



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:51 PM UTC

PDB ID : 9AT2 / pdb_00009at2
Title : Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PAN3 inhibitor
Authors : Geeraerts, Z.; Yeh, S.-R.
Deposited on : 2024-02-26
Resolution : 2.25 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

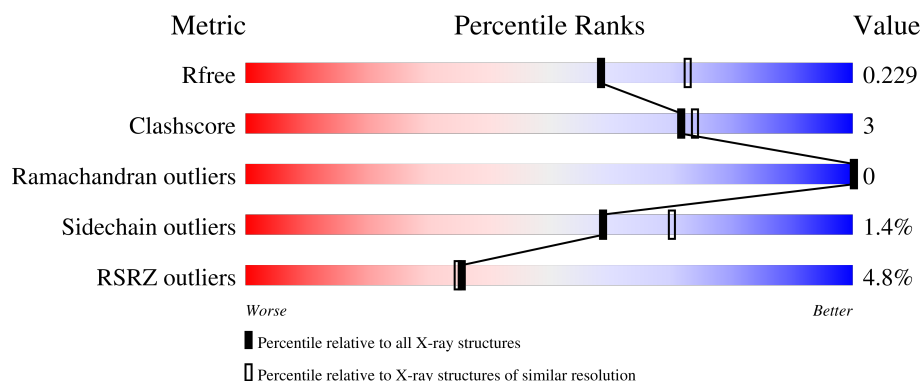
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	
1	B	380	
1	C	380	
1	D	380	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12007 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
			2936	1886	515	524	11			
1	B	346	Total	C	N	O	S	0	0	0
			2941	1890	516	524	11			
1	C	336	Total	C	N	O	S	0	0	0
			2860	1843	502	504	11			
1	D	342	Total	C	N	O	S	0	0	0
			2907	1870	509	517	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

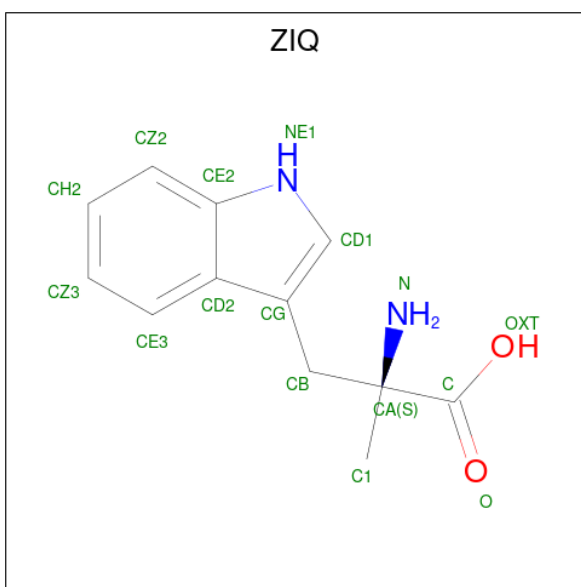
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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391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

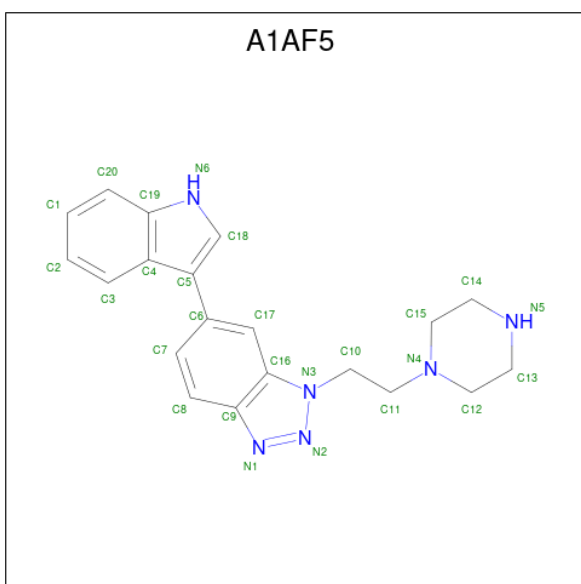
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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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-(1H-indol-3-yl)-1-[2-(piperazin-1-yl)ethyl]-1H-1,2,3-benzotriazole (CCD ID: A1AF5) (formula: C₂₀H₂₂N₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			26	20	6		
4	B	1	Total	C	N	0	0
			26	20	6		
4	C	1	Total	C	N	0	0
			26	20	6		
4	D	1	Total	C	N	0	0
			26	20	6		

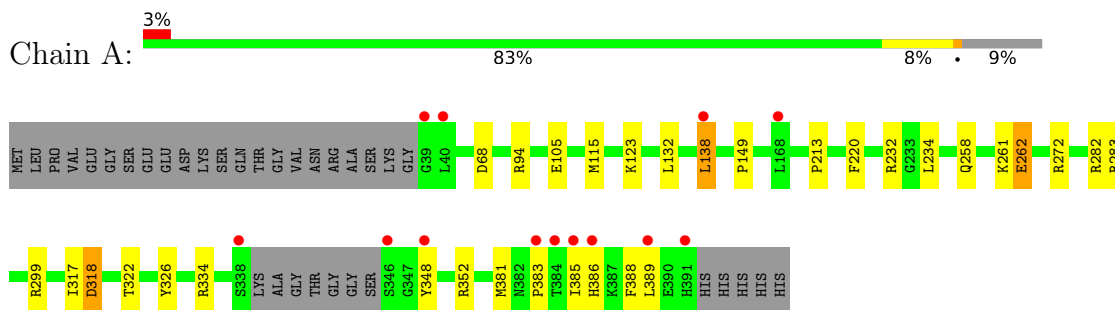
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	9	Total	O	0	0
			9	9		
5	C	3	Total	O	0	0
			3	3		
5	D	3	Total	O	0	0
			3	3		

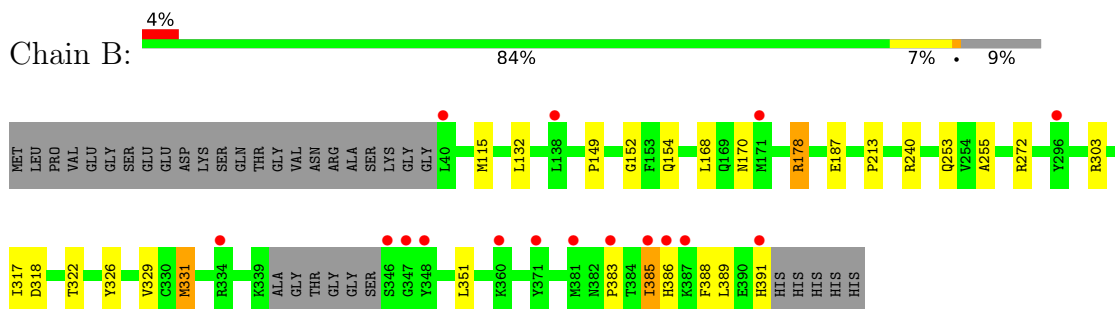
3 Residue-property plots

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.

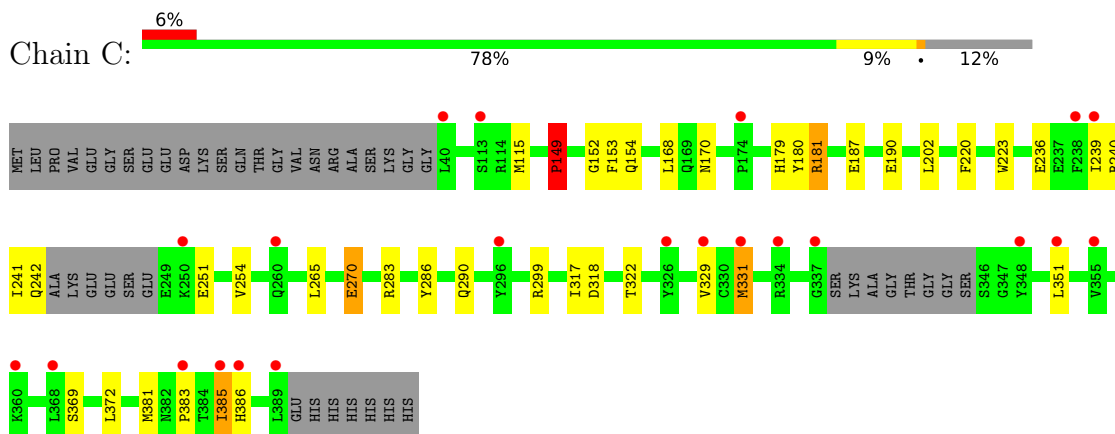
- Molecule 1: Tryptophan 2,3-dioxygenase



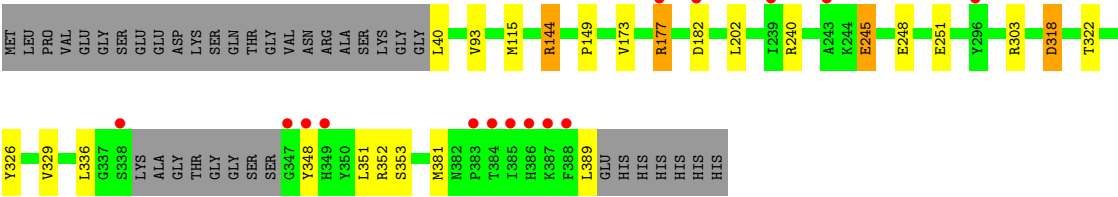
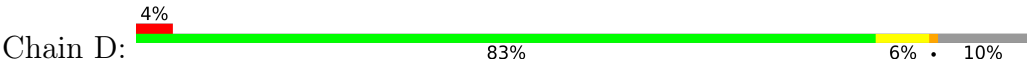
- Molecule 1: Tryptophan 2,3-dioxygenase



- 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	144.04Å 155.11Å 88.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.67 – 2.25 88.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (88.67-2.25) 99.8 (88.67-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.202 , 0.223 0.207 , 0.229	Depositor DCC
R_{free} test set	4874 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.9	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	12007	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: A1AF5, ZIQ, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	0/3005	1.04	4/4044 (0.1%)
1	B	0.62	2/3010 (0.1%)	1.03	1/4050 (0.0%)
1	C	0.55	0/2927	0.99	2/3939 (0.1%)
1	D	0.82	3/2975 (0.1%)	1.09	6/4004 (0.1%)
All	All	0.66	5/11917 (0.0%)	1.04	13/16037 (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	6
1	B	0	2
1	C	0	1
1	D	0	3
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	ARG	CZ-NH2	19.45	1.58	1.33
1	D	177	ARG	NE-CZ	16.30	1.50	1.33
1	D	177	ARG	CD-NE	14.44	1.66	1.46
1	B	255	ALA	CA-C	-6.20	1.45	1.52
1	B	253	GLN	C-N	5.18	1.40	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	ARG	NE-CZ-NH2	19.49	136.74	119.20
1	D	177	ARG	NE-CZ-NH1	-17.45	104.05	121.50
1	C	318	ASP	CA-CB-CG	6.59	119.19	112.60
1	D	318	ASP	CA-CB-CG	6.39	118.99	112.60
1	D	182	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	105	GLU	CB-CG-CD	5.68	122.25	112.60
1	C	149	PRO	N-CA-CB	-5.60	96.44	102.60
1	A	318	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	177	ARG	N-CA-CB	-5.40	103.92	112.08
1	A	68	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	262	GLU	CB-CG-CD	5.06	121.21	112.60
1	D	177	ARG	CD-NE-CZ	-5.01	117.39	124.40
1	B	178	ARG	NE-CZ-NH2	-5.00	114.70	119.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	282	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	94	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	240	ARG	Sidechain
1	C	181	ARG	Sidechain
1	D	144	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	240	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	2936	0	2917	19	0
1	B	2941	0	2927	16	0
1	C	2860	0	2854	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2907	0	2896	15	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	1	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	26	0	0	0	0
4	B	26	0	0	0	0
4	C	26	0	0	0	0
4	D	26	0	0	0	0
5	A	8	0	0	0	0
5	B	9	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
All	All	12007	0	11714	78	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 (78) 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	1.60	0.84
1:D:93:VAL:HG21	1:D:115:MET:HE3	1.61	0.82
1:C:383:PRO:HA	1:C:386:HIS:HB2	1.65	0.78
2:A:401:HEM:HBB2	2:A:401:HEM:HMB2	1.69	0.75
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.17	0.75
1:A:318:ASP:O	1:A:322:THR:HG23	1.89	0.73
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.20	0.72
1:A:138:LEU:HD13	1:C:299:ARG:NH1	2.05	0.71
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.20	0.71
1:C:239:ILE:HA	1:C:242:GLN:HE21	1.57	0.69
1:C:223:TRP:CG	1:C:290:GLN:HE21	2.12	0.67
1:A:220:PHE:HD1	1:A:385:ILE:HG12	1.63	0.63
1:C:220:PHE:HD1	1:C:385:ILE:HG21	1.67	0.59
1:C:381:MET:HG3	1:C:386:HIS:HD2	1.68	0.58
1:A:138:LEU:HD13	1:C:299:ARG:HH12	1.68	0.55
1:C:223:TRP:CD1	1:C:290:GLN:HE21	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:GLU:HG2	1:C:286:TYR:CD2	2.42	0.55
1:A:381:MET:SD	1:A:389:LEU:HD12	2.47	0.55
1:A:348:TYR:CZ	1:A:352:ARG:HD2	2.42	0.54
1:C:236:GLU:O	1:C:240:ARG:HG2	2.08	0.54
1:D:348:TYR:CZ	1:D:352:ARG:HD2	2.44	0.52
1:C:179:HIS:CE1	1:C:181:ARG:HB2	2.46	0.51
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	1.93	0.51
1:B:326:TYR:OH	1:D:322:THR:HG22	2.10	0.51
1:C:329:VAL:HG22	1:C:351:LEU:HB3	1.93	0.49
1:C:223:TRP:CG	1:C:290:GLN:NE2	2.79	0.49
2:B:401:HEM:HBC2	2:B:401:HEM:HHD	1.94	0.48
1:D:144:ARG:HE	1:D:336:LEU:HD22	1.79	0.48
1:B:168:LEU:HB3	1:B:170:ASN:OD1	2.14	0.48
1:C:241:ILE:HD12	1:C:254:VAL:HG13	1.95	0.47
1:D:303:ARG:HD3	1:D:389:LEU:HA	1.96	0.47
1:B:383:PRO:HA	1:B:386:HIS:HB2	1.97	0.47
1:A:234:LEU:HD13	1:A:261:LYS:HG3	1.97	0.47
1:D:381:MET:SD	1:D:389:LEU:HD12	2.55	0.47
1:C:187:GLU:HG3	1:C:190:GLU:OE2	2.15	0.47
1:D:115:MET:HA	1:D:115:MET:HE2	1.97	0.47
1:B:272:ARG:NH2	1:B:272:ARG:HG2	2.30	0.46
1:D:202:LEU:C	1:D:202:LEU:HD13	2.41	0.46
1:B:329:VAL:HG22	1:B:351:LEU:HB3	1.97	0.46
1:A:348:TYR:CE2	1:A:352:ARG:HD2	2.52	0.45
1:A:383:PRO:CA	1:A:386:HIS:HB3	2.37	0.45
1:B:385:ILE:HG22	1:B:388:PHE:CD1	2.52	0.45
1:C:149:PRO:HD2	1:D:40:LEU:HB3	1.99	0.45
1:C:270:GLU:HG2	1:C:286:TYR:CE2	2.51	0.44
1:D:248:GLU:HA	1:D:251:GLU:HB2	1.98	0.44
1:D:348:TYR:CE2	1:D:352:ARG:HD2	2.53	0.44
1:B:115:MET:HE3	1:B:317:ILE:HD13	1.96	0.44
1:A:258:GLN:O	1:A:262:GLU:HG2	2.18	0.44
1:A:326:TYR:OH	1:C:322:THR:HG22	2.18	0.43
2:A:401:HEM:HBB2	2:A:401:HEM:CMB	2.44	0.43
1:C:265:LEU:HD13	1:C:265:LEU:HA	1.92	0.43
1:C:168:LEU:HB3	1:C:170:ASN:OD1	2.18	0.43
1:A:283:ARG:NH2	1:A:283:ARG:CG	2.81	0.43
1:D:245:GLU:CD	1:D:245:GLU:H	2.25	0.43
1:A:283:ARG:HH21	1:A:283:ARG:HG2	1.83	0.42
1:A:381:MET:HG3	1:A:385:ILE:HG23	2.00	0.42
1:C:331:MET:HE3	1:C:331:MET:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:THR:HG22	1:D:326:TYR:OH	2.19	0.42
1:C:202:LEU:CD2	1:C:283:ARG:NH2	2.83	0.42
1:C:223:TRP:CD1	1:C:290:GLN:NE2	2.87	0.42
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.96	0.42
1:B:303:ARG:HD3	1:B:389:LEU:HA	2.01	0.41
1:D:173:VAL:HG11	1:D:353:SER:OG	2.20	0.41
1:A:283:ARG:CG	1:A:283:ARG:HH21	2.32	0.41
1:B:152:GLY:C	1:B:154:GLN:N	2.77	0.41
2:C:401:HEM:HBC2	2:C:401:HEM:HHD	2.01	0.41
1:B:272:ARG:HG2	1:B:272:ARG:HH21	1.83	0.41
1:C:241:ILE:HB	1:C:254:VAL:HG22	2.02	0.41
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.93	0.41
1:C:180:TYR:CZ	1:C:181:ARG:HG3	2.56	0.41
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.95	0.41
1:A:213:PRO:HB2	1:A:388:PHE:HE2	1.85	0.41
1:B:331:MET:HE3	1:B:331:MET:HB2	1.81	0.41
2:D:401:HEM:HBB2	2:D:401:HEM:CMB	2.51	0.41
1:D:329:VAL:HG22	1:D:351:LEU:HB3	2.02	0.40
1:C:369:SER:O	1:C:372:LEU:HG	2.21	0.40
1:B:213:PRO:HB2	1:B:388:PHE:HE2	1.86	0.40
1:C:152:GLY:C	1:C:154:GLN:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	334 (98%)	8 (2%)	0	100	100
1	B	342/380 (90%)	336 (98%)	6 (2%)	0	100	100
1	C	330/380 (87%)	324 (98%)	6 (2%)	0	100	100
1	D	338/380 (89%)	330 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1352/1520 (89%)	1324 (98%)	28 (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	322/348 (92%)	319 (99%)	3 (1%)	70	79
1	B	323/348 (93%)	317 (98%)	6 (2%)	50	61
1	C	314/348 (90%)	308 (98%)	6 (2%)	50	61
1	D	319/348 (92%)	316 (99%)	3 (1%)	70	79
All	All	1278/1392 (92%)	1260 (99%)	18 (1%)	59	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	138	LEU
1	A	149	PRO
1	B	149	PRO
1	B	187	GLU
1	B	318	ASP
1	B	331	MET
1	B	385	ILE
1	B	391	HIS
1	C	149	PRO
1	C	153	PHE
1	C	251	GLU
1	C	270	GLU
1	C	331	MET
1	C	385	ILE
1	D	149	PRO
1	D	245	GLU

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Mol	Chain	Res	Type
1	D	318	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	170	ASN
1	A	189	ASN
1	A	309	GLN
1	B	183	ASN
1	B	197	GLN
1	B	258	GLN
1	B	260	GLN
1	B	309	GLN
1	B	382	ASN
1	C	189	ASN
1	C	242	GLN
1	C	258	GLN
1	C	260	GLN
1	C	309	GLN
1	C	382	ASN
1	C	386	HIS
1	D	44	ASN
1	D	189	ASN
1	D	290	GLN
1	D	309	GLN
1	D	376	HIS
1	D	382	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	ZIQ	D	402	-	14,17,17	0.69	0	20,25,25	1.11	2 (10%)
4	A1AF5	D	403	-	30,30,30	0.74	0	42,42,42	0.71	1 (2%)
4	A1AF5	A	403	-	30,30,30	0.70	1 (3%)	42,42,42	0.76	1 (2%)
3	ZIQ	C	402	-	14,17,17	0.56	0	20,25,25	1.26	2 (10%)
2	HEM	C	401	1	50,50,50	1.68	8 (16%)	67,82,82	1.72	15 (22%)
2	HEM	A	401	1	50,50,50	1.67	11 (22%)	67,82,82	1.72	13 (19%)
2	HEM	D	401	1	50,50,50	1.63	13 (26%)	67,82,82	1.61	13 (19%)
3	ZIQ	A	402	-	14,17,17	0.58	0	20,25,25	1.25	3 (15%)
3	ZIQ	B	402	-	14,17,17	0.77	0	20,25,25	1.53	3 (15%)
4	A1AF5	B	403	-	30,30,30	0.58	0	42,42,42	0.75	1 (2%)
2	HEM	B	401	1	50,50,50	1.59	8 (16%)	67,82,82	1.69	14 (20%)
4	A1AF5	C	403	-	30,30,30	0.59	0	42,42,42	0.72	1 (2%)

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	ZIQ	D	402	-	-	4/11/11/11	0/2/2/2
4	A1AF5	D	403	-	-	2/9/17/17	1/5/5/5
4	A1AF5	A	403	-	-	2/9/17/17	0/5/5/5
3	ZIQ	C	402	-	-	4/11/11/11	0/2/2/2
2	HEM	C	401	1	-	2/14/54/54	-
2	HEM	A	401	1	-	2/14/54/54	-
2	HEM	D	401	1	-	2/14/54/54	-
3	ZIQ	A	402	-	-	4/11/11/11	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZIQ	B	402	-	-	1/11/11/11	0/2/2/2
4	A1AF5	B	403	-	-	2/9/17/17	1/5/5/5
2	HEM	B	401	1	-	2/14/54/54	-
4	A1AF5	C	403	-	-	0/9/17/17	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	FE-NB	5.51	2.11	1.94
2	B	401	HEM	FE-NB	5.24	2.11	1.94
2	A	401	HEM	FE-NB	4.82	2.09	1.94
2	C	401	HEM	FE-NC	4.31	2.09	1.95
2	B	401	HEM	FE-NC	4.22	2.09	1.95
2	B	401	HEM	C1B-NB	-4.03	1.33	1.40
2	C	401	HEM	C4D-ND	-4.00	1.33	1.40
2	A	401	HEM	C1B-NB	-3.78	1.33	1.40
2	D	401	HEM	FE-NB	3.70	2.06	1.94
2	C	401	HEM	C1B-NB	-3.62	1.34	1.40
2	D	401	HEM	FE-NC	3.61	2.07	1.95
2	D	401	HEM	C1C-C2C	-3.51	1.38	1.45
2	A	401	HEM	FE-NC	3.43	2.06	1.95
2	A	401	HEM	C1C-C2C	-3.40	1.38	1.45
2	D	401	HEM	C1B-NB	-3.32	1.34	1.40
2	C	401	HEM	C1C-C2C	-3.26	1.38	1.45
2	A	401	HEM	C1D-ND	-3.18	1.32	1.38
2	D	401	HEM	C4B-NB	-3.04	1.32	1.38
2	D	401	HEM	C4D-ND	-2.78	1.35	1.40
2	B	401	HEM	C4D-ND	-2.68	1.35	1.40
2	D	401	HEM	C3C-C4C	-2.67	1.41	1.46
2	B	401	HEM	C1C-NC	-2.65	1.34	1.39
2	A	401	HEM	C4B-NB	-2.60	1.33	1.38
2	D	401	HEM	O1D-CGD	2.59	1.30	1.22
2	D	401	HEM	C1C-NC	-2.58	1.34	1.39
2	D	401	HEM	FE-NA	2.57	2.03	1.95
2	C	401	HEM	C4B-NB	-2.45	1.34	1.38
2	B	401	HEM	C4B-NB	-2.40	1.34	1.38
4	A	403	A1AF5	C17-C6	-2.36	1.36	1.39
2	B	401	HEM	C1C-C2C	-2.34	1.40	1.45
2	C	401	HEM	C3C-C4C	-2.33	1.41	1.46
2	A	401	HEM	C3C-C4C	-2.28	1.42	1.46
2	A	401	HEM	C1C-NC	-2.27	1.35	1.39
2	D	401	HEM	C4A-NA	-2.25	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	FE-NA	2.15	2.02	1.95
2	B	401	HEM	C1D-ND	-2.14	1.34	1.38
2	C	401	HEM	FE-ND	-2.08	1.88	1.94
2	D	401	HEM	C1A-C2A	-2.07	1.40	1.44
2	A	401	HEM	C1A-C2A	-2.06	1.40	1.44
2	D	401	HEM	FE-ND	-2.05	1.88	1.94
2	A	401	HEM	FE-ND	-2.02	1.88	1.94

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	ZIQ	CB-CA-C	4.90	115.83	109.10
2	C	401	HEM	CHC-C4B-NB	4.77	129.56	124.42
2	A	401	HEM	CHC-C4B-NB	4.62	129.40	124.42
2	A	401	HEM	CHA-C4D-ND	4.58	130.03	124.37
2	D	401	HEM	CHD-C1D-ND	4.19	128.93	124.42
2	B	401	HEM	CHD-C1D-ND	4.15	128.89	124.42
2	D	401	HEM	CHB-C1B-NB	4.03	129.35	124.37
2	A	401	HEM	C1B-NB-C4B	3.92	109.86	105.21
2	B	401	HEM	CHC-C4B-NB	3.85	128.57	124.42
2	B	401	HEM	C1B-NB-C4B	3.85	109.76	105.21
2	D	401	HEM	CHC-C4B-NB	3.81	128.53	124.42
2	A	401	HEM	CBD-CAD-C3D	-3.77	102.10	112.53
2	C	401	HEM	CBD-CAD-C3D	-3.71	102.27	112.53
3	C	402	ZIQ	CB-CA-C	3.65	114.12	109.10
2	A	401	HEM	CHD-C1D-ND	3.63	128.33	124.42
3	A	402	ZIQ	O-C-CA	-3.57	116.37	122.78
2	C	401	HEM	CHD-C1D-ND	3.56	128.25	124.42
2	C	401	HEM	C1B-NB-C4B	3.46	109.31	105.21
2	B	401	HEM	CBD-CAD-C3D	-3.46	102.97	112.53
3	C	402	ZIQ	O-C-CA	-3.37	116.73	122.78
3	D	402	ZIQ	O-C-CA	-3.37	116.73	122.78
2	C	401	HEM	CHA-C4D-ND	3.36	128.52	124.37
3	B	402	ZIQ	O-C-CA	-3.31	116.84	122.78
2	A	401	HEM	CHB-C1B-NB	3.29	128.44	124.37
2	B	401	HEM	CHA-C4D-ND	3.26	128.40	124.37
2	D	401	HEM	CHA-C4D-ND	3.25	128.39	124.37
2	D	401	HEM	CBD-CAD-C3D	-3.23	103.60	112.53
2	C	401	HEM	CHB-C1B-NB	3.23	128.36	124.37
2	B	401	HEM	CHB-C1B-NB	3.18	128.29	124.37
2	D	401	HEM	C1B-NB-C4B	2.96	108.71	105.21
2	B	401	HEM	CHD-C4C-NC	2.91	127.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CHD-C4C-NC	2.90	127.61	124.45
2	C	401	HEM	CHD-C4C-NC	2.89	127.59	124.45
4	B	403	A1AF5	C17-C16-N3	2.85	134.40	131.30
2	D	401	HEM	C4C-NC-C1C	2.80	110.39	105.82
4	C	403	A1AF5	C17-C16-N3	2.76	134.30	131.30
2	A	401	HEM	C4C-NC-C1C	2.67	110.18	105.82
2	D	401	HEM	CHD-C4C-NC	2.67	127.36	124.45
4	A	403	A1AF5	C17-C16-N3	2.65	134.18	131.30
2	B	401	HEM	CHD-C1D-C2D	-2.62	120.88	125.03
3	D	402	ZIQ	CB-CA-C	2.55	112.61	109.10
4	D	403	A1AF5	C17-C16-N3	2.53	134.06	131.30
2	C	401	HEM	C4C-NC-C1C	2.49	109.89	105.82
2	D	401	HEM	CHB-C1B-C2B	-2.47	119.92	126.95
2	D	401	HEM	CHD-C1D-C2D	-2.46	121.15	125.03
2	D	401	HEM	CAD-C3D-C4D	2.45	128.97	124.70
2	A	401	HEM	CHA-C4D-C3D	-2.38	120.84	125.23
2	B	401	HEM	O2A-CGA-CBA	2.37	121.49	114.00
2	A	401	HEM	CHD-C1D-C2D	-2.37	121.29	125.03
2	C	401	HEM	CMD-C2D-C1D	2.37	128.73	125.03
2	A	401	HEM	CMD-C2D-C1D	2.35	128.70	125.03
3	A	402	ZIQ	C1-CA-CB	-2.33	107.55	110.82
2	B	401	HEM	C4C-NC-C1C	2.26	109.51	105.82
2	D	401	HEM	C1A-CHA-C4D	-2.23	121.01	126.25
2	A	401	HEM	C3B-C4B-NB	-2.22	107.87	109.47
2	C	401	HEM	C4B-C3B-C2B	-2.20	105.26	107.28
2	C	401	HEM	CHD-C1D-C2D	-2.19	121.56	125.03
2	D	401	HEM	CHA-C4D-C3D	-2.19	121.19	125.23
2	B	401	HEM	CAD-C3D-C4D	2.18	128.50	124.70
2	C	401	HEM	CAC-C3C-C4C	2.18	130.02	124.82
3	B	402	ZIQ	C1-CA-CB	-2.16	107.79	110.82
2	B	401	HEM	C3B-C4B-NB	-2.13	107.94	109.47
2	B	401	HEM	O2A-CGA-O1A	-2.13	117.86	123.33
2	C	401	HEM	C4D-ND-C1D	2.11	107.71	105.21
2	C	401	HEM	C1A-CHA-C4D	-2.11	121.28	126.25
2	B	401	HEM	CAC-C3C-C4C	2.07	129.75	124.82
2	C	401	HEM	CAC-C3C-C2C	-2.05	121.75	128.43
2	A	401	HEM	C4C-CHD-C1D	-2.05	121.66	126.02
3	A	402	ZIQ	CB-CA-C	2.04	111.90	109.10

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	ZIQ	O-C-CA-C1
3	A	402	ZIQ	OXT-C-CA-C1
3	C	402	ZIQ	OXT-C-CA-N
3	D	402	ZIQ	O-C-CA-C1
3	D	402	ZIQ	OXT-C-CA-C1
4	A	403	A1AF5	C10-C11-N4-C12
4	A	403	A1AF5	C10-C11-N4-C15
3	A	402	ZIQ	O-C-CA-CB
3	A	402	ZIQ	OXT-C-CA-CB
3	D	402	ZIQ	O-C-CA-CB
3	D	402	ZIQ	OXT-C-CA-CB
4	B	403	A1AF5	C10-C11-N4-C12
4	B	403	A1AF5	C10-C11-N4-C15
3	B	402	ZIQ	O-C-CA-C1
3	C	402	ZIQ	O-C-CA-C1
2	D	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O1A
4	D	403	A1AF5	C10-C11-N4-C12
4	D	403	A1AF5	C10-C11-N4-C15
2	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O2A
3	C	402	ZIQ	OXT-C-CA-C1
2	C	401	HEM	CAA-CBA-CGA-O2A
3	C	402	ZIQ	OXT-C-CA-CB

All (2) ring outliers are listed below:

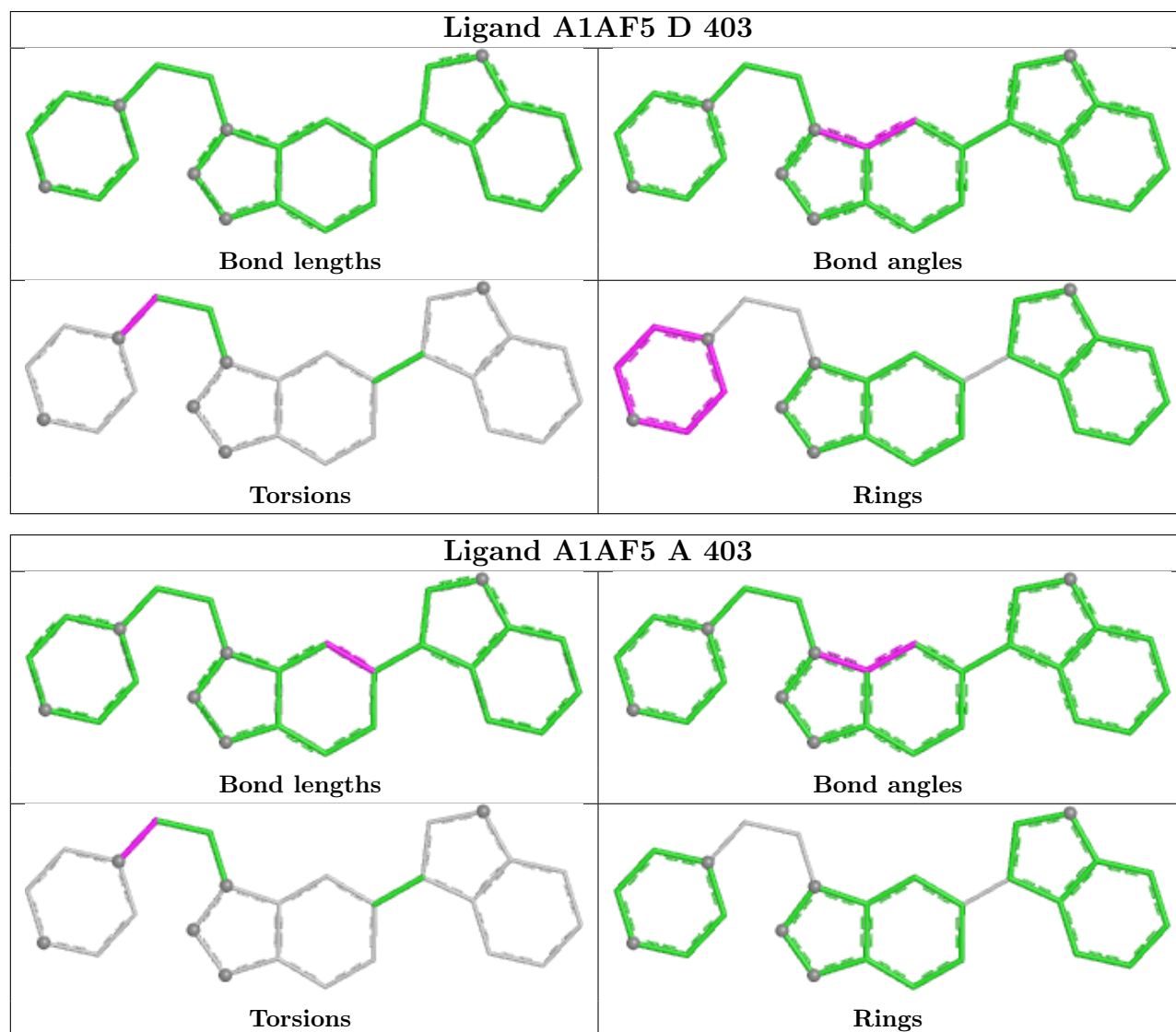
Mol	Chain	Res	Type	Atoms
4	B	403	A1AF5	C12-C13-C14-C15-N4-N5
4	D	403	A1AF5	C12-C13-C14-C15-N4-N5

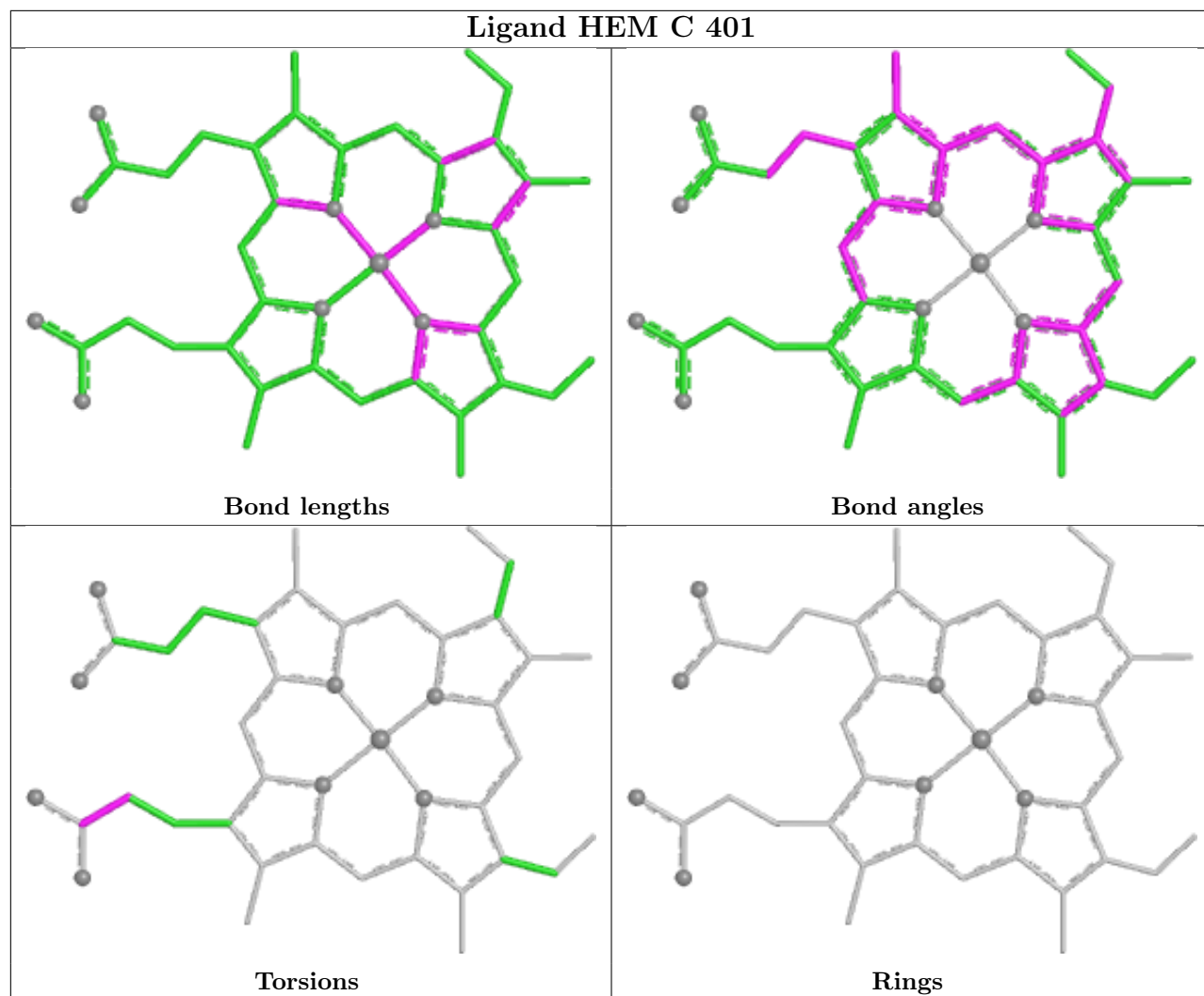
4 monomers are involved in 6 short contacts:

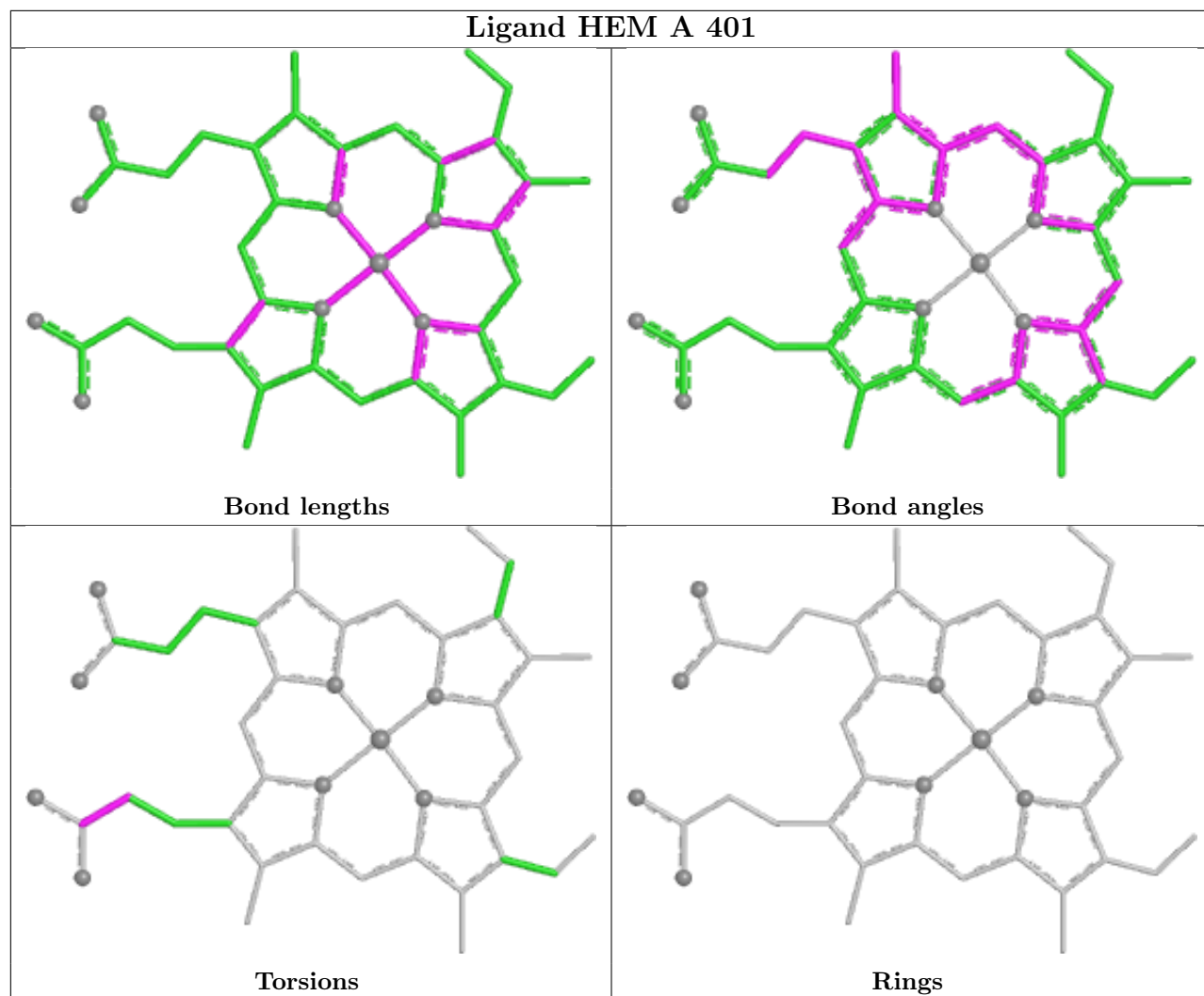
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	HEM	1	0
2	A	401	HEM	2	0
2	D	401	HEM	2	0
2	B	401	HEM	1	0

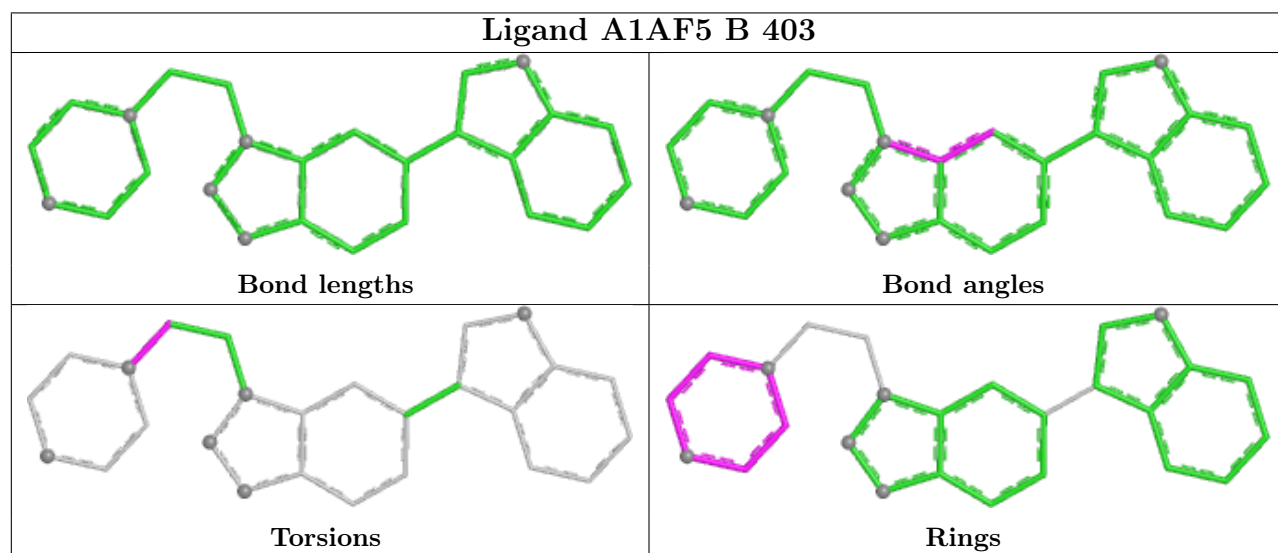
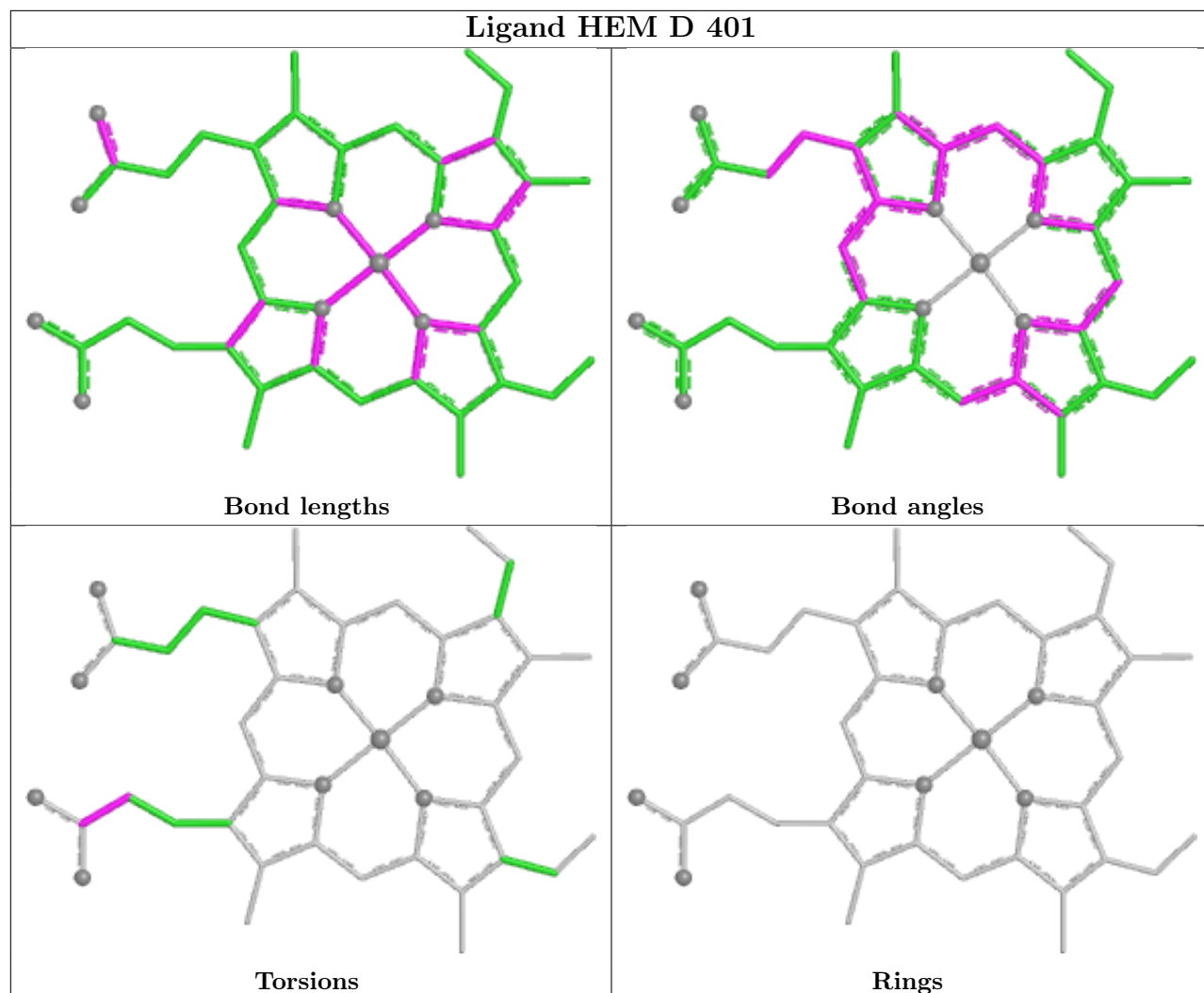
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

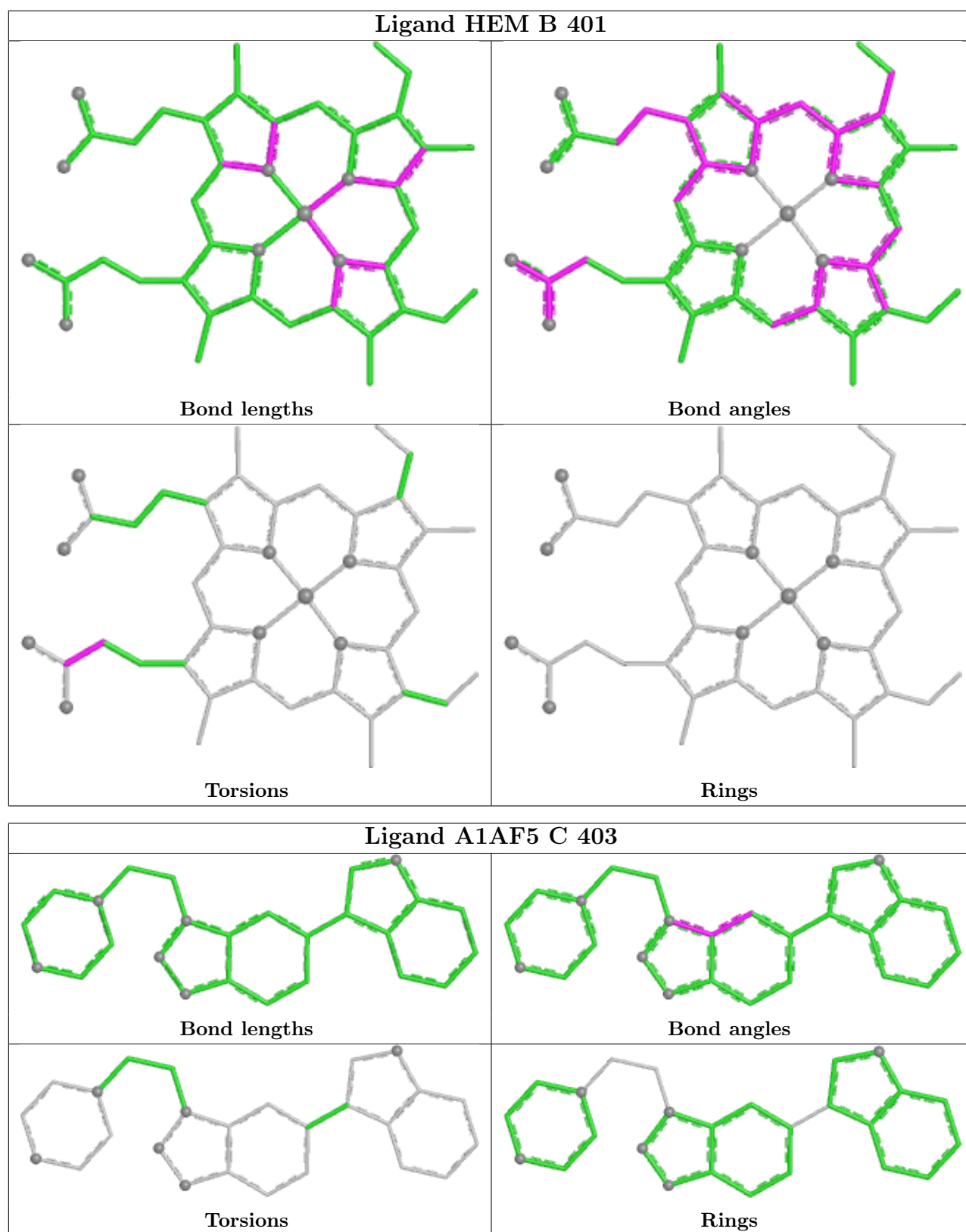
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.30	13 (3%) 44 44	50, 71, 134, 209	0
1	B	346/380 (91%)	0.36	16 (4%) 37 36	50, 77, 138, 223	0
1	C	336/380 (88%)	0.58	22 (6%) 25 23	55, 97, 193, 252	0
1	D	342/380 (90%)	0.34	15 (4%) 39 38	50, 78, 154, 233	0
All	All	1370/1520 (90%)	0.39	66 (4%) 35 35	50, 80, 159, 252	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ILE	4.7
1	C	40	LEU	4.4
1	D	385	ILE	4.2
1	B	386	HIS	4.1
1	B	383	PRO	4.1
1	C	326	TYR	3.9
1	A	138	LEU	3.9
1	D	386	HIS	3.9
1	A	386	HIS	3.8
1	B	385	ILE	3.8
1	A	40	LEU	3.7
1	C	389	LEU	3.6
1	C	250	LYS	3.5
1	C	296	TYR	3.5
1	C	385	ILE	3.5
1	A	384	THR	3.4
1	A	338	SER	3.4
1	D	348	TYR	3.4
1	B	296	TYR	3.3
1	D	338	SER	3.2
1	D	383	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	347	GLY	3.1
1	C	383	PRO	3.1
1	C	174	PRO	3.1
1	C	348	TYR	3.0
1	B	40	LEU	3.0
1	A	391	HIS	2.9
1	D	347	GLY	2.8
1	A	168	LEU	2.8
1	D	384	THR	2.8
1	D	239	ILE	2.7
1	C	368	LEU	2.7
1	C	337	GLY	2.7
1	C	260	GLN	2.6
1	B	348	TYR	2.6
1	D	388	PHE	2.6
1	B	391	HIS	2.6
1	D	177	ARG	2.5
1	A	348	TYR	2.5
1	A	346	SER	2.5
1	D	296	TYR	2.5
1	C	334	ARG	2.4
1	C	329	VAL	2.4
1	B	138	LEU	2.4
1	B	334	ARG	2.4
1	C	355	VAL	2.4
1	B	381	MET	2.4
1	A	389	LEU	2.3
1	D	243	ALA	2.3
1	C	113	SER	2.3
1	C	386	HIS	2.3
1	B	360	LYS	2.3
1	D	182	ASP	2.2
1	B	171	MET	2.2
1	C	360	LYS	2.2
1	C	239	ILE	2.2
1	C	331	MET	2.2
1	D	349	HIS	2.2
1	B	371	TYR	2.1
1	D	387	LYS	2.1
1	B	387	LYS	2.0
1	C	351	LEU	2.0
1	A	39	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	238	PHE	2.0
1	B	346	SER	2.0
1	A	383	PRO	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](#)

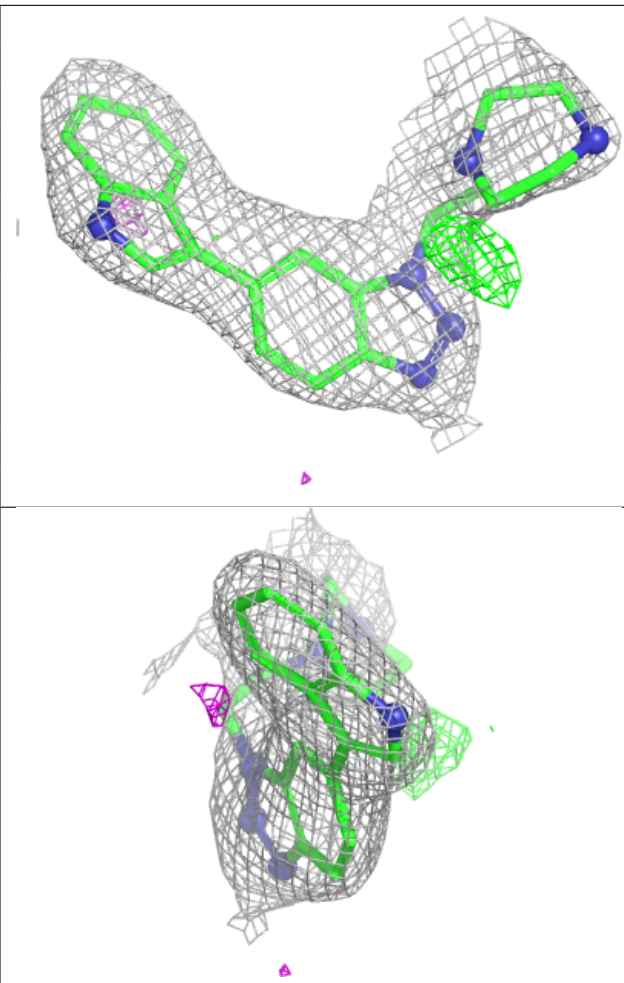
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1AF5	A	403	26/26	0.86	0.15	76,95,153,157	0
4	A1AF5	B	403	26/26	0.87	0.17	78,93,144,146	0
4	A1AF5	C	403	26/26	0.87	0.14	102,124,162,167	0
4	A1AF5	D	403	26/26	0.88	0.15	69,81,125,130	0
2	HEM	C	401	43/43	0.95	0.12	78,92,117,129	0
3	ZIQ	A	402	16/16	0.95	0.09	52,60,77,81	0
3	ZIQ	B	402	16/16	0.95	0.10	64,74,79,85	0
3	ZIQ	C	402	16/16	0.95	0.10	81,92,112,116	0
3	ZIQ	D	402	16/16	0.96	0.08	67,71,81,83	0
2	HEM	B	401	43/43	0.97	0.09	62,76,95,103	0
2	HEM	A	401	43/43	0.97	0.08	57,70,84,98	0
2	HEM	D	401	43/43	0.98	0.07	55,65,78,103	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.

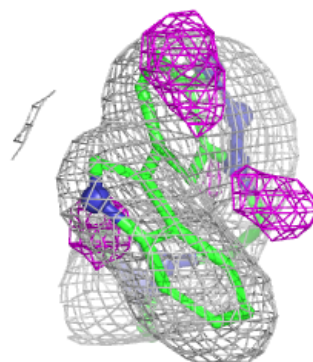
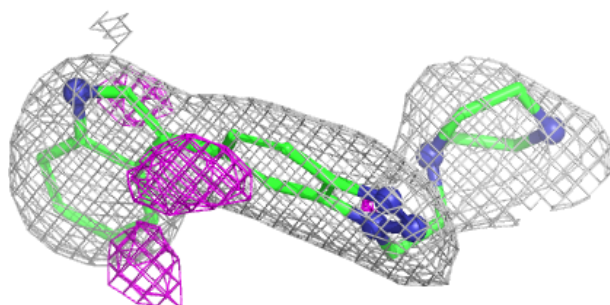
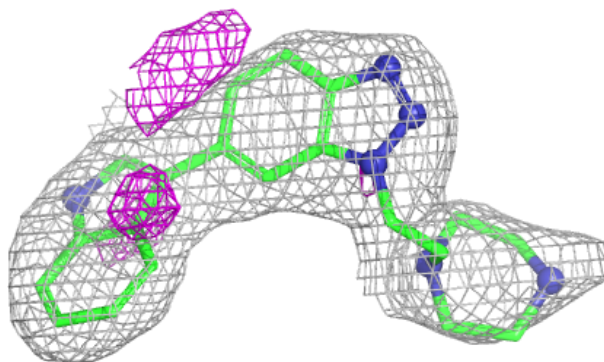
Electron density around A1AF5 A 403:

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

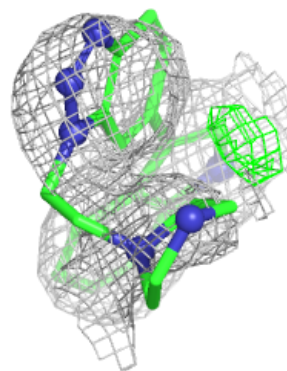
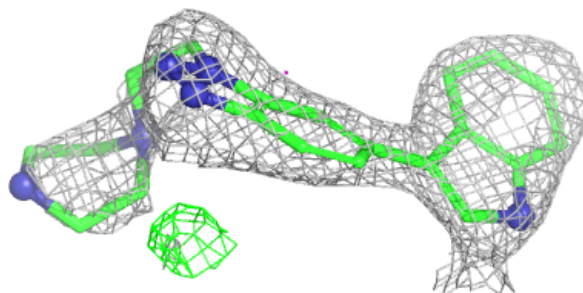
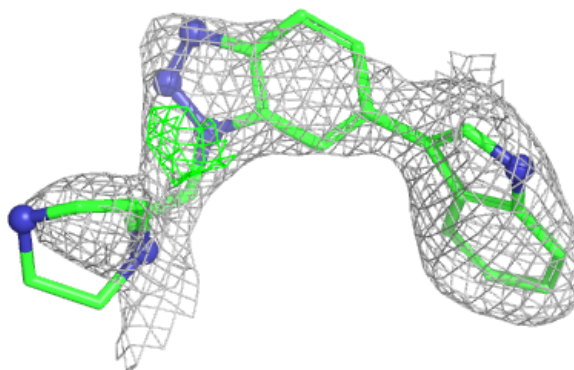


Electron density around A1AF5 B 403:

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

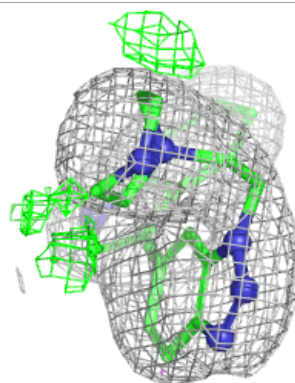
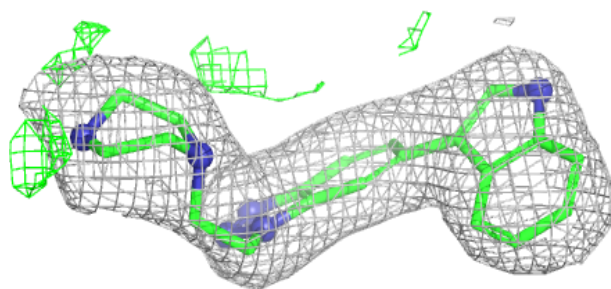
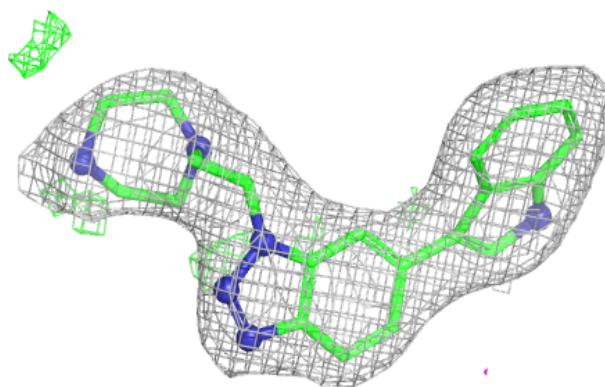
**Electron density around A1AF5 C 403:**

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



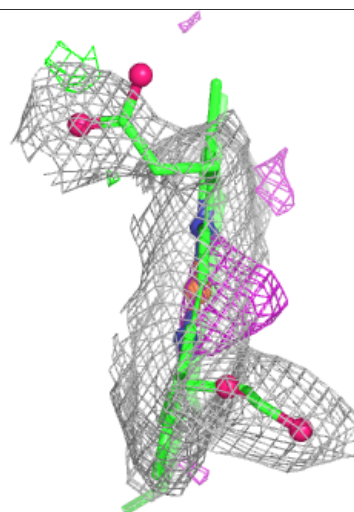
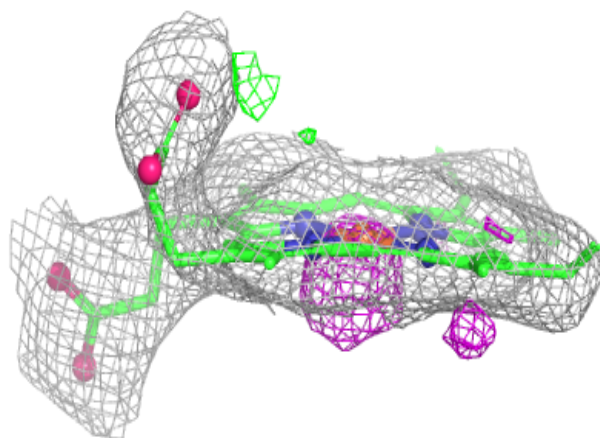
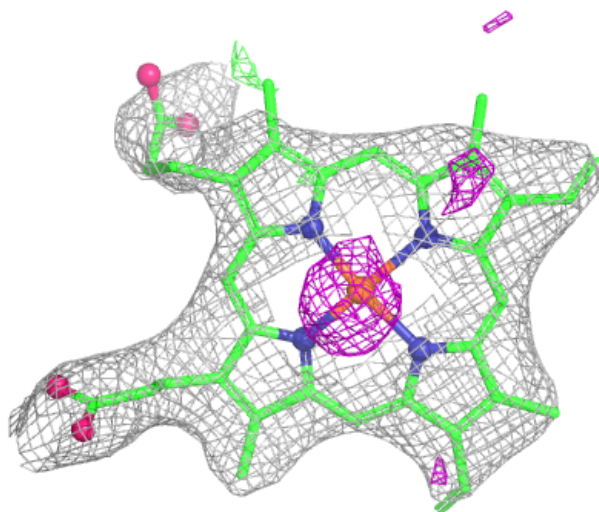
Electron density around A1AF5 D 403:

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



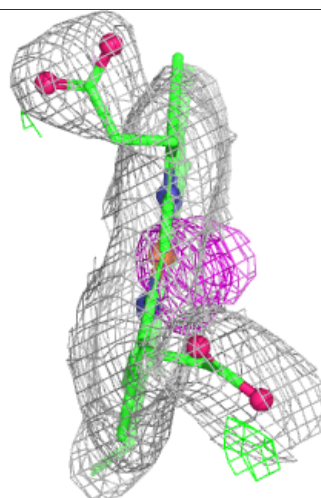
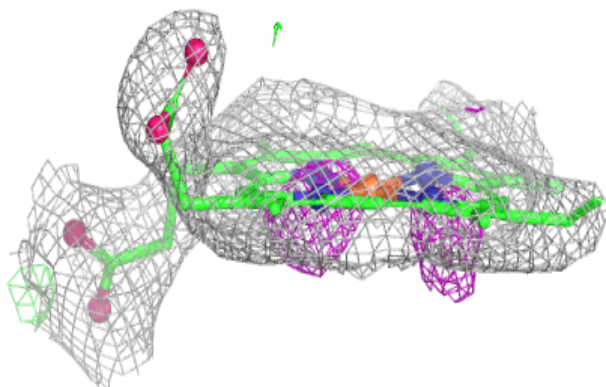
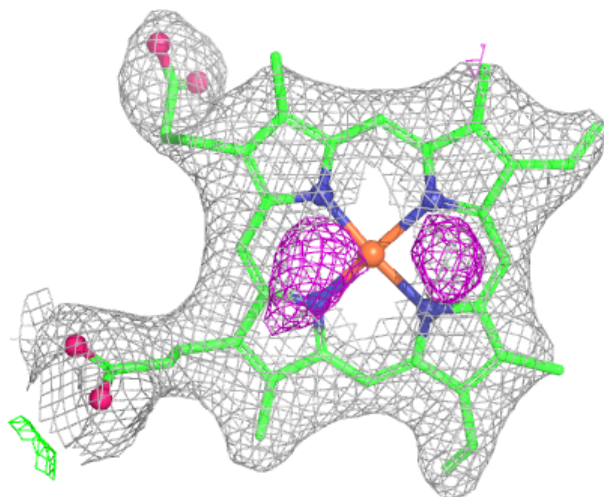
Electron density around HEM C 401:

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



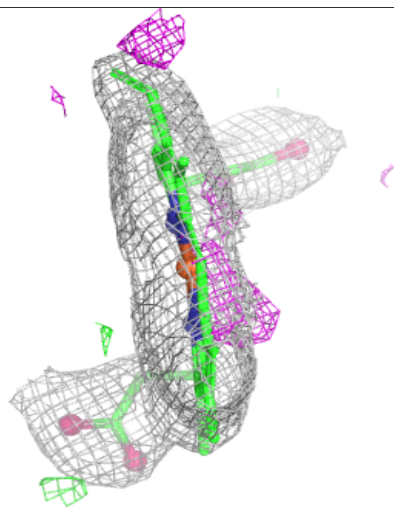
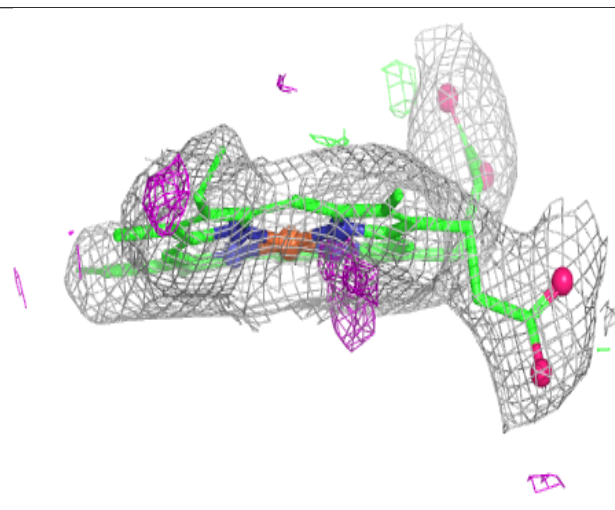
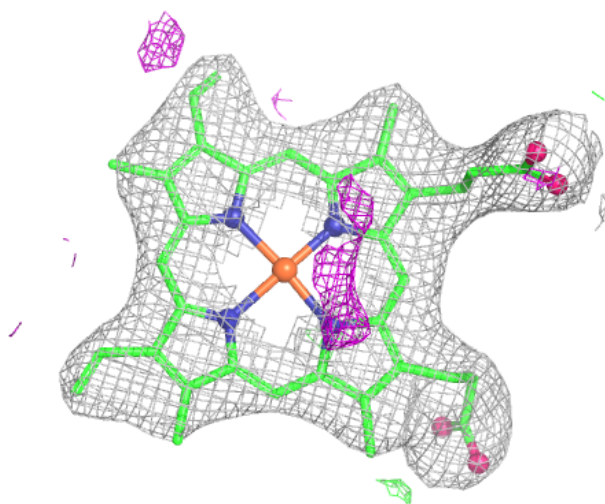
Electron density around HEM B 401:

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



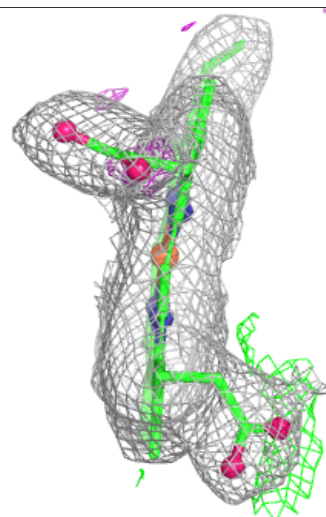
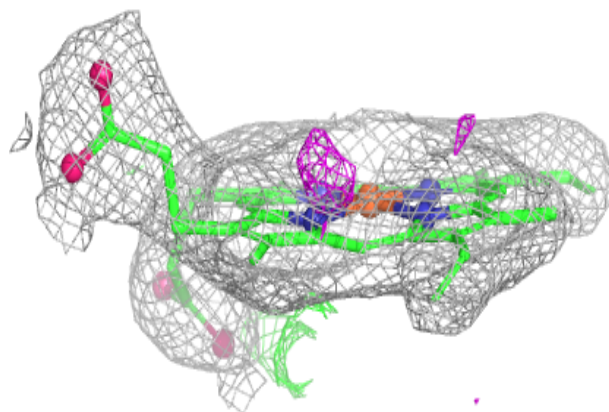
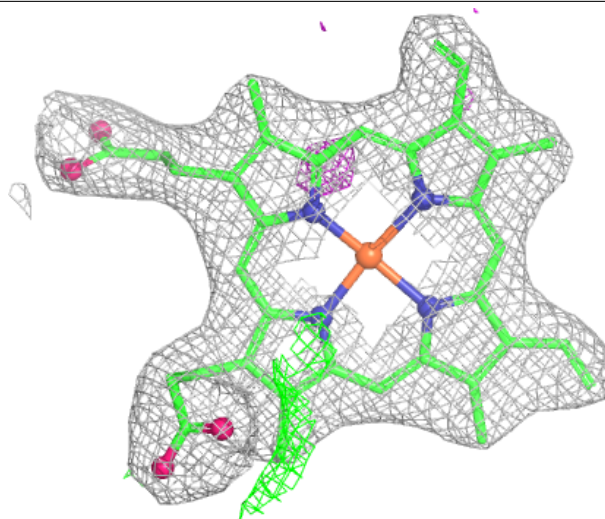
Electron density around HEM A 401:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.