



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 8W2K / pdb_00008w2k
Title : Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PAN3F inhibitor
Authors : Geeraerts, Z.; Yeh, S.-R.
Deposited on : 2024-02-20
Resolution : 2.45 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

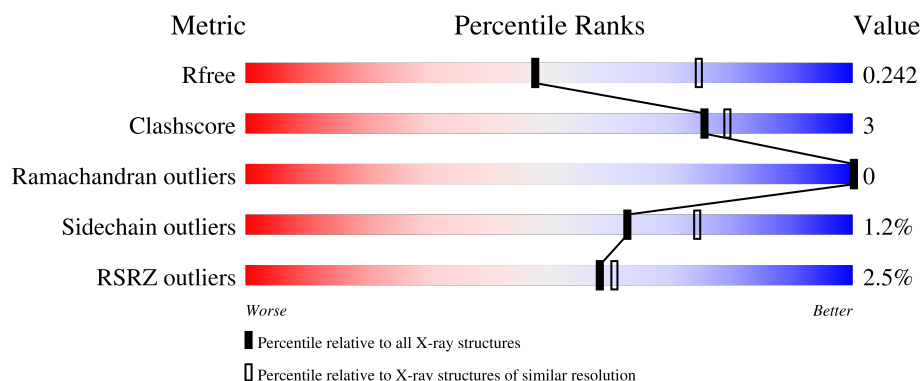
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	 2% 81% 10% 9%
1	B	380	 2% 83% 7% 9%
1	C	380	 3% 81% 8% 10%
1	D	380	 2% 84% 6% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12031 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	346	Total	C	N	O	S	0	0	0
			2941	1890	516	524	11			
1	C	341	Total	C	N	O	S	0	0	0
			2898	1865	508	514	11			
1	D	342	Total	C	N	O	S	0	0	0
			2904	1867	508	518	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

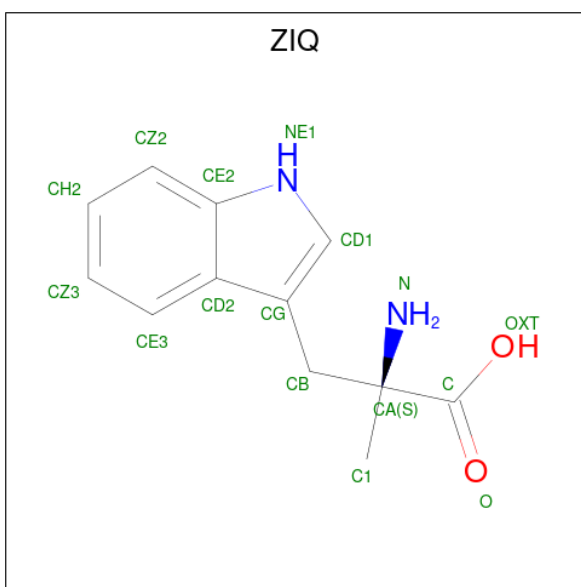
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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391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

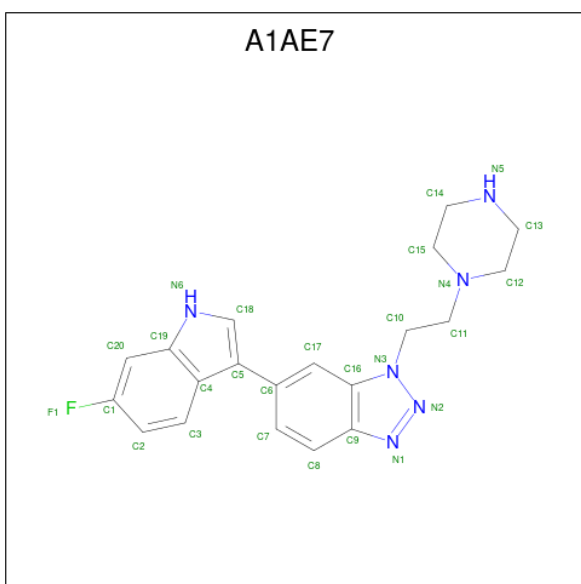
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- WORLDWIDE
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)-6-(6-fluoro-1H-indol-3-yl)-1-[2-(piperazin-1-yl)ethyl]-1H-benzotriazole (CCD ID: A1AE7) (formula: C₂₀H₂₁FN₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			27	20	1	6		
4	B	1	Total	C	F	N	0	0
			27	20	1	6		
4	C	1	Total	C	F	N	0	0
			27	20	1	6		
4	D	1	Total	C	F	N	0	0
			27	20	1	6		

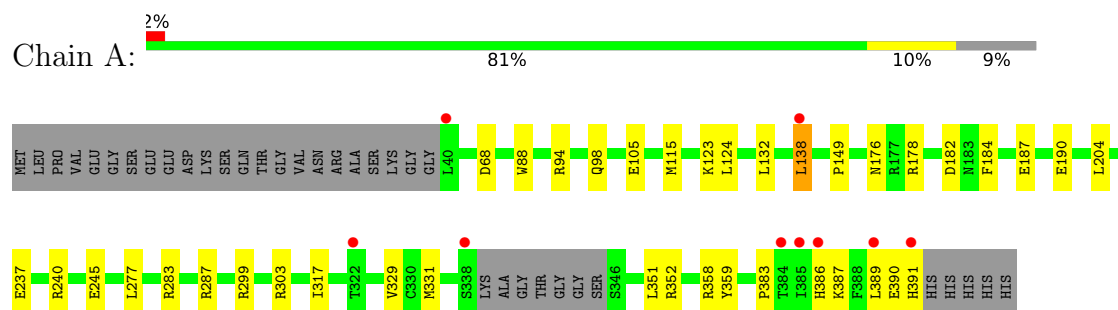
- Molecule 5 is water.

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

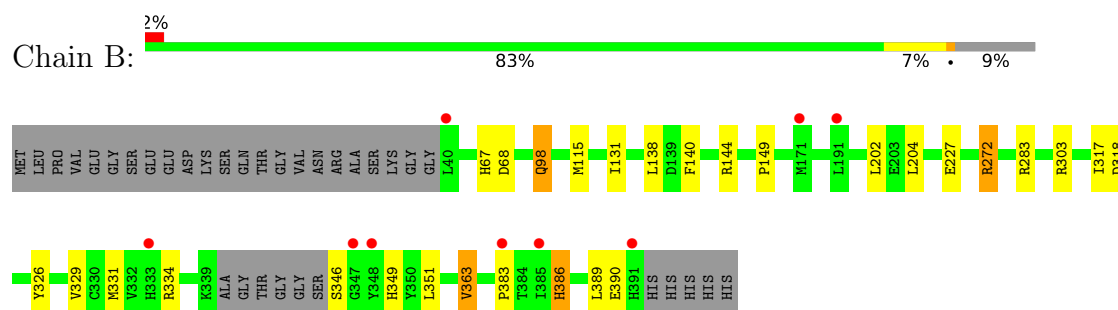
3 Residue-property plots [i](#)

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.

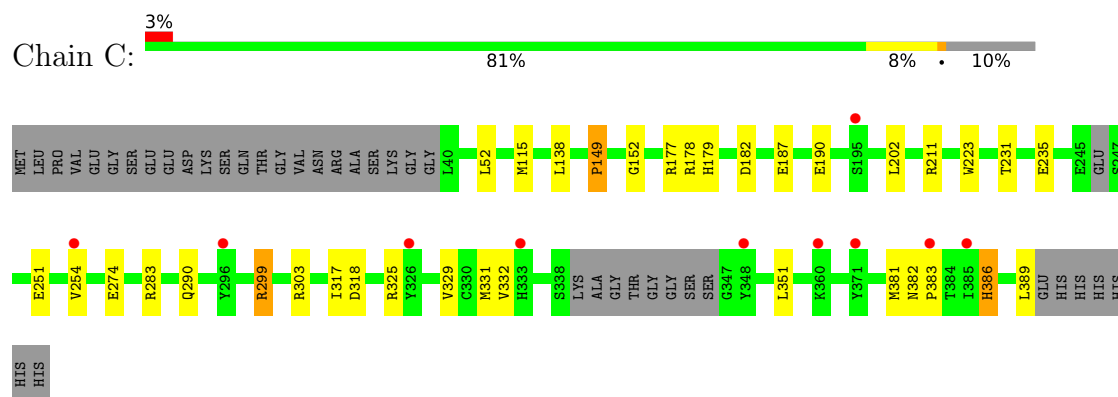
- Molecule 1: Tryptophan 2,3-dioxygenase



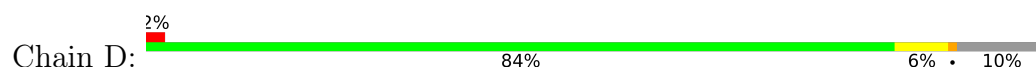
- Molecule 1: Tryptophan 2,3-dioxygenase

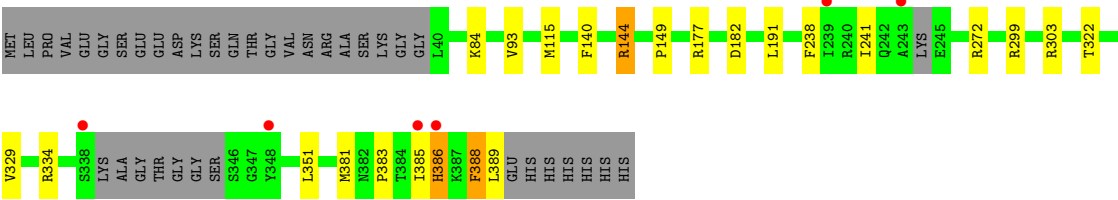


- Molecule 1: Tryptophan 2,3-dioxygenase



- 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	144.08Å 154.84Å 88.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.54 – 2.45 77.54 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (77.54-2.45) 97.9 (77.54-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.199 , 0.244 0.202 , 0.242	Depositor DCC
R_{free} test set	3662 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12031	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, A1AE7

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	0.63	0/3001	1.08	4/4039 (0.1%)
1	B	0.61	0/3010	1.07	6/4050 (0.1%)
1	C	0.56	0/2965	1.03	2/3989 (0.1%)
1	D	0.62	0/2971	1.07	2/3998 (0.1%)
All	All	0.61	0/11947	1.06	14/16076 (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	2
1	C	0	4
1	D	0	5
All	All	0	16

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	GLN	CB-CA-C	-6.57	99.89	110.79
1	D	182	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	105	GLU	CB-CG-CD	5.77	122.41	112.60
1	B	363	VAL	N-CA-CB	5.71	117.61	110.47
1	B	68	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	388	PHE	CA-CB-CG	5.56	119.36	113.80
1	B	318	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	227	GLU	CB-CG-CD	5.51	121.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	123	LYS	N-CA-CB	5.44	118.11	110.12
1	A	245	GLU	CB-CG-CD	5.35	121.70	112.60
1	C	149	PRO	N-CA-CB	-5.26	96.82	102.60
1	A	68	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	98	GLN	N-CA-CB	5.18	117.74	110.12

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ARG	Sidechain
1	A	287	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	352	ARG	Sidechain
1	A	94	ARG	Sidechain
1	B	272	ARG	Sidechain
1	B	334	ARG	Sidechain
1	C	177	ARG	Sidechain
1	C	178	ARG	Sidechain
1	C	211	ARG	Sidechain
1	C	299	ARG	Sidechain
1	D	144	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	272	ARG	Sidechain
1	D	299	ARG	Sidechain
1	D	334	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	20	0
1	B	2941	0	2927	16	0
1	C	2898	0	2889	25	0
1	D	2904	0	2887	11	0
2	A	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	0	0
2	C	43	0	30	3	0
2	D	43	0	30	1	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	27	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
All	All	12031	0	11737	70	0

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

All (70) 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:A:383:PRO:HA	1:A:386:HIS:HB3	1.31	1.08
1:A:138:LEU:HD13	1:C:299:ARG:HH12	1.19	1.03
1:C:381:MET:HG2	1:C:386:HIS:HB3	1.57	0.87
1:D:93:VAL:HG21	1:D:115:MET:HE3	1.58	0.83
1:A:138:LEU:HD22	1:C:299:ARG:HH22	1.51	0.74
1:C:329:VAL:HG22	1:C:351:LEU:HB3	1.69	0.73
2:A:401:HEM:HBC2	2:A:401:HEM:HHD	1.78	0.66
1:A:383:PRO:CA	1:A:386:HIS:HB3	2.19	0.64
1:B:383:PRO:HA	1:B:386:HIS:HB3	1.78	0.64
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.28	0.63
1:B:329:VAL:HG22	1:B:351:LEU:HB3	1.82	0.60
1:C:179:HIS:HB3	1:C:182:ASP:CB	2.31	0.59
1:C:383:PRO:HA	1:C:386:HIS:CE1	2.38	0.58
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.33	0.58
1:D:329:VAL:HG22	1:D:351:LEU:HB3	1.86	0.57
1:A:237:GLU:OE2	1:A:240:ARG:NH2	2.33	0.57
1:C:179:HIS:HB3	1:C:182:ASP:HB3	1.87	0.56
1:D:238:PHE:HA	1:D:241:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:VAL:HG22	1:C:351:LEU:CB	2.36	0.55
1:A:303:ARG:HD3	1:A:389:LEU:HA	1.88	0.55
1:D:115:MET:HA	1:D:115:MET:HE2	1.88	0.55
1:C:231:THR:O	1:C:235:GLU:HG3	2.09	0.53
1:A:329:VAL:HG22	1:A:351:LEU:HB3	1.91	0.52
1:C:303:ARG:HD3	1:C:389:LEU:HA	1.92	0.52
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.40	0.51
1:B:303:ARG:HD3	1:B:389:LEU:HA	1.93	0.51
1:C:325:ARG:O	1:C:329:VAL:HG23	2.11	0.50
1:C:251:GLU:O	1:C:254:VAL:HG12	2.11	0.50
1:C:52:LEU:O	1:D:84:LYS:NZ	2.45	0.50
1:A:176:ASN:O	1:A:178:ARG:HG3	2.12	0.49
1:D:303:ARG:HD3	1:D:389:LEU:HA	1.93	0.49
1:C:331:MET:HE3	2:C:401:HEM:HAB	1.95	0.49
1:C:383:PRO:HA	1:C:386:HIS:NE2	2.28	0.49
1:D:140:PHE:CE2	1:D:144:ARG:HD3	2.48	0.49
1:B:272:ARG:NH2	1:B:272:ARG:HG2	2.27	0.49
2:A:401:HEM:HHD	2:A:401:HEM:CBC	2.42	0.48
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	1.96	0.48
1:A:187:GLU:O	1:A:190:GLU:HB3	2.14	0.48
1:B:329:VAL:HG22	1:B:351:LEU:CB	2.43	0.48
1:B:346:SER:HB2	1:B:349:HIS:ND1	2.28	0.48
1:B:202:LEU:CD2	1:B:283:ARG:NH1	2.76	0.47
1:D:383:PRO:HA	1:D:386:HIS:CG	2.49	0.47
1:B:98:GLN:HG2	1:B:204:LEU:HD21	1.97	0.46
1:D:385:ILE:O	1:D:388:PHE:HD1	1.99	0.46
1:C:386:HIS:ND1	1:C:386:HIS:C	2.74	0.46
1:C:179:HIS:HB3	1:C:182:ASP:HB2	1.97	0.45
1:A:98:GLN:HG2	1:A:204:LEU:HD21	1.97	0.45
1:C:152:GLY:HA3	2:C:401:HEM:C1D	2.52	0.45
1:B:326:TYR:OH	1:D:322:THR:HG22	2.18	0.44
2:A:401:HEM:HBC2	2:A:401:HEM:CHD	2.43	0.44
1:B:140:PHE:CE2	1:B:144:ARG:HD3	2.53	0.44
1:C:332:VAL:HG22	2:C:401:HEM:C1B	2.53	0.44
1:B:386:HIS:CE1	1:B:390:GLU:HG2	2.53	0.43
1:C:202:LEU:HD21	1:C:283:ARG:HB3	2.00	0.43
1:A:331:MET:HE3	1:A:331:MET:HB2	1.83	0.43
1:C:223:TRP:CG	1:C:290:GLN:HE21	2.37	0.42
1:B:331:MET:HE2	1:B:331:MET:HB2	1.80	0.42
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.95	0.42
1:A:387:LYS:O	1:A:390:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:HG3	1:A:359:TYR:CD1	2.54	0.42
1:C:223:TRP:CD1	1:C:290:GLN:HE21	2.37	0.42
2:A:401:HEM:HBB2	2:A:401:HEM:CMB	2.50	0.42
1:C:187:GLU:O	1:C:190:GLU:HB3	2.19	0.42
1:A:88:TRP:CD1	1:B:67:HIS:CE1	3.09	0.41
1:A:124:LEU:HD22	1:B:131:ILE:CD1	2.50	0.41
1:D:381:MET:SD	1:D:389:LEU:HD12	2.60	0.41
1:A:124:LEU:HD22	1:B:131:ILE:HD11	2.02	0.41
1:C:115:MET:HE3	1:C:317:ILE:HD12	2.03	0.41
1:A:383:PRO:C	1:A:386:HIS:H	2.29	0.40
1:A:182:ASP:C	1:A:184:PHE:H	2.29	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%)	332 (97%)	9 (3%)	0	100	100
1	B	342/380 (90%)	334 (98%)	8 (2%)	0	100	100
1	C	335/380 (88%)	327 (98%)	8 (2%)	0	100	100
1	D	336/380 (88%)	327 (97%)	9 (3%)	0	100	100
All	All	1354/1520 (89%)	1320 (98%)	34 (2%)	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%)	318 (99%)	4 (1%)	63	74
1	B	323/348 (93%)	319 (99%)	4 (1%)	63	74
1	C	318/348 (91%)	313 (98%)	5 (2%)	55	69
1	D	319/348 (92%)	316 (99%)	3 (1%)	70	81
All	All	1282/1392 (92%)	1266 (99%)	16 (1%)	63	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	149	PRO
1	A	277	LEU
1	A	391	HIS
1	B	138	LEU
1	B	149	PRO
1	B	363	VAL
1	B	386	HIS
1	C	138	LEU
1	C	149	PRO
1	C	274	GLU
1	C	382	ASN
1	C	386	HIS
1	D	149	PRO
1	D	191	LEU
1	D	386	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	107	ASN
1	A	218	HIS
1	A	290	GLN
1	A	309	GLN
1	A	376	HIS
1	B	183	ASN
1	B	189	ASN
1	B	290	GLN

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Mol	Chain	Res	Type
1	B	309	GLN
1	C	98	GLN
1	C	309	GLN
1	C	382	ASN
1	D	44	ASN
1	D	258	GLN
1	D	309	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A1AE7	B	403	-	31,31,31	0.62	0	44,44,44	1.01	2 (4%)
2	HEM	A	401	1	50,50,50	1.63	9 (18%)	67,82,82	1.66	14 (20%)
4	A1AE7	C	403	-	31,31,31	0.53	0	44,44,44	0.90	1 (2%)
4	A1AE7	D	403	-	31,31,31	0.86	2 (6%)	44,44,44	1.02	3 (6%)
3	ZIQ	A	402	-	14,17,17	0.94	1 (7%)	20,25,25	1.09	1 (5%)

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	1.69	11 (22%)	67,82,82	1.79	18 (26%)
3	ZIQ	C	402	-	14,17,17	0.68	0	20,25,25	1.11	2 (10%)
3	ZIQ	B	402	-	14,17,17	0.66	0	20,25,25	1.30	2 (10%)
3	ZIQ	D	402	-	14,17,17	0.65	0	20,25,25	1.11	2 (10%)
4	A1AE7	A	403	-	31,31,31	0.77	1 (3%)	44,44,44	0.83	1 (2%)
2	HEM	B	401	1	50,50,50	1.47	5 (10%)	67,82,82	1.73	16 (23%)
2	HEM	C	401	1	50,50,50	1.57	7 (14%)	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
4	A1AE7	B	403	-	-	0/9/26/26	0/5/5/5
2	HEM	A	401	1	-	2/14/54/54	-
4	A1AE7	C	403	-	-	0/9/26/26	0/5/5/5
4	A1AE7	D	403	-	-	1/9/26/26	0/5/5/5
3	ZIQ	A	402	-	-	7/11/11/11	0/2/2/2
2	HEM	D	401	1	-	2/14/54/54	-
3	ZIQ	C	402	-	-	4/11/11/11	0/2/2/2
3	ZIQ	B	402	-	-	1/11/11/11	0/2/2/2
3	ZIQ	D	402	-	-	4/11/11/11	0/2/2/2
4	A1AE7	A	403	-	-	2/9/26/26	0/5/5/5
2	HEM	B	401	1	-	2/14/54/54	-
2	HEM	C	401	1	-	3/14/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	FE-NB	5.36	2.11	1.94
2	A	401	HEM	FE-NB	4.99	2.10	1.94
2	B	401	HEM	FE-NB	4.81	2.09	1.94
2	D	401	HEM	FE-NB	4.73	2.09	1.94
2	C	401	HEM	FE-NC	4.54	2.10	1.95
2	B	401	HEM	FE-NC	4.48	2.10	1.95
2	D	401	HEM	FE-NC	4.08	2.08	1.95
2	B	401	HEM	C1B-NB	-3.51	1.34	1.40
2	C	401	HEM	C1B-NB	-3.47	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C1D-ND	-3.47	1.32	1.38
2	A	401	HEM	C1B-NB	-3.36	1.34	1.40
2	A	401	HEM	FE-NC	3.32	2.06	1.95
2	D	401	HEM	C1C-C2C	-3.17	1.39	1.45
2	C	401	HEM	C1C-C2C	-2.97	1.39	1.45
2	D	401	HEM	C3C-C4C	-2.96	1.40	1.46
2	D	401	HEM	C4B-NB	-2.94	1.33	1.38
4	D	403	A1AE7	C17-C6	-2.92	1.35	1.39
2	A	401	HEM	C1C-NC	-2.91	1.34	1.39
2	A	401	HEM	C3C-C4C	-2.83	1.41	1.46
4	A	403	A1AE7	C17-C6	-2.80	1.35	1.39
2	A	401	HEM	C1C-C2C	-2.80	1.39	1.45
3	A	402	ZIQ	O-C	2.78	1.30	1.22
2	B	401	HEM	C1C-C2C	-2.77	1.39	1.45
2	A	401	HEM	C4B-NB	-2.75	1.33	1.38
2	D	401	HEM	C4D-ND	-2.71	1.35	1.40
2	D	401	HEM	C1B-NB	-2.68	1.35	1.40
2	D	401	HEM	C1C-NC	-2.64	1.34	1.39
2	D	401	HEM	FE-ND	-2.58	1.87	1.94
2	C	401	HEM	C4D-ND	-2.57	1.35	1.40
2	C	401	HEM	C4B-NB	-2.54	1.33	1.38
4	D	403	A1AE7	C20-C1	-2.32	1.33	1.37
2	D	401	HEM	FE-NA	2.24	2.02	1.95
2	A	401	HEM	FE-NA	2.11	2.02	1.95
2	B	401	HEM	C4D-ND	-2.08	1.36	1.40
2	C	401	HEM	C3C-C4C	-2.04	1.42	1.46
2	D	401	HEM	O1D-CGD	2.02	1.28	1.22

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CHA-C4D-ND	4.66	130.13	124.37
2	D	401	HEM	CHD-C1D-ND	4.61	129.38	124.42
2	B	401	HEM	C1B-NB-C4B	4.60	110.66	105.21
2	C	401	HEM	CHC-C4B-NB	4.59	129.36	124.42
2	D	401	HEM	CHC-C4B-NB	4.48	129.25	124.42
2	B	401	HEM	CHC-C4B-NB	4.45	129.22	124.42
2	D	401	HEM	CHA-C4D-ND	4.17	129.53	124.37
2	D	401	HEM	CHB-C1B-NB	4.02	129.34	124.37
2	C	401	HEM	C1B-NB-C4B	3.93	109.86	105.21
2	D	401	HEM	C1B-NB-C4B	3.90	109.82	105.21
2	C	401	HEM	CHD-C1D-ND	3.85	128.57	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	C1B-NB-C4B	3.78	109.68	105.21
2	A	401	HEM	CHC-C4B-NB	3.75	128.46	124.42
2	B	401	HEM	CHD-C1D-ND	3.71	128.42	124.42
2	D	401	HEM	CBD-CAD-C3D	-3.55	102.72	112.53
4	B	403	A1AE7	C17-C16-N3	3.48	135.09	131.30
3	B	402	ZIQ	O-C-CA	-3.48	116.55	122.78
2	C	401	HEM	CHB-C1B-NB	3.46	128.65	124.37
2	B	401	HEM	CHD-C4C-NC	3.41	128.17	124.45
3	D	402	ZIQ	O-C-CA	-3.38	116.71	122.78
3	B	402	ZIQ	CB-CA-C	3.35	113.71	109.10
4	C	403	A1AE7	C17-C16-N3	3.31	134.90	131.30
3	A	402	ZIQ	O-C-CA	-3.29	116.88	122.78
2	A	401	HEM	CBD-CAD-C3D	-3.24	103.57	112.53
3	C	402	ZIQ	O-C-CA	-3.24	116.97	122.78
2	B	401	HEM	CHA-C4D-ND	3.20	128.32	124.37
2	B	401	HEM	CHB-C1B-NB	3.16	128.28	124.37
2	C	401	HEM	CHA-C4D-ND	3.08	128.18	124.37
2	A	401	HEM	C4C-NC-C1C	2.99	110.70	105.82
2	A	401	HEM	CHD-C1D-ND	2.98	127.63	124.42
2	A	401	HEM	CHD-C4C-NC	2.98	127.70	124.45
2	B	401	HEM	CBD-CAD-C3D	-2.88	104.58	112.53
3	D	402	ZIQ	CB-CA-C	2.86	113.03	109.10
3	C	402	ZIQ	CB-CA-C	2.79	112.94	109.10
2	A	401	HEM	CHB-C1B-NB	2.77	127.80	124.37
2	B	401	HEM	C3B-C4B-NB	-2.72	107.51	109.47
4	D	403	A1AE7	C17-C16-N3	2.68	134.21	131.30
2	A	401	HEM	CHA-C4D-C3D	-2.58	120.47	125.23
2	D	401	HEM	CHD-C4C-NC	2.57	127.25	124.45
2	B	401	HEM	CHD-C1D-C2D	-2.55	121.00	125.03
4	A	403	A1AE7	C17-C16-N3	2.55	134.07	131.30
2	C	401	HEM	C4C-NC-C1C	2.55	109.97	105.82
2	B	401	HEM	CAC-C3C-C4C	2.54	130.89	124.82
2	C	401	HEM	CAC-C3C-C2C	-2.54	120.18	128.43
2	D	401	HEM	CMD-C2D-C1D	2.53	128.99	125.03
2	C	401	HEM	CHD-C4C-NC	2.50	127.18	124.45
2	B	401	HEM	O2A-CGA-O1A	-2.50	116.91	123.33
2	D	401	HEM	CHD-C1D-C2D	-2.45	121.16	125.03
2	D	401	HEM	C4C-NC-C1C	2.44	109.81	105.82
2	D	401	HEM	C4B-C3B-C2B	-2.44	105.03	107.28
2	B	401	HEM	C3B-C2B-C1B	2.35	108.18	106.41
2	D	401	HEM	CAC-C3C-C4C	2.34	130.40	124.82
2	C	401	HEM	C4B-C3B-C2B	-2.33	105.13	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CAD-C3D-C4D	2.33	128.76	124.70
2	B	401	HEM	O2A-CGA-CBA	2.33	121.36	114.00
2	C	401	HEM	CAC-C3C-C4C	2.31	130.34	124.82
2	B	401	HEM	CAC-C3C-C2C	-2.30	120.96	128.43
2	A	401	HEM	O2D-CGD-CBD	2.27	121.18	114.00
2	A	401	HEM	O2A-CGA-CBA	2.24	121.08	114.00
2	D	401	HEM	C4C-CHD-C1D	-2.23	121.27	126.02
2	A	401	HEM	C4B-C3B-C2B	-2.18	105.27	107.28
2	B	401	HEM	C4C-NC-C1C	2.18	109.38	105.82
4	D	403	A1AE7	F1-C1-C20	-2.16	115.21	118.28
2	A	401	HEM	C1A-CHA-C4D	-2.16	121.17	126.25
2	C	401	HEM	C3B-C2B-C1B	2.16	108.03	106.41
2	C	401	HEM	CBD-CAD-C3D	-2.14	106.61	112.53
2	D	401	HEM	CAD-C3D-C2D	-2.13	123.89	127.87
2	D	401	HEM	CAC-C3C-C2C	-2.12	121.55	128.43
2	A	401	HEM	CMD-C2D-C1D	2.10	128.32	125.03
2	C	401	HEM	CHA-C1A-NA	2.09	127.65	123.86
4	B	403	A1AE7	C7-C6-C5	-2.09	118.36	120.98
2	C	401	HEM	C1A-CHA-C4D	-2.06	121.41	126.25
2	B	401	HEM	C1A-CHA-C4D	-2.06	121.41	126.25
2	D	401	HEM	C4D-ND-C1D	2.04	107.62	105.21
2	C	401	HEM	C4C-C3C-C2C	2.04	108.58	106.81
2	D	401	HEM	CHA-C4D-C3D	-2.04	121.47	125.23
4	D	403	A1AE7	C8-C7-C6	2.00	122.94	120.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	ZIQ	OXT-C-CA-N
3	D	402	ZIQ	OXT-C-CA-C1
4	D	403	A1AE7	N3-C10-C11-N4
3	D	402	ZIQ	O-C-CA-C1
3	D	402	ZIQ	O-C-CA-CB
3	D	402	ZIQ	OXT-C-CA-CB
4	A	403	A1AE7	C10-C11-N4-C12
4	A	403	A1AE7	C10-C11-N4-C15
3	A	402	ZIQ	CA-CB-CG-CD2
3	A	402	ZIQ	CA-CB-CG-CD1
3	A	402	ZIQ	OXT-C-CA-C1
2	C	401	HEM	C3D-CAD-CBD-CGD
3	A	402	ZIQ	O-C-CA-C1

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Mol	Chain	Res	Type	Atoms
3	C	402	ZIQ	O-C-CA-C1
3	A	402	ZIQ	O-C-CA-CB
3	A	402	ZIQ	OXT-C-CA-CB
2	D	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
3	B	402	ZIQ	O-C-CA-C1
2	B	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
3	C	402	ZIQ	OXT-C-CA-C1
3	A	402	ZIQ	C-CA-CB-CG
3	C	402	ZIQ	O-C-CA-CB

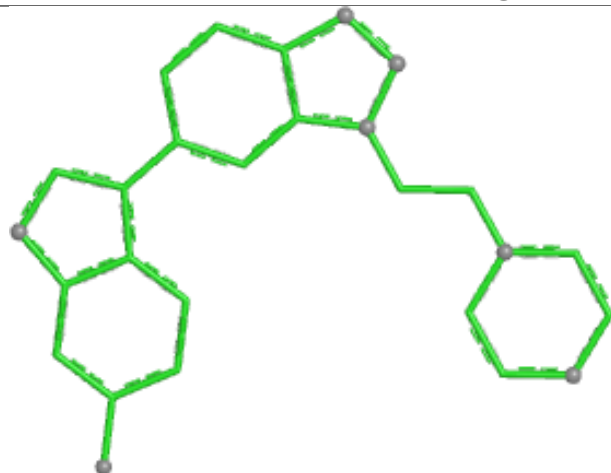
There are no ring outliers.

3 monomers are involved in 8 short contacts:

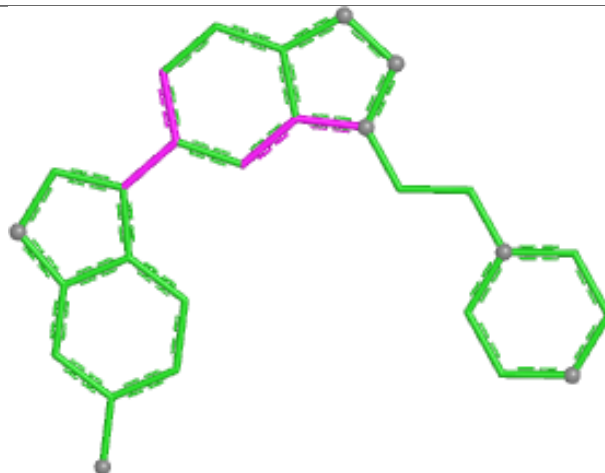
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	4	0
2	D	401	HEM	1	0
2	C	401	HEM	3	0

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.

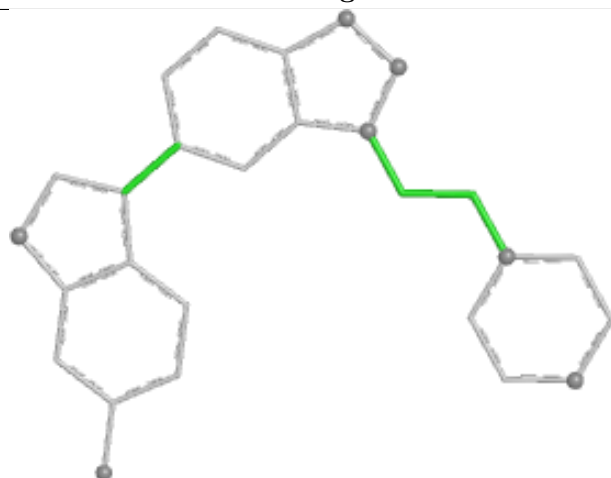
Ligand A1AE7 B 403



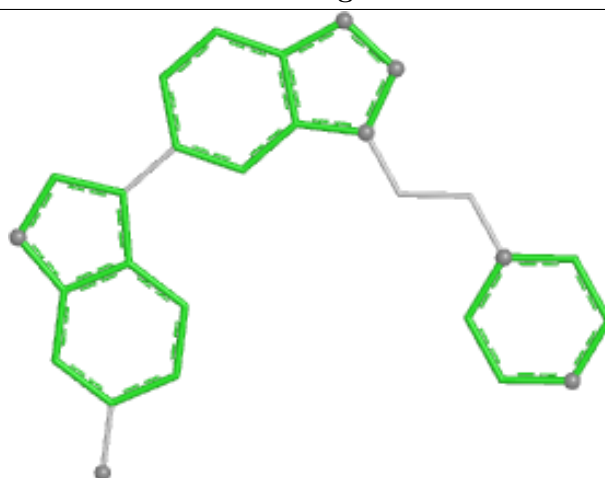
Bond lengths



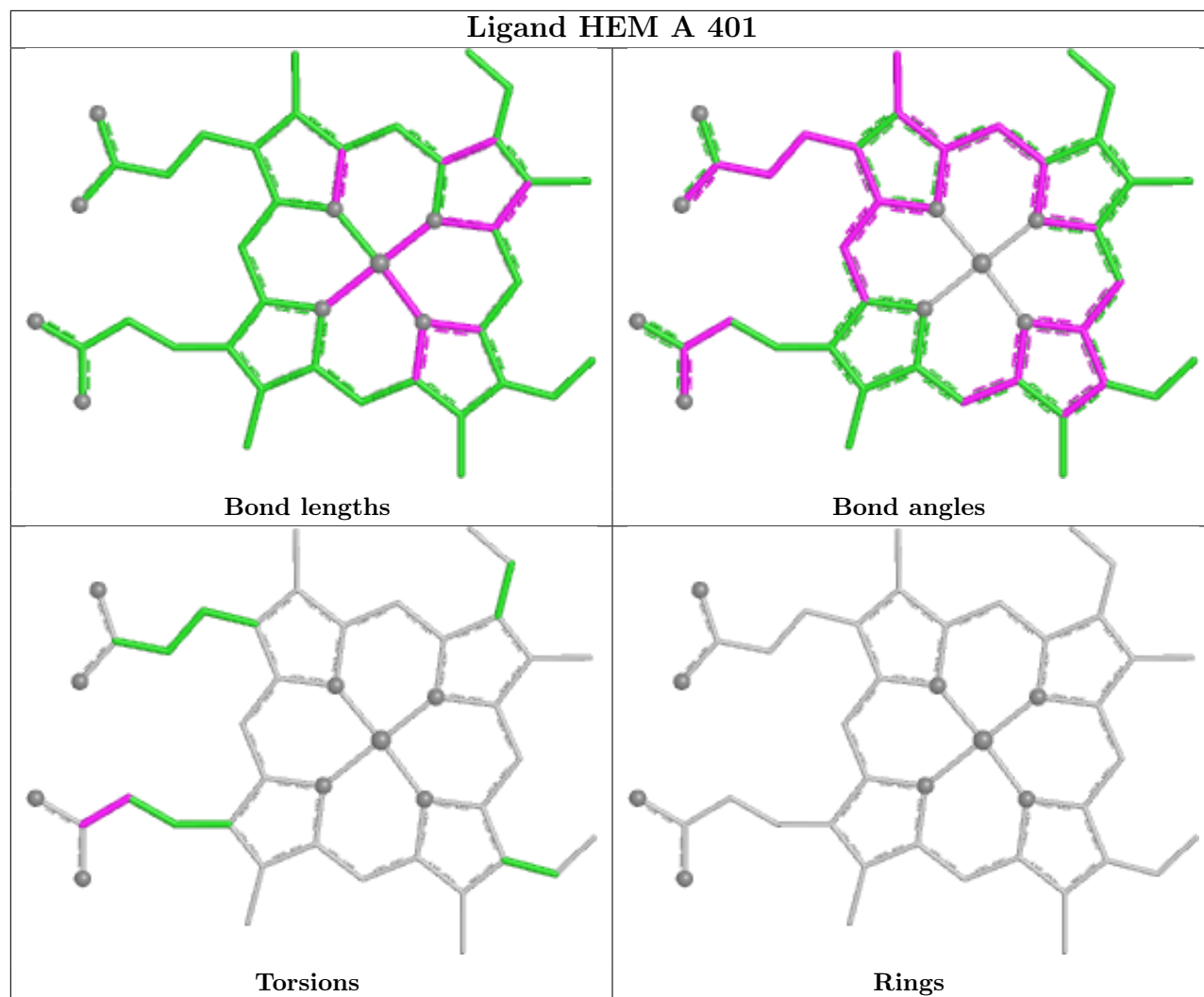
Bond angles



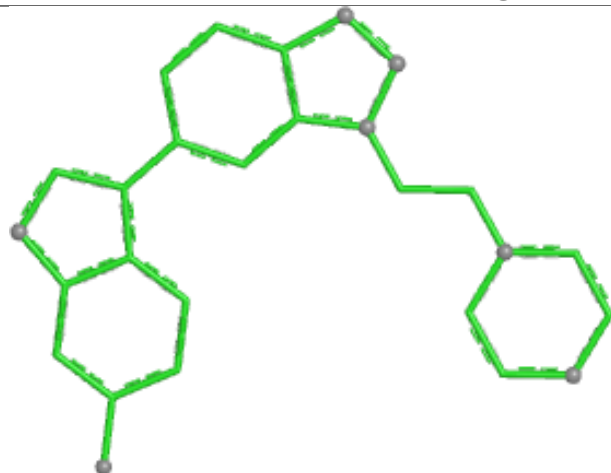
Torsions



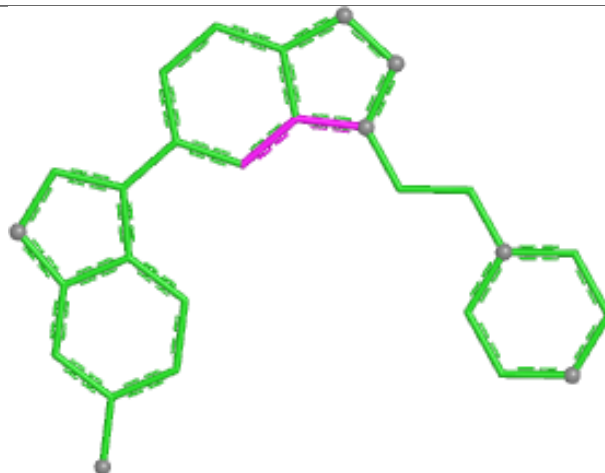
Rings



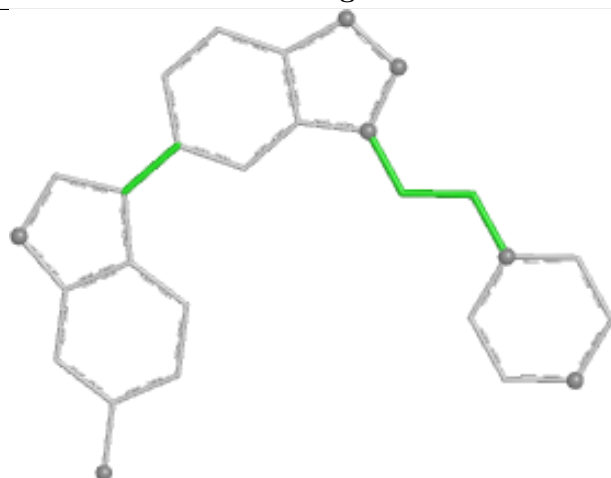
Ligand A1AE7 C 403



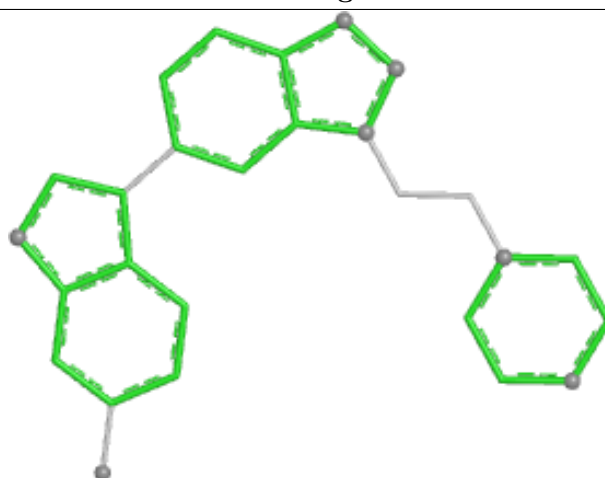
Bond lengths



Bond angles

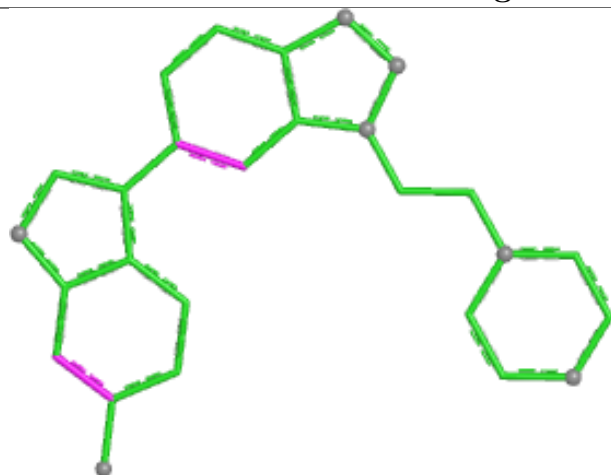


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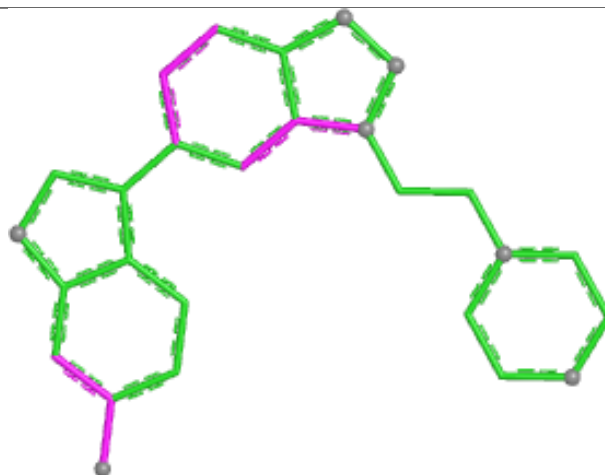


Rings

Ligand A1AE7 D 403



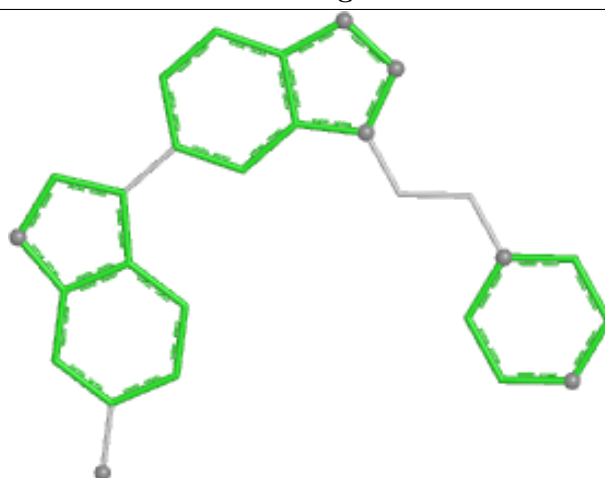
Bond lengths



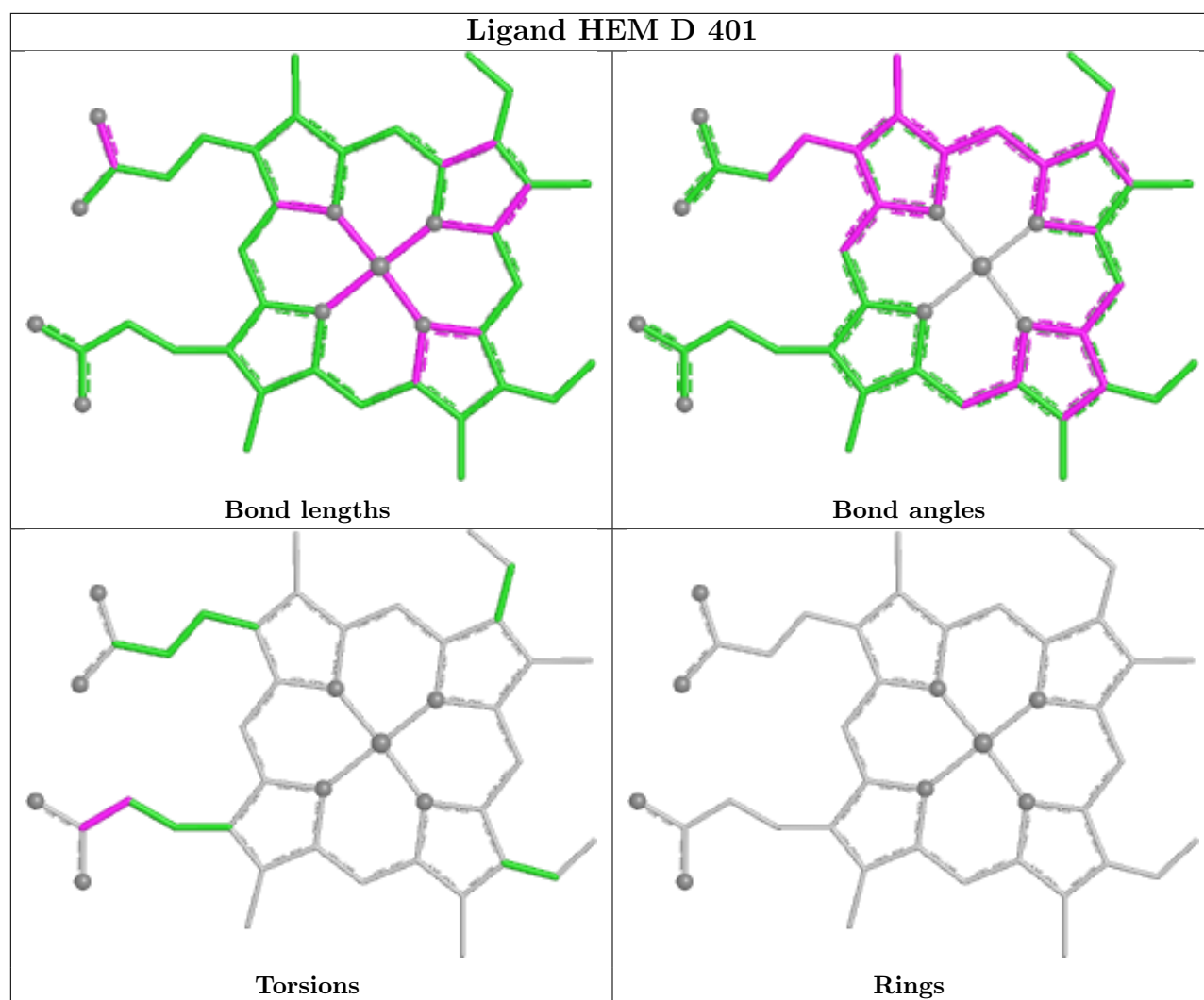
Bond angles



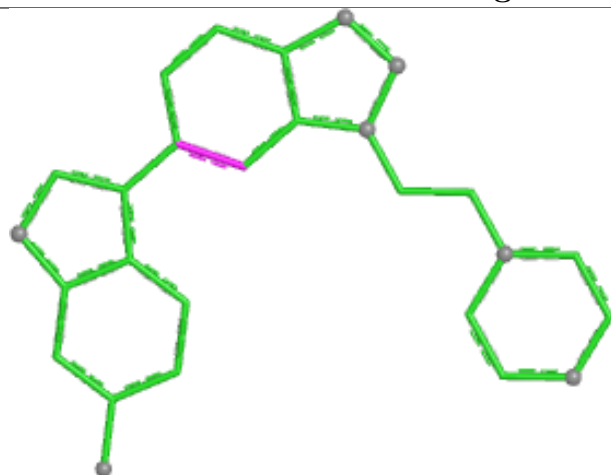
Torsions



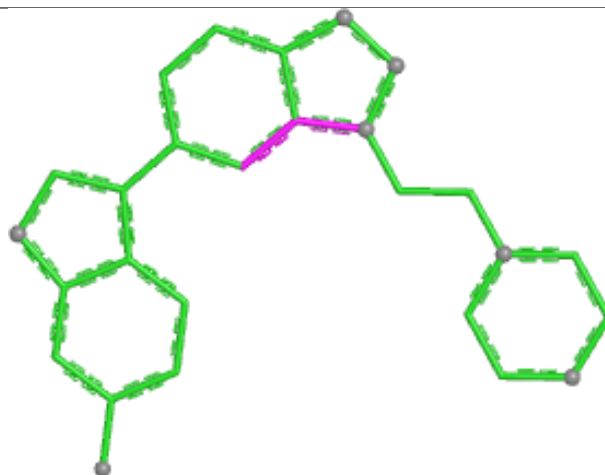
Rings



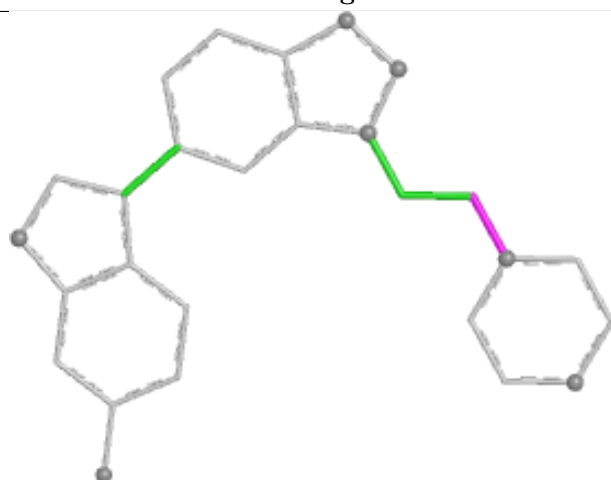
Ligand A1AE7 A 403



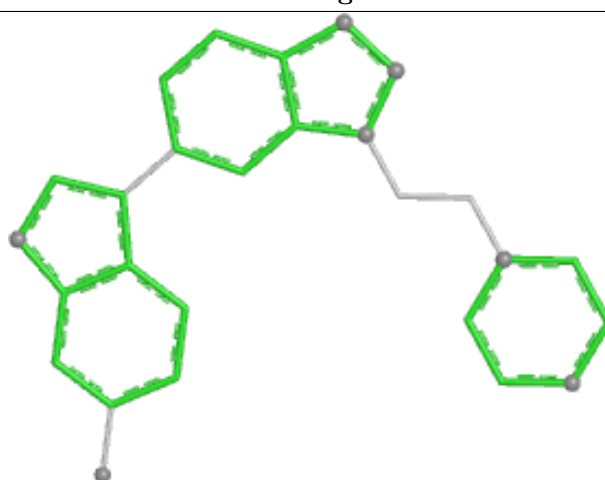
Bond lengths



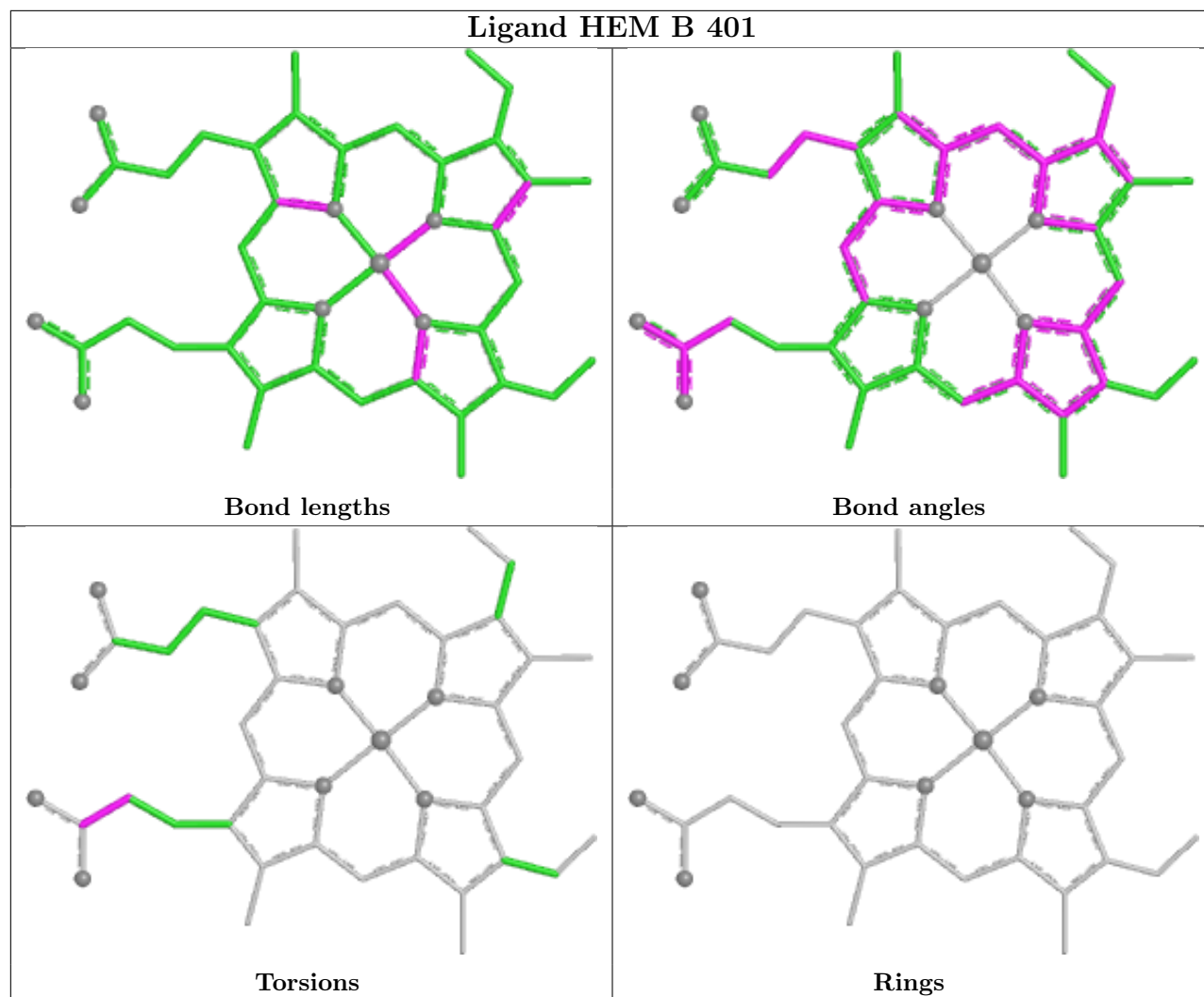
Bond angles

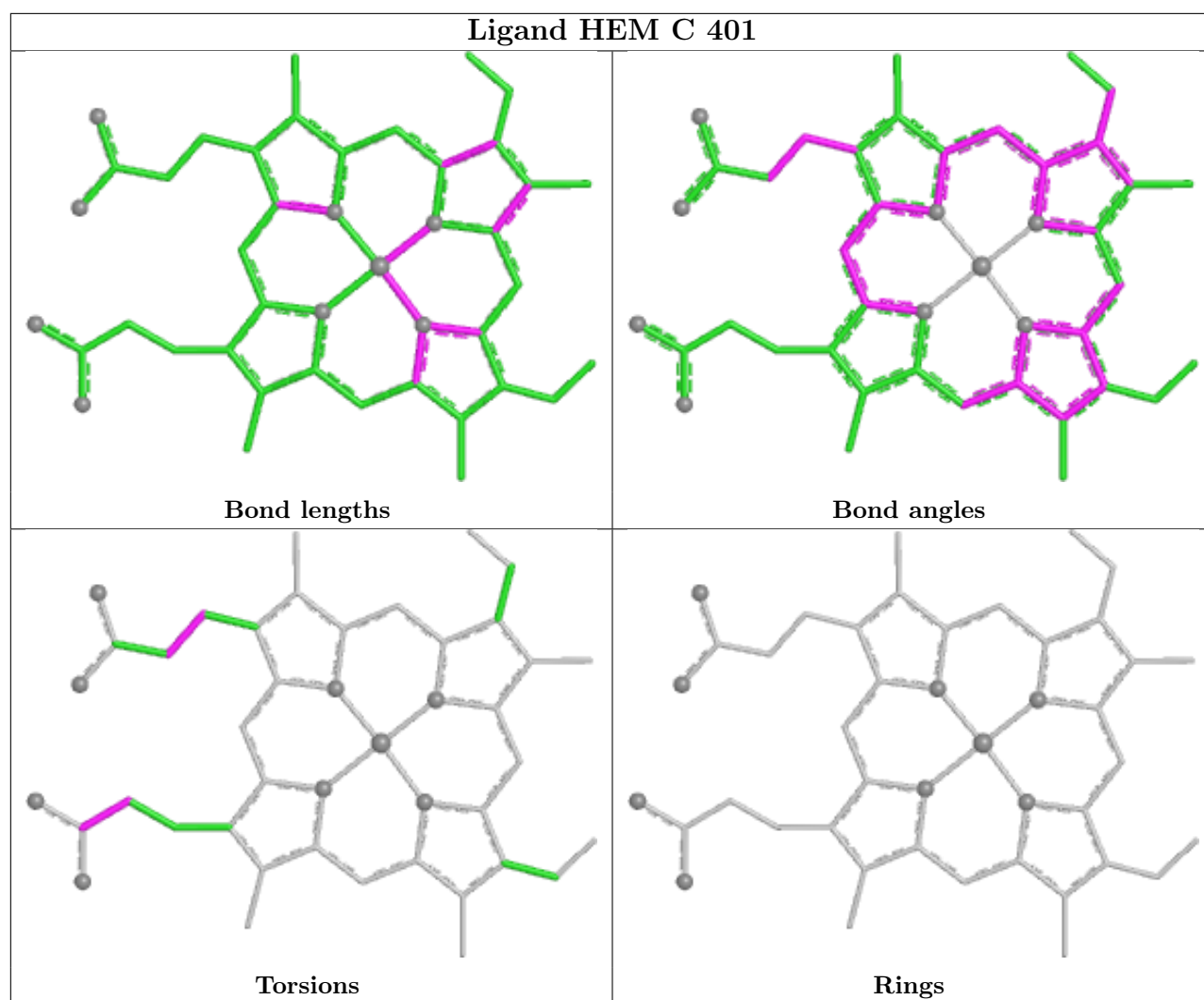


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.02	9 (2%) 57 58	49, 74, 139, 194	0
1	B	346/380 (91%)	0.07	9 (2%) 57 58	51, 78, 139, 196	0
1	C	341/380 (89%)	0.26	10 (2%) 53 55	57, 102, 199, 241	0
1	D	342/380 (90%)	0.04	6 (1%) 67 69	49, 79, 159, 248	0
All	All	1374/1520 (90%)	0.10	34 (2%) 58 61	49, 81, 166, 248	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	243	ALA	4.6
1	D	385	ILE	4.4
1	C	385	ILE	3.5
1	A	385	ILE	3.5
1	D	239	ILE	3.2
1	D	338	SER	3.1
1	B	348	TYR	3.0
1	D	386	HIS	3.0
1	C	326	TYR	2.9
1	B	391	HIS	2.9
1	A	338	SER	2.8
1	A	386	HIS	2.8
1	B	385	ILE	2.8
1	A	40	LEU	2.8
1	C	383	PRO	2.7
1	C	195	SER	2.6
1	B	40	LEU	2.6
1	C	371	TYR	2.6
1	D	348	TYR	2.5
1	C	360	LYS	2.5
1	B	383	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	389	LEU	2.3
1	B	333	HIS	2.3
1	A	322	THR	2.3
1	C	254	VAL	2.2
1	A	138	LEU	2.2
1	B	347	GLY	2.2
1	A	391	HIS	2.1
1	B	191	LEU	2.1
1	C	333	HIS	2.1
1	A	384	THR	2.1
1	C	348	TYR	2.1
1	B	171	MET	2.0
1	C	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(Å ²)	Q<0.9
4	A1AE7	A	403	27/27	0.84	0.21	87,121,194,206	0
4	A1AE7	B	403	27/27	0.84	0.19	85,115,185,192	0
4	A1AE7	D	403	27/27	0.84	0.17	79,111,168,176	0
4	A1AE7	C	403	27/27	0.85	0.15	115,155,199,205	0
3	ZIQ	C	402	16/16	0.91	0.12	83,95,121,124	0
3	ZIQ	A	402	16/16	0.92	0.10	56,62,75,85	0
2	HEM	C	401	43/43	0.94	0.12	88,108,140,159	0
2	HEM	B	401	43/43	0.96	0.10	73,92,110,128	0
3	ZIQ	D	402	16/16	0.96	0.08	71,78,86,92	0
3	ZIQ	B	402	16/16	0.96	0.07	70,75,88,91	0

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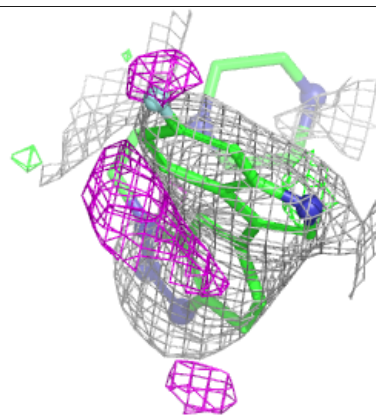
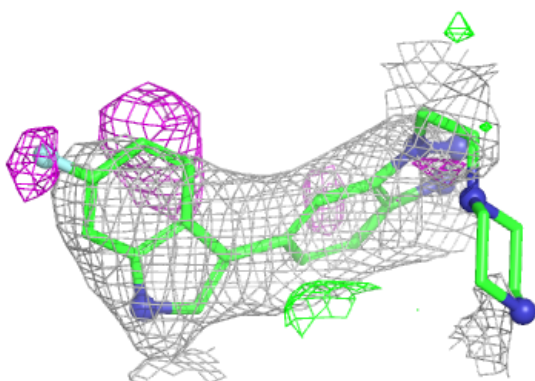
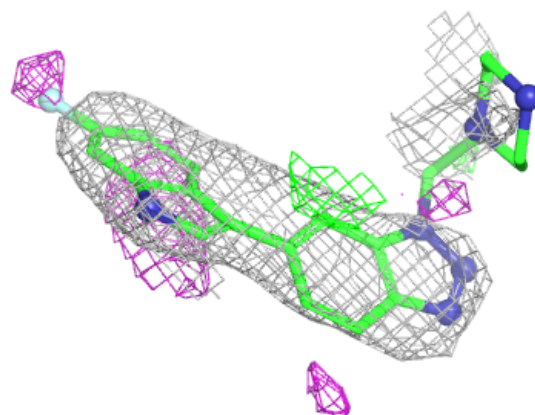
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	401	43/43	0.97	0.09	62,73,89,113	0
2	HEM	D	401	43/43	0.98	0.07	60,67,79,92	0

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.

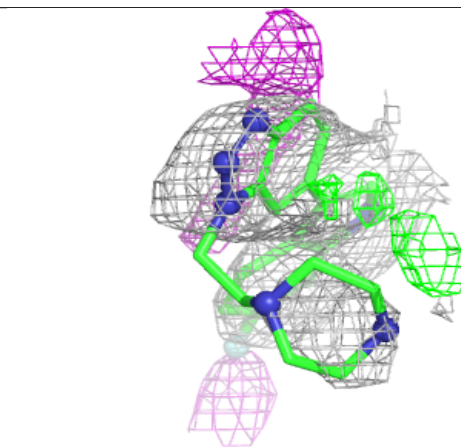
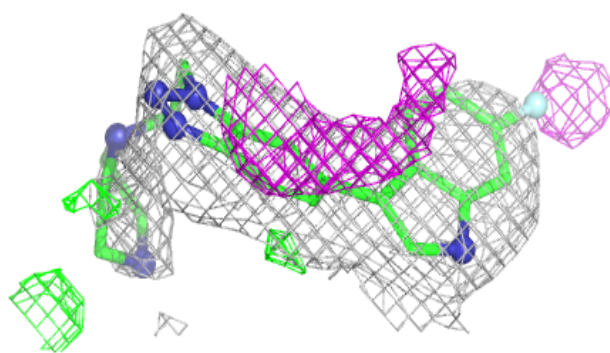
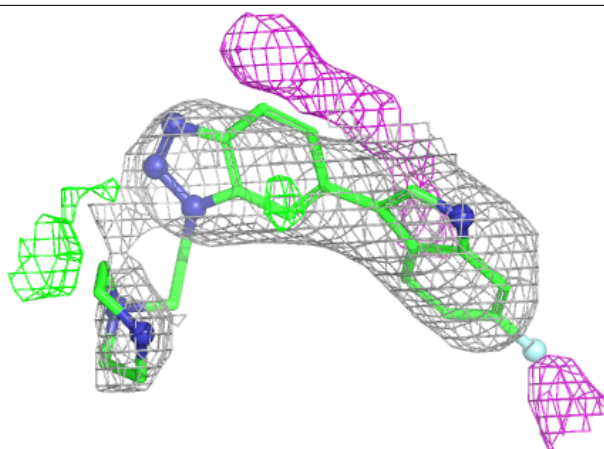
Electron density around A1AE7 A 403:

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

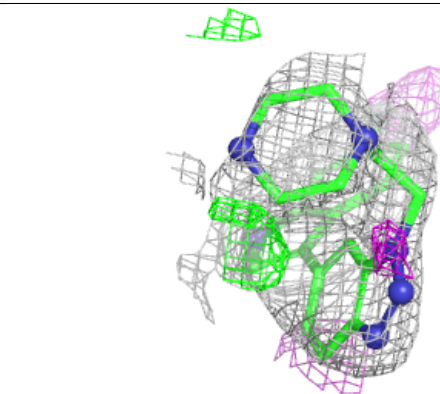
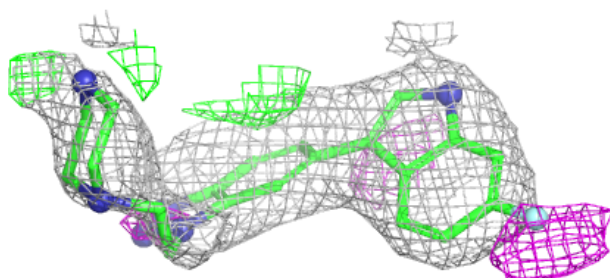
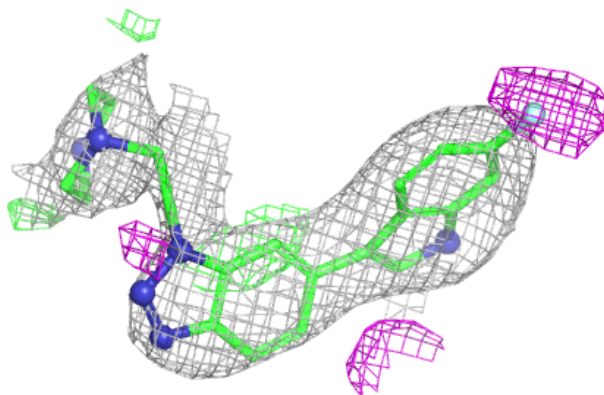


Electron density around A1AE7 B 403:

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

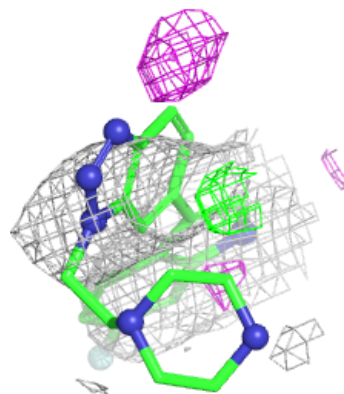
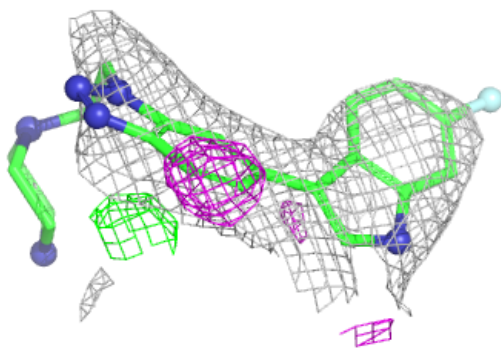
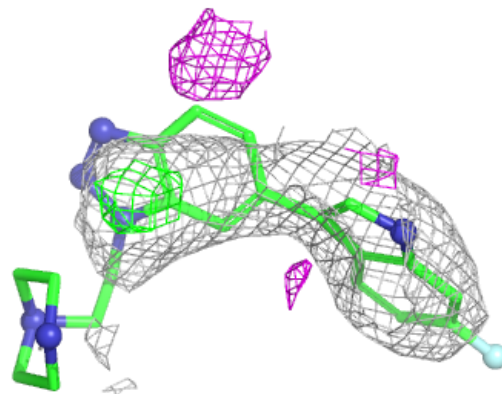
**Electron density around A1AE7 D 403:**

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



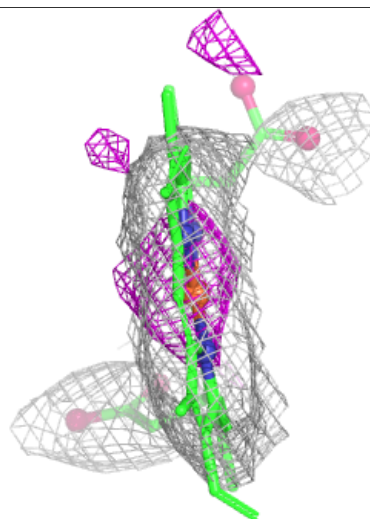
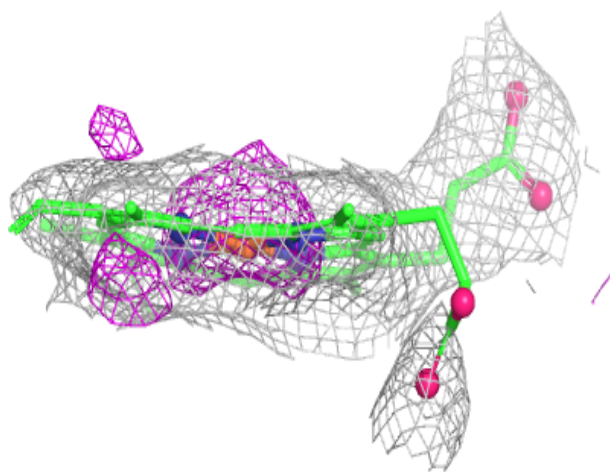
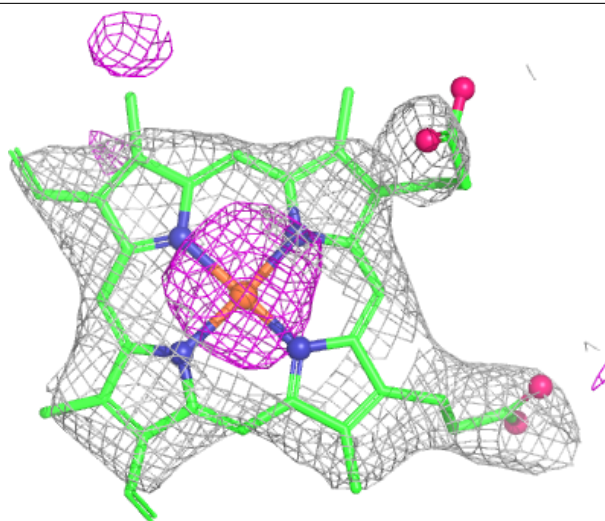
Electron density around A1AE7 C 403:

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



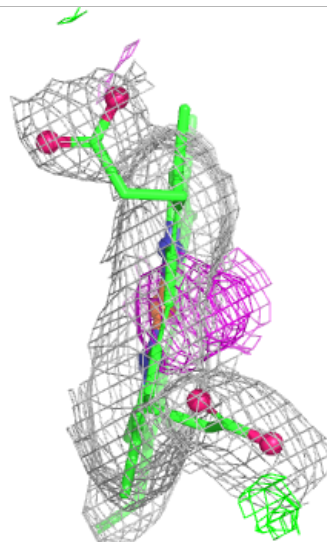
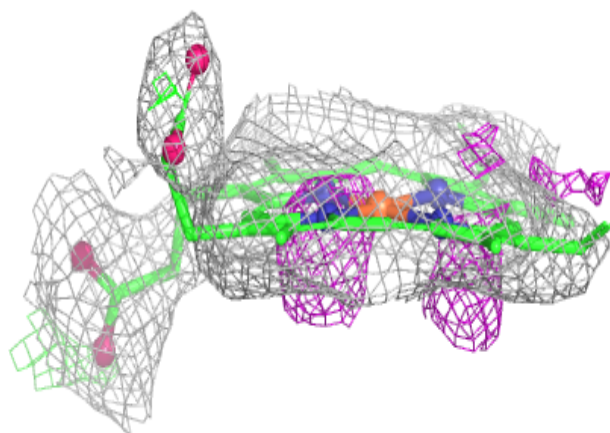
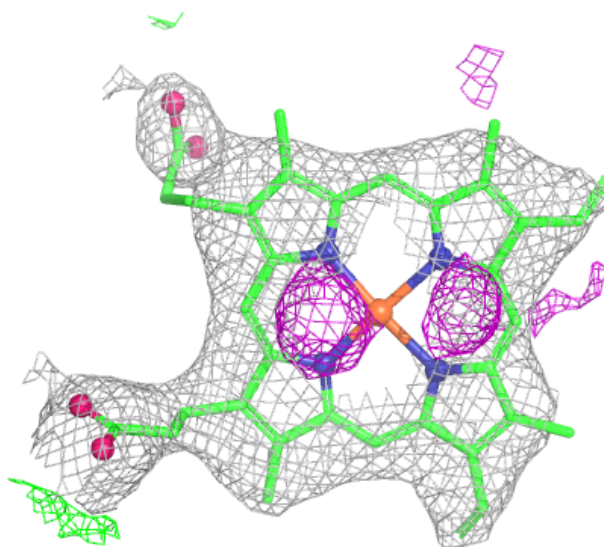
Electron density around HEM C 401:

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



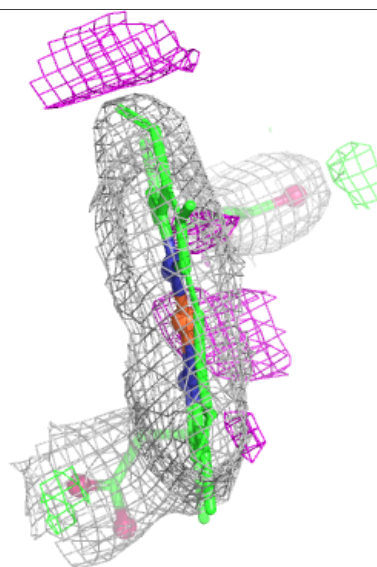
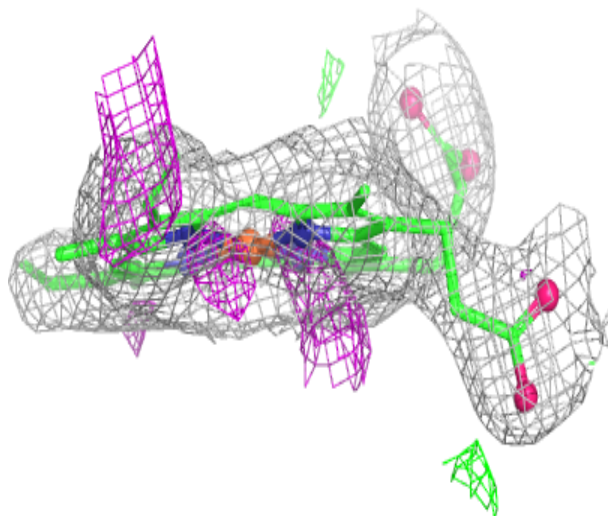
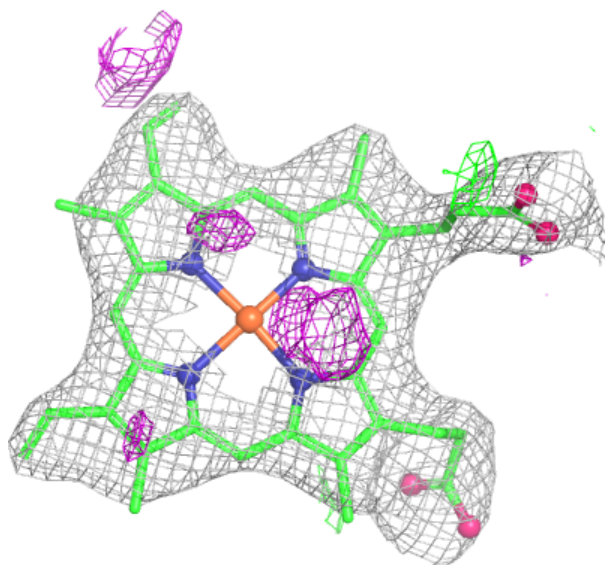
Electron density around HEM B 401:

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



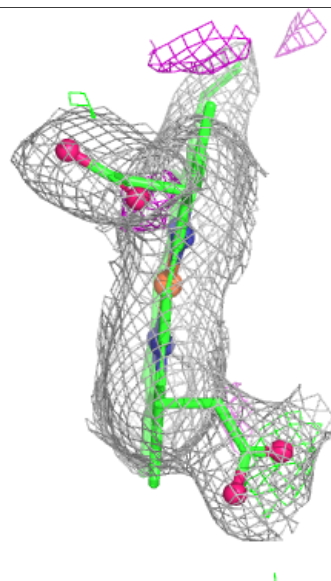
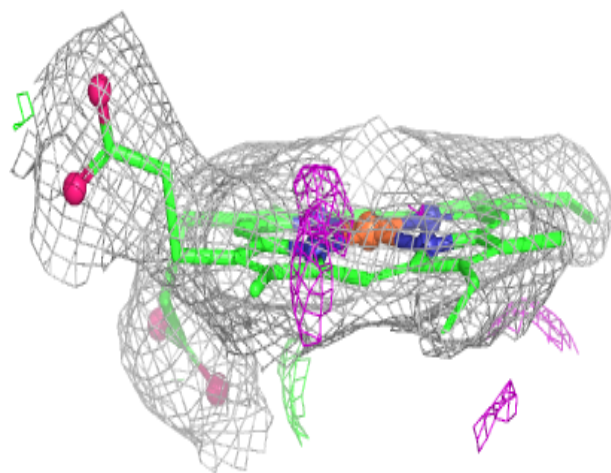
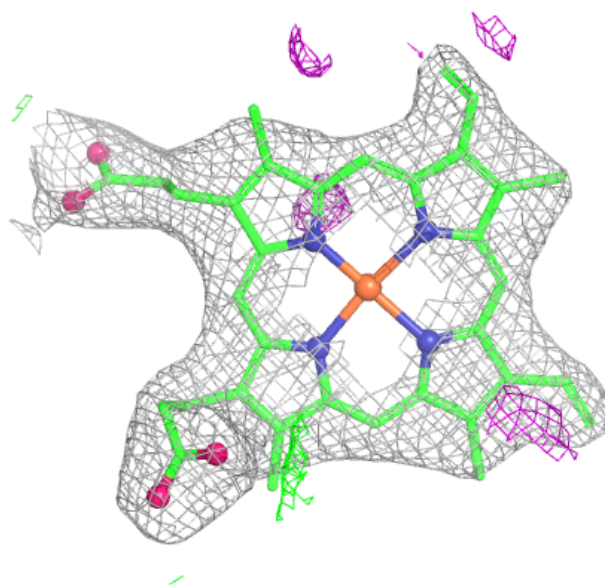
Electron density around HEM A 401:

$2mF_o-DF_c$ (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.