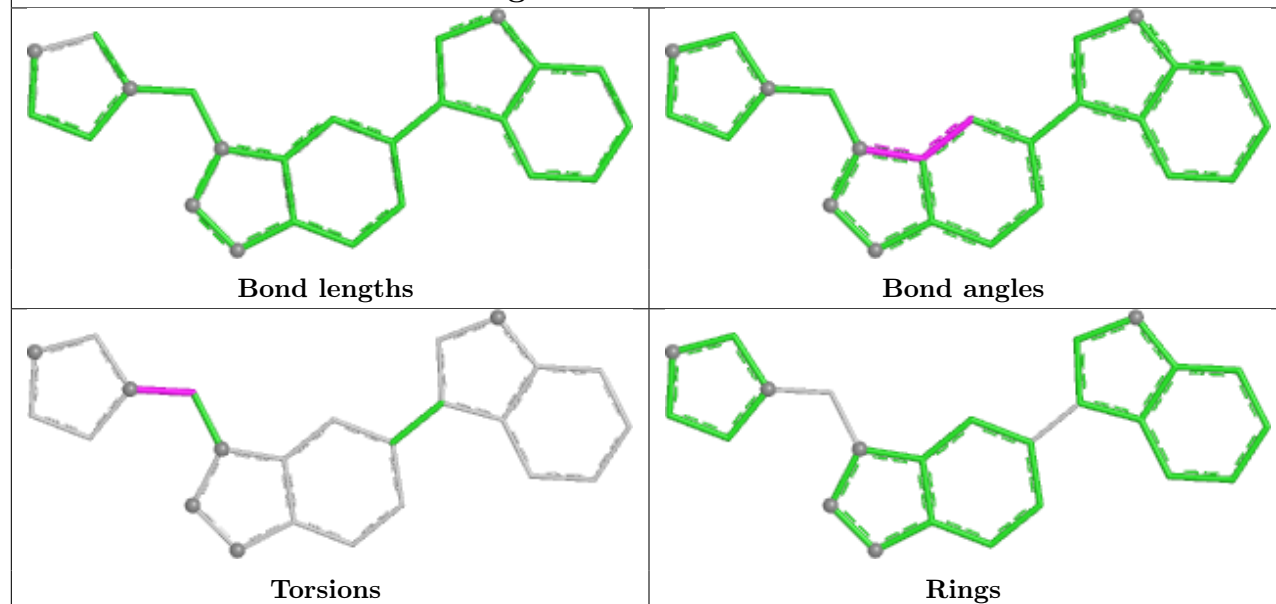
There are no ring outliers.

3 monomers are involved in 11 short contacts:

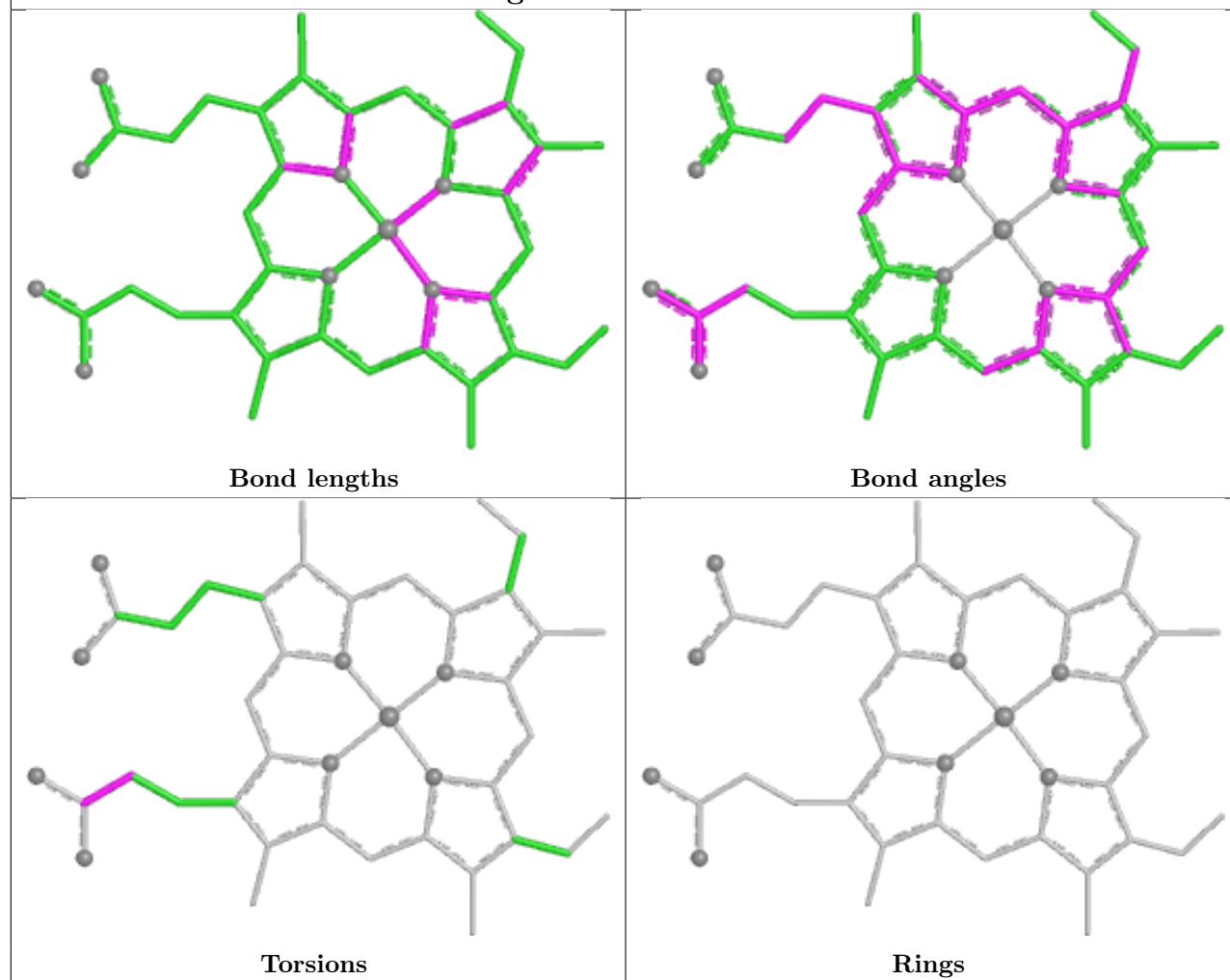
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	3	0
2	C	401	HEM	6	0
2	D	401	HEM	2	0

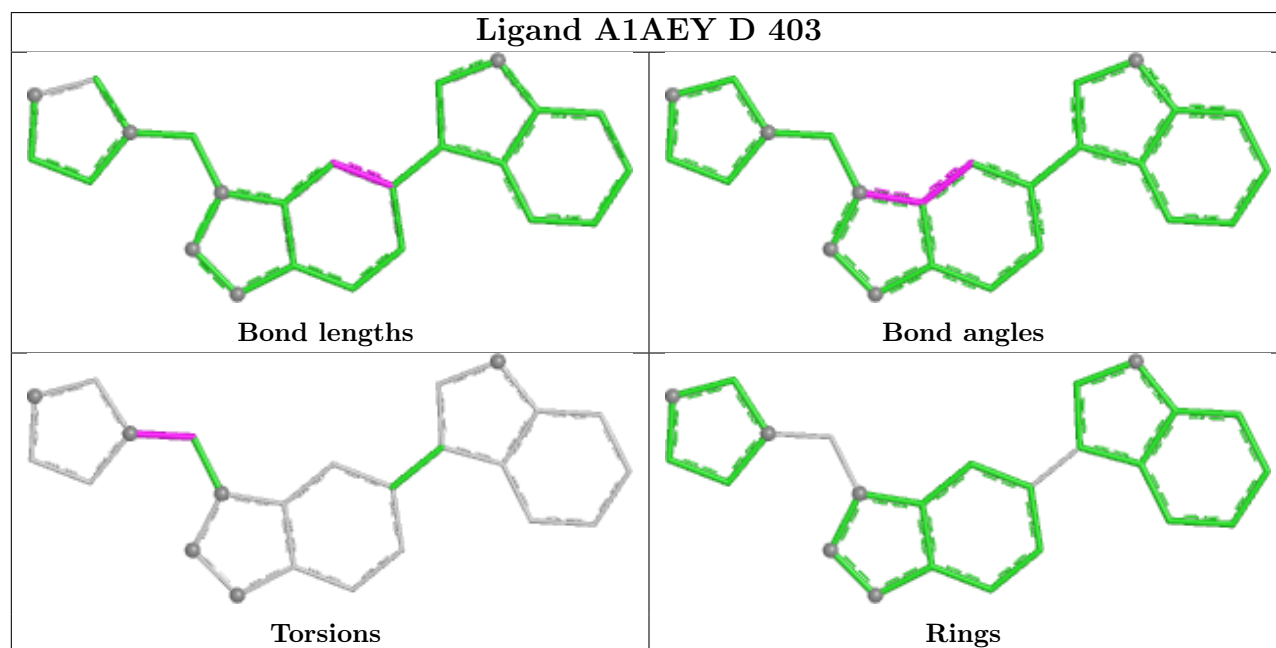
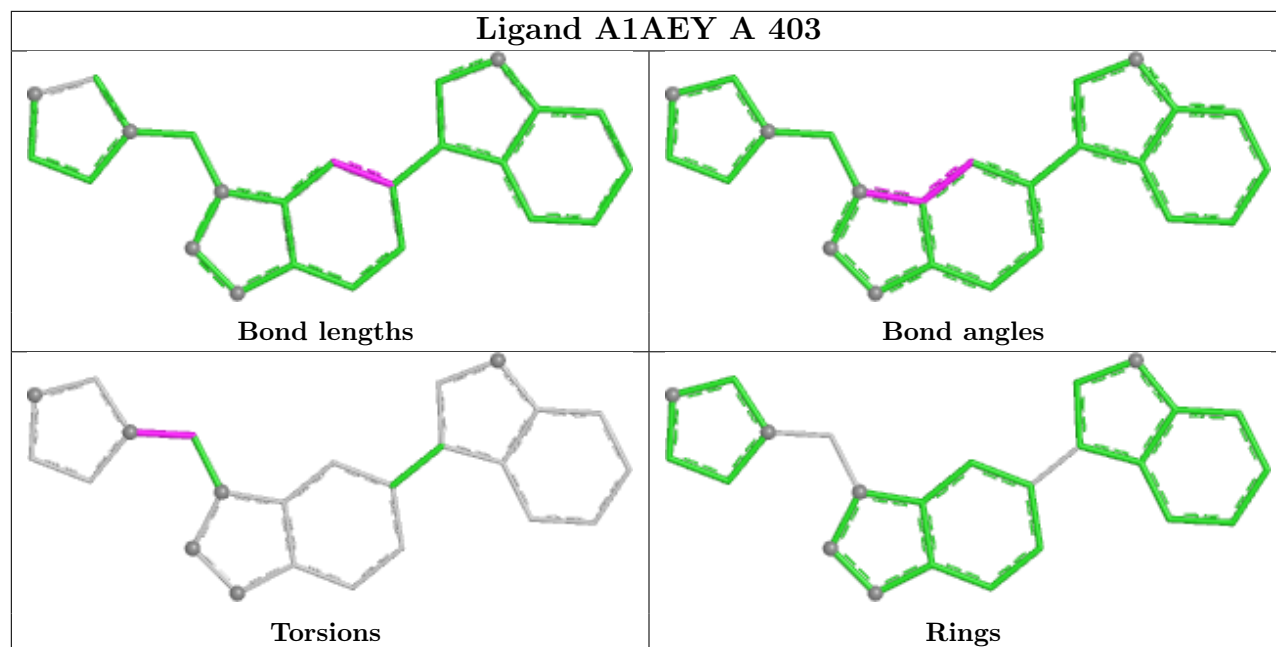
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

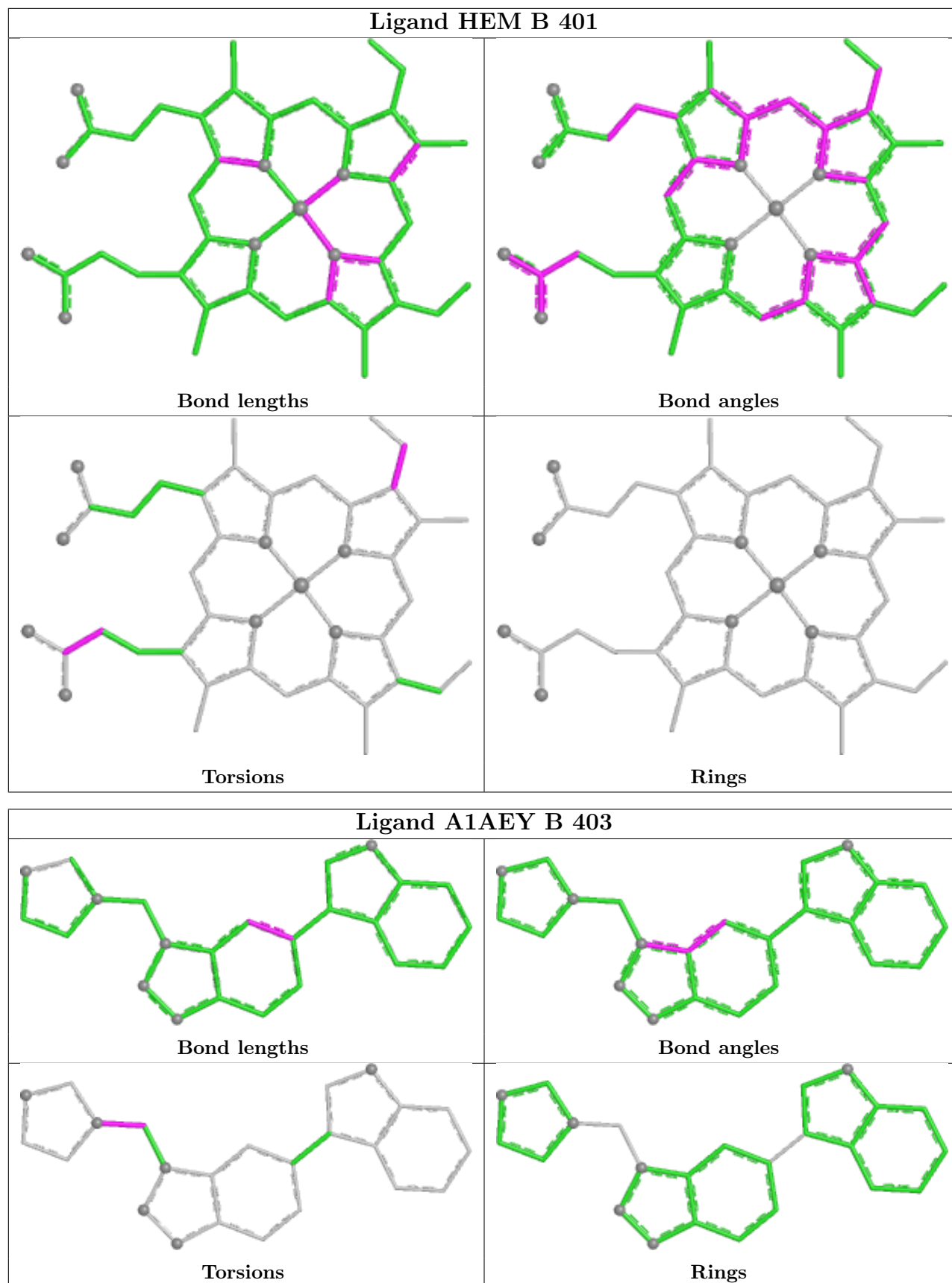
Ligand A1AEY C 403

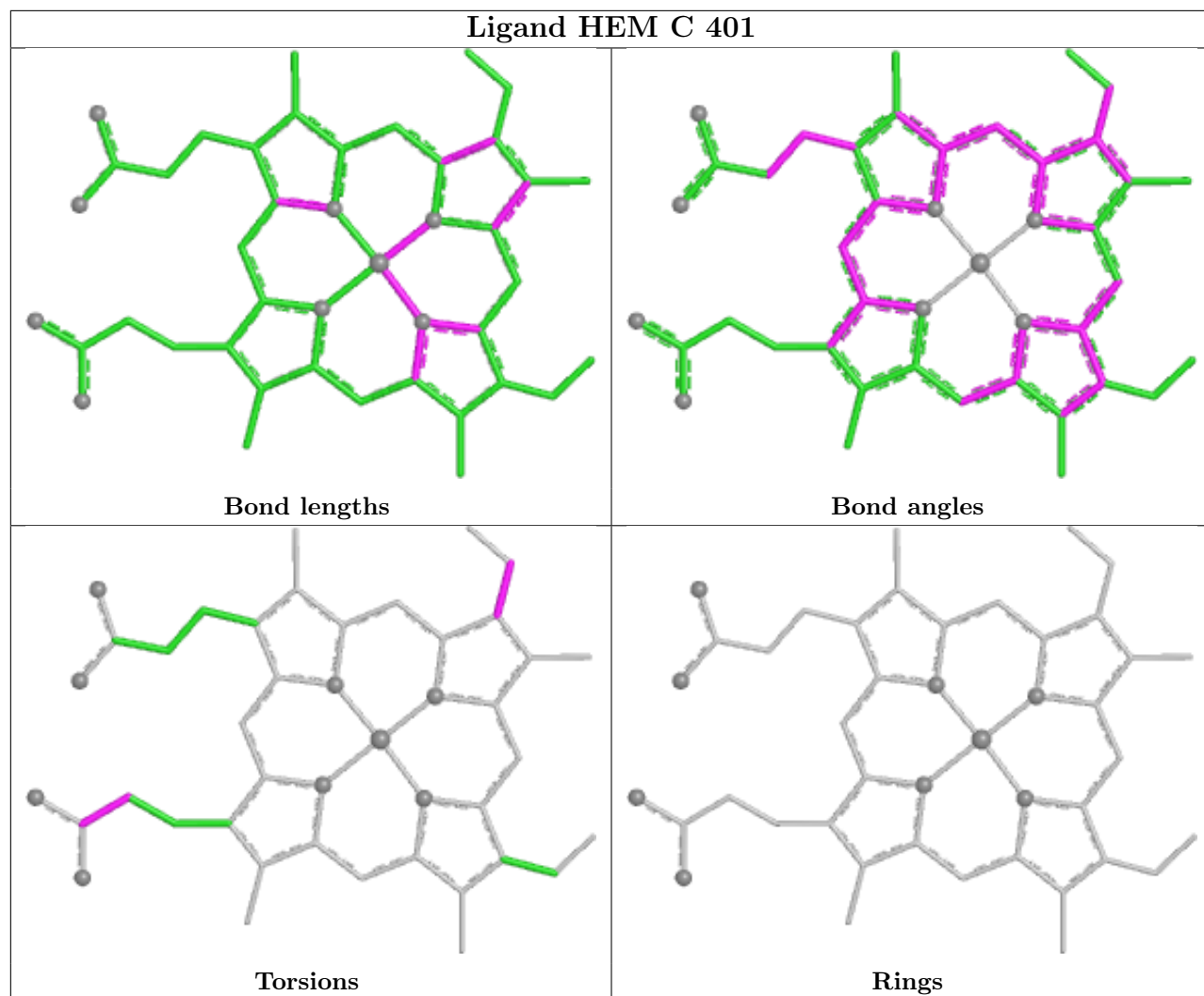


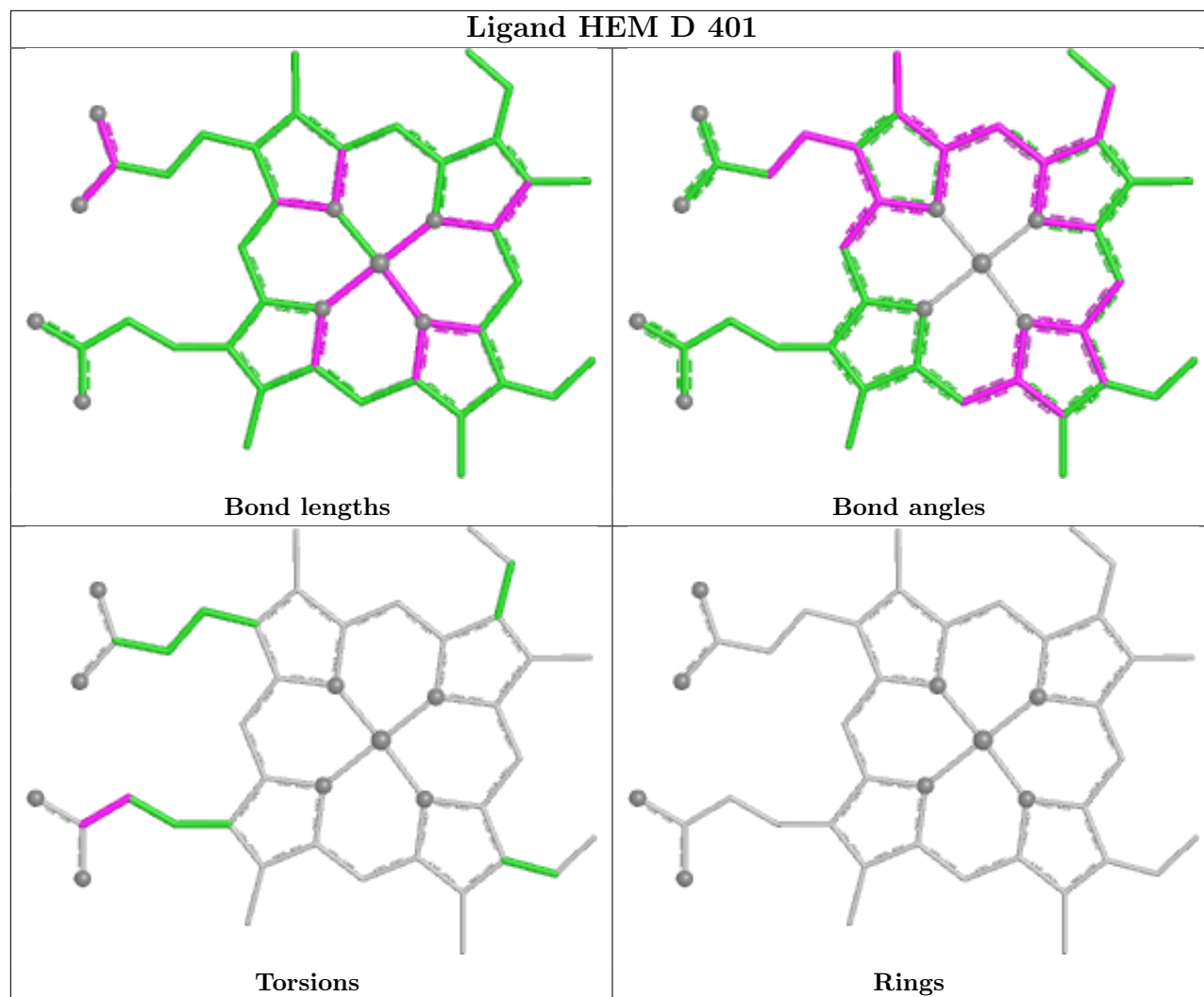
Ligand HEM A 401











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	346/380 (91%)	0.45	17 (4%) 35 37	46, 69, 125, 176	0
1	B	343/380 (90%)	0.56	27 (7%) 18 20	48, 72, 129, 174	0
1	C	335/380 (88%)	0.76	31 (9%) 14 15	54, 94, 183, 246	0
1	D	343/380 (90%)	0.46	20 (5%) 29 30	49, 74, 141, 204	0
All	All	1367/1520 (89%)	0.56	95 (6%) 23 24	46, 76, 149, 246	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	385	ILE	5.2
1	A	138	LEU	4.2
1	A	385	ILE	4.1
1	D	386	HIS	4.0
1	C	385	ILE	3.9
1	D	239	ILE	3.9
1	A	40	LEU	3.7
1	C	326	TYR	3.6
1	D	383	PRO	3.5
1	B	351	LEU	3.5
1	B	296	TYR	3.5
1	B	348	TYR	3.5
1	B	385	ILE	3.4
1	D	348	TYR	3.4
1	B	386	HIS	3.3
1	C	333	HIS	3.3
1	A	386	HIS	3.3
1	C	368	LEU	3.2
1	C	296	TYR	3.1
1	B	391	HIS	3.1
1	B	168	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	329	VAL	3.0
1	C	348	TYR	3.0
1	B	247	SER	2.9
1	A	389	LEU	2.9
1	B	383	PRO	2.8
1	C	371	TYR	2.8
1	D	371	TYR	2.8
1	C	351	LEU	2.8
1	B	40	LEU	2.8
1	D	338	SER	2.7
1	C	174	PRO	2.7
1	B	138	LEU	2.7
1	B	180	TYR	2.7
1	C	257	PHE	2.6
1	B	193	LEU	2.6
1	A	368	LEU	2.6
1	C	250	LYS	2.6
1	D	389	LEU	2.6
1	B	388	PHE	2.6
1	C	369	SER	2.6
1	D	384	THR	2.5
1	D	347	GLY	2.5
1	C	386	HIS	2.5
1	C	239	ILE	2.5
1	C	243	ALA	2.4
1	C	383	PRO	2.4
1	C	147	LEU	2.4
1	C	355	VAL	2.4
1	C	354	THR	2.4
1	B	333	HIS	2.4
1	C	138	LEU	2.4
1	C	388	PHE	2.4
1	A	333	HIS	2.4
1	A	391	HIS	2.4
1	C	238	PHE	2.3
1	C	168	LEU	2.3
1	A	339	LYS	2.3
1	A	153	PHE	2.3
1	D	388	PHE	2.3
1	D	296	TYR	2.3
1	C	360	LYS	2.3
1	C	338	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	153	PHE	2.3
1	B	173	VAL	2.2
1	B	368	LEU	2.2
1	D	368	LEU	2.2
1	D	366	PHE	2.2
1	B	389	LEU	2.2
1	D	40	LEU	2.2
1	D	138	LEU	2.2
1	B	197	GLN	2.2
1	B	369	SER	2.2
1	A	384	THR	2.2
1	B	349	HIS	2.2
1	B	371	TYR	2.2
1	B	169	GLN	2.1
1	B	171	MET	2.1
1	B	329	VAL	2.1
1	C	337	GLY	2.1
1	B	330	CYS	2.1
1	C	180	TYR	2.1
1	C	384	THR	2.1
1	D	170	ASN	2.1
1	D	350	TYR	2.1
1	A	143	PHE	2.1
1	A	243	ALA	2.1
1	A	338	SER	2.1
1	A	351	LEU	2.0
1	A	241	ILE	2.0
1	A	254	VAL	2.0
1	D	254	VAL	2.0
1	C	113	SER	2.0
1	B	334	ARG	2.0
1	C	280	GLY	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

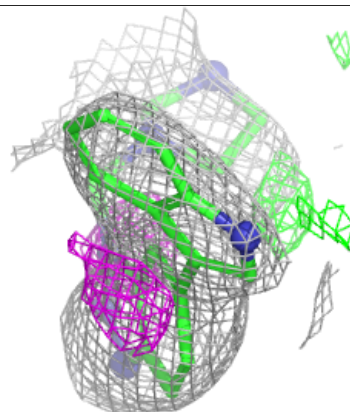
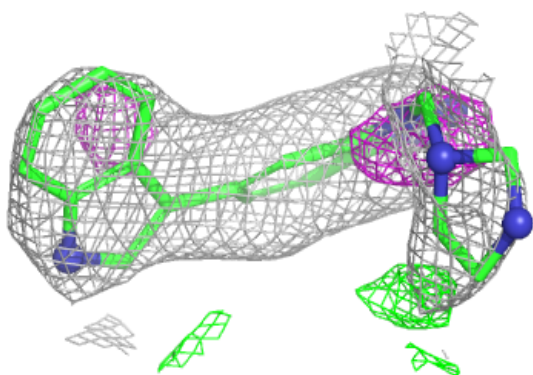
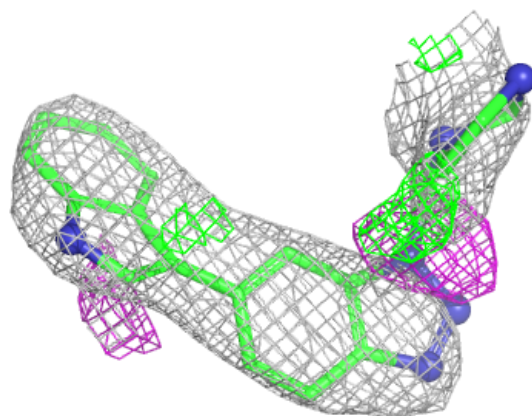
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	A1AEY	A	403	24/24	0.82	0.18	97,112,147,149	0
4	A1AEY	C	403	24/24	0.82	0.15	115,133,148,149	0
4	A1AEY	B	403	24/24	0.85	0.16	88,107,128,136	0
4	A1AEY	D	403	24/24	0.85	0.17	85,99,137,143	0
2	HEM	C	401	43/43	0.91	0.16	89,104,127,138	0
2	HEM	B	401	43/43	0.95	0.12	74,85,105,111	0
3	ZIQ	C	402	16/16	0.95	0.09	75,86,91,95	0
3	ZIQ	A	402	16/16	0.97	0.07	49,56,66,71	0
3	ZIQ	B	402	16/16	0.97	0.08	60,70,77,83	0
2	HEM	A	401	43/43	0.97	0.09	60,68,79,94	0
3	ZIQ	D	402	16/16	0.97	0.07	59,67,71,73	0
2	HEM	D	401	43/43	0.98	0.08	58,64,80,90	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.

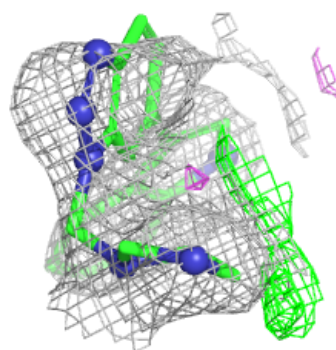
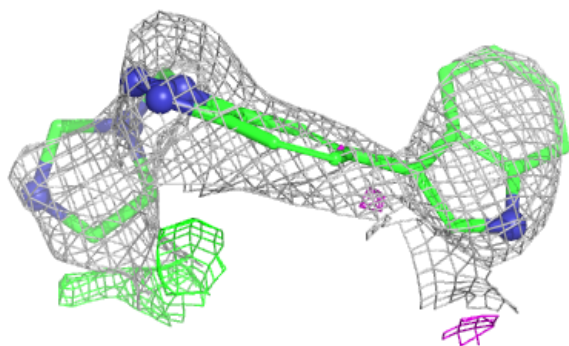
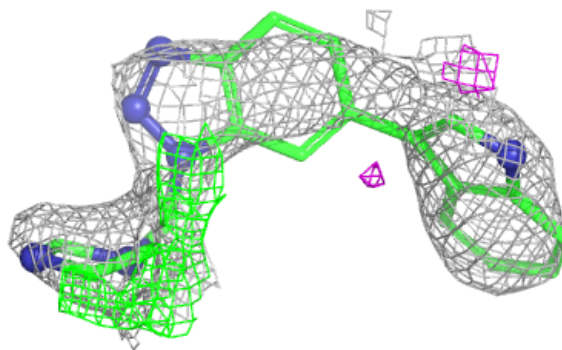
Electron density around A1AEY A 403:

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



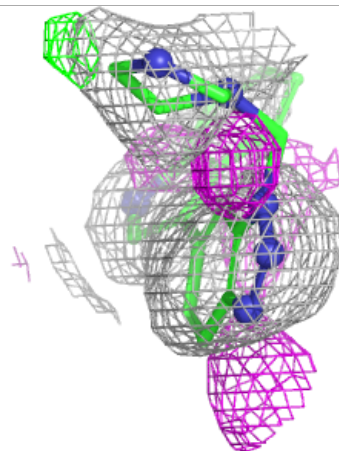
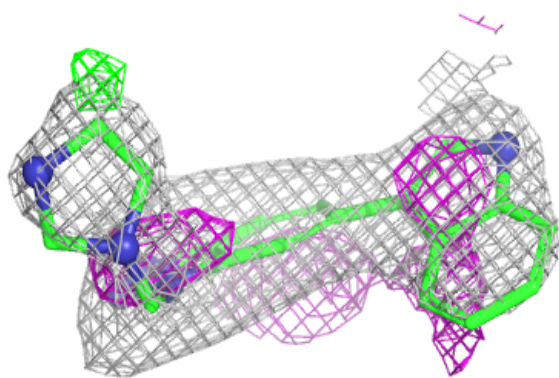
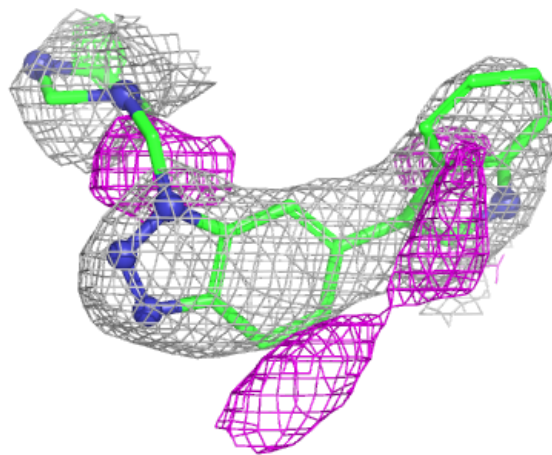
Electron density around A1AEY C 403:

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



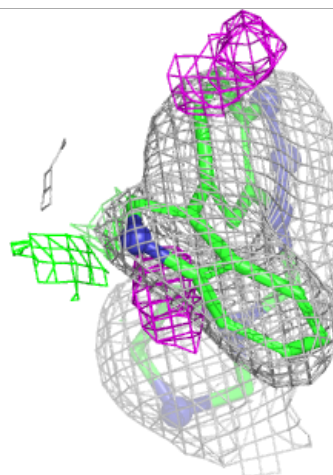
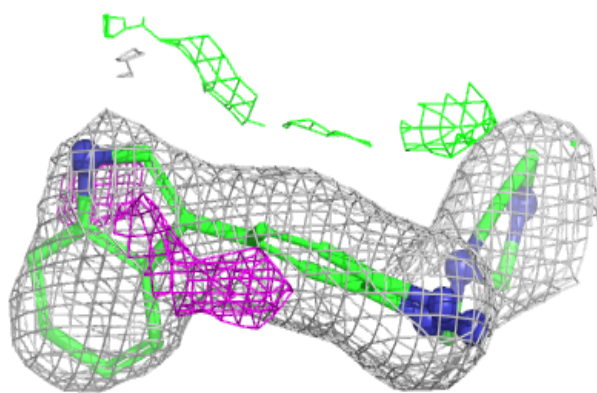
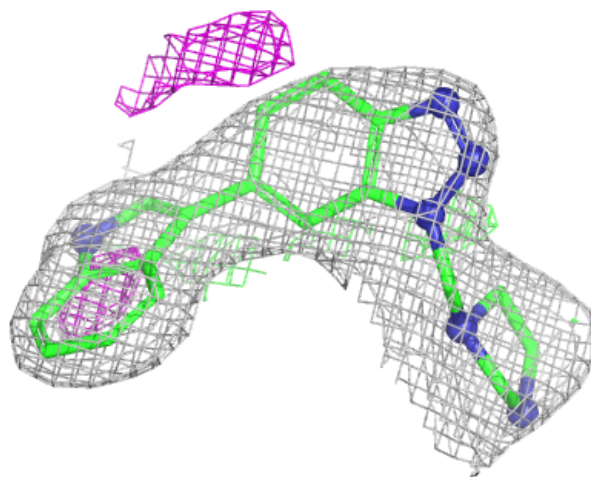
Electron density around A1AEY B 403:

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



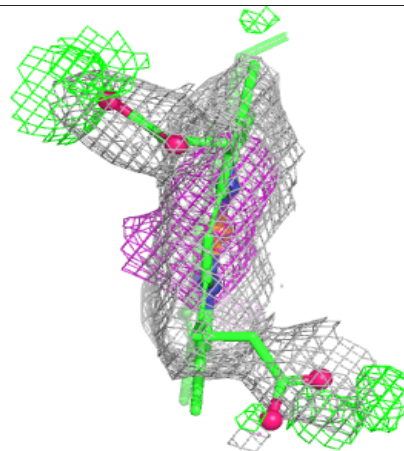
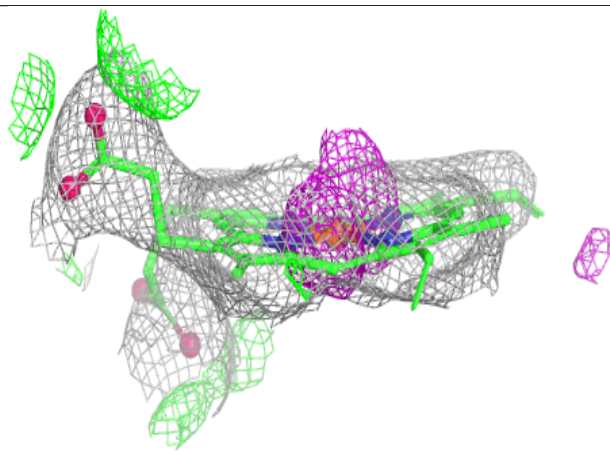
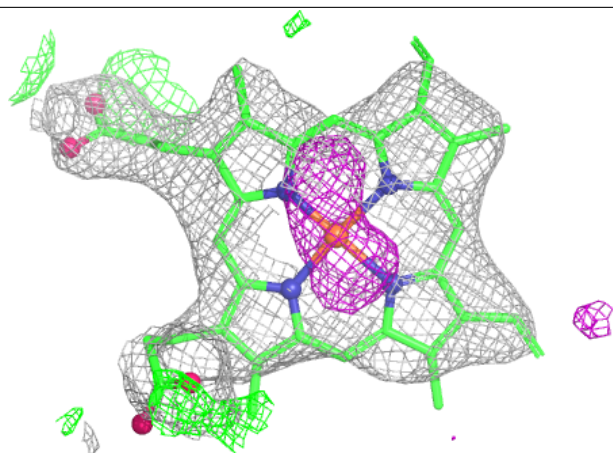
Electron density around A1AEY D 403:

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



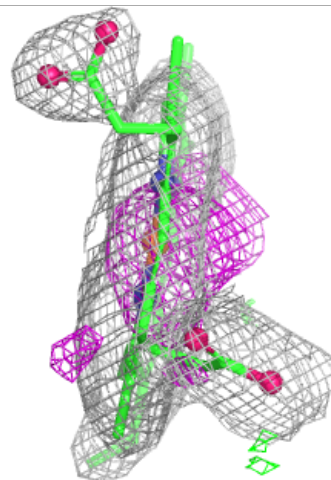
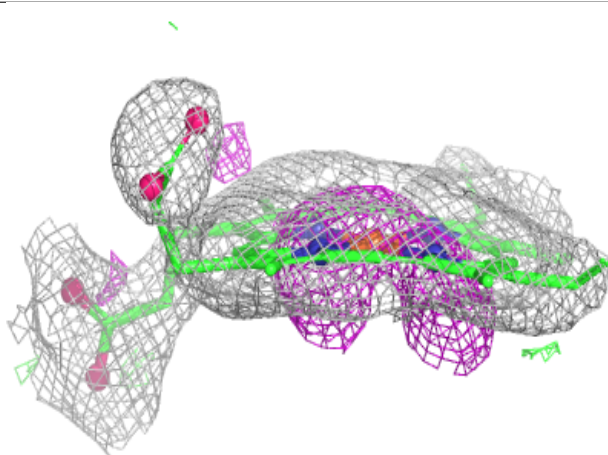
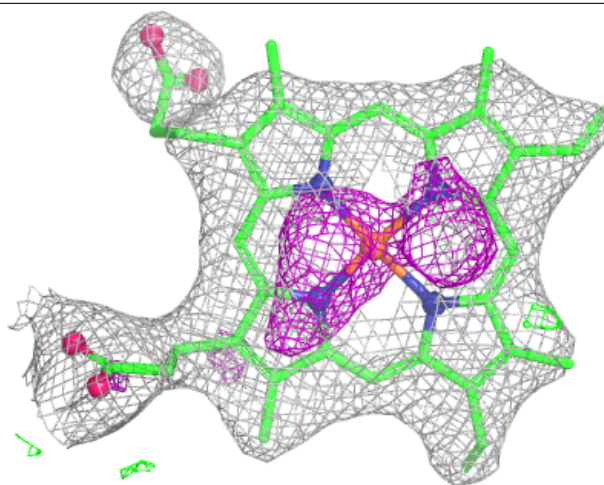
Electron density around HEM C 401:

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



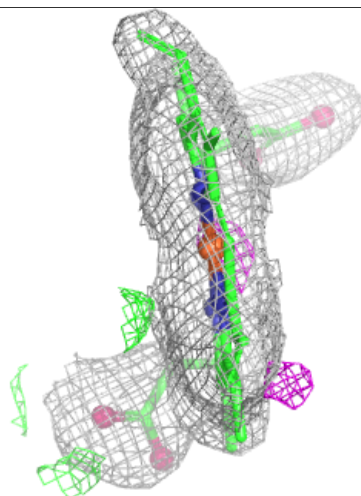
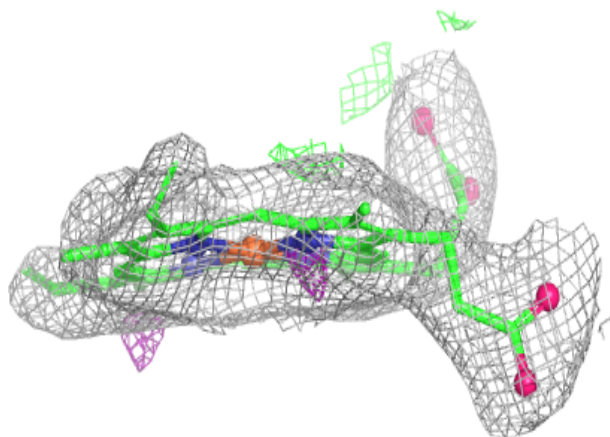
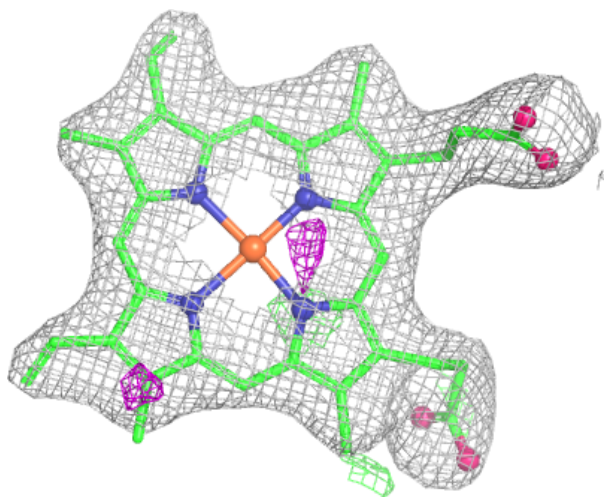
Electron density around HEM B 401:

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



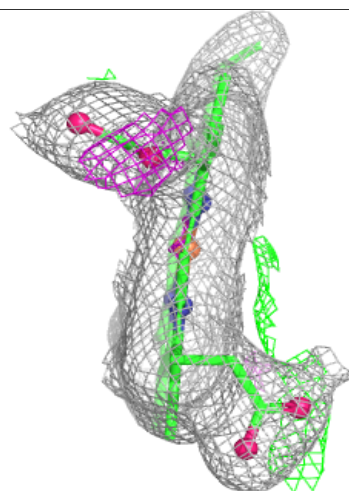
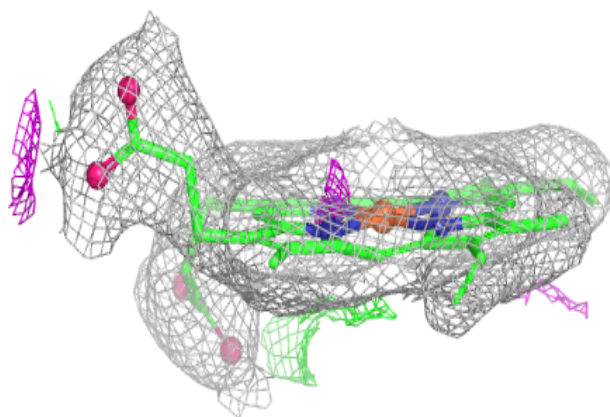
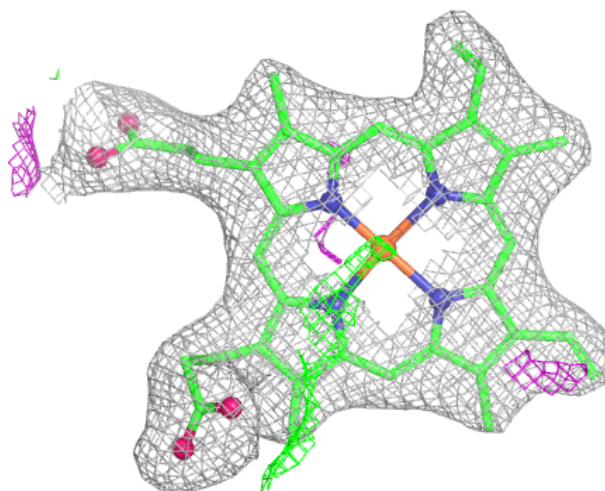
Electron density around HEM A 401:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.