



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:47 PM UTC

PDB ID : 8VTQ / pdb_00008vtq
Title : Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PPN3 inhibitor
Authors : Geeraerts, Z.; Yeh, S.-R.
Deposited on : 2024-01-26
Resolution : 2.05 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

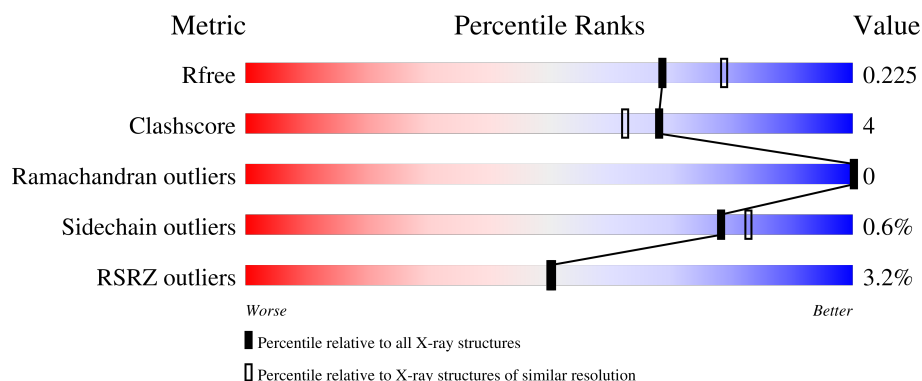
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

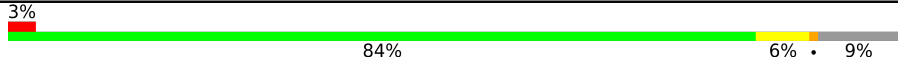
The reported resolution of this entry is 2.05 Å.

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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 12206 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.

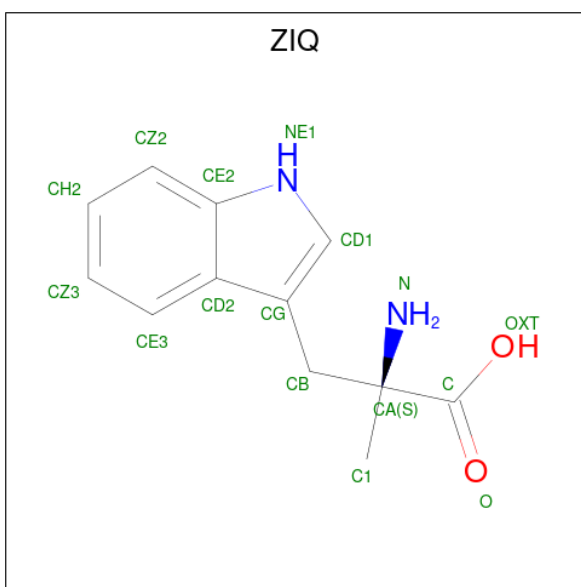
- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2947	1893	517	526	11			
1	B	347	Total	C	N	O	S	0	0	0
			2946	1893	517	525	11			
1	C	344	Total	C	N	O	S	0	0	0
			2918	1876	511	520	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:

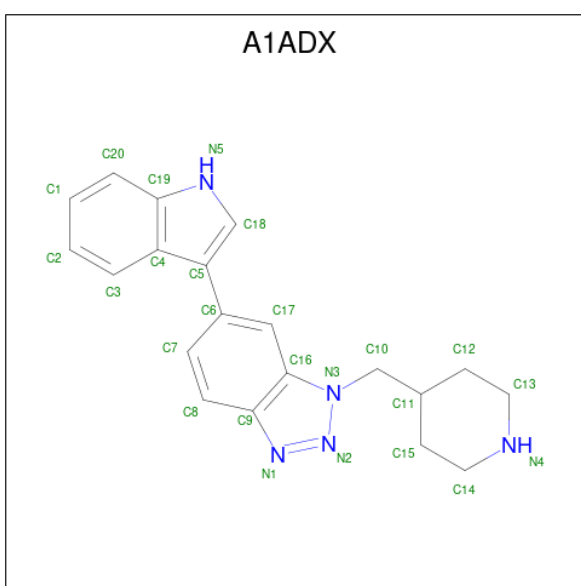
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression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

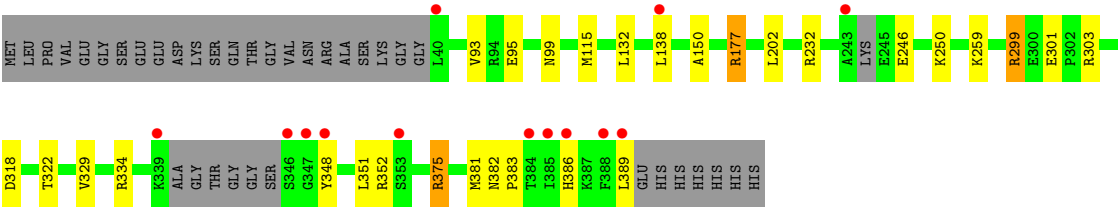
- Molecule 4 is (6M)-6-(1H-indol-3-yl)-1-[(piperidin-4-yl)methyl]-1H-benzotriazole (CCD ID: A1ADX) (formula: C₂₀H₂₁N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			25	20	5		
4	B	1	Total	C	N	0	0
			25	20	5		
4	C	1	Total	C	N	0	0
			25	20	5		
4	D	1	Total	C	N	0	0
			25	20	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	36	Total	O	0	0
			36	36		
5	C	20	Total	O	0	0
			20	20		
5	D	41	Total	O	0	0
			41	41		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.82Å 154.73Å 88.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.56 – 2.05 105.34 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (105.56-2.05) 99.1 (105.34-2.05)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.191 , 0.218 0.200 , 0.225	Depositor DCC
R_{free} test set	6077 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12206	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZIQ, A1ADX

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	0.67	0/3016	1.05	3/4058 (0.1%)
1	B	0.65	0/3015	1.06	3/4057 (0.1%)
1	C	0.60	0/2985	1.02	2/4016 (0.0%)
1	D	0.72	1/2980 (0.0%)	1.06	3/4009 (0.1%)
All	All	0.66	1/11996 (0.0%)	1.05	11/16140 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	5
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	ARG	CZ-NH2	11.82	1.48	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	ARG	NE-CZ-NH2	10.25	128.43	119.20
1	D	177	ARG	NE-CZ-NH1	-7.62	113.88	121.50
1	B	318	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	268	PHE	CA-CB-CG	-5.83	107.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	PHE	CA-CB-CG	-5.69	108.11	113.80
1	C	318	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	318	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	105	GLU	CB-CG-CD	5.31	121.63	112.60
1	B	388	PHE	CA-CB-CG	5.31	119.11	113.80
1	C	149	PRO	N-CA-CB	-5.03	97.07	102.60
1	A	386	HIS	CA-CB-CG	5.00	118.81	113.80

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	ARG	Sidechain
1	A	303	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	375	ARG	Sidechain
1	A	94	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	334	ARG	Sidechain
1	B	358	ARG	Sidechain
1	B	94	ARG	Sidechain
1	C	178	ARG	Sidechain
1	C	232	ARG	Sidechain
1	C	299	ARG	Sidechain
1	C	375	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	232	ARG	Sidechain
1	D	299	ARG	Sidechain
1	D	334	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	2947	0	2932	17	0
1	B	2946	0	2932	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2918	0	2905	32	0
1	D	2913	0	2900	20	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	2	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	25	0	0	0	0
4	B	25	0	0	1	0
4	C	25	0	0	0	0
4	D	25	0	0	0	0
5	A	49	0	0	0	0
5	B	36	0	0	0	0
5	C	20	0	0	0	0
5	D	41	0	0	0	0
All	All	12206	0	11789	86	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 (86) 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:C:383:PRO:HA	1:C:386:HIS:HB3	1.43	1.00
1:A:383:PRO:HA	1:A:386:HIS:HB3	1.46	0.94
1:B:383:PRO:HA	1:B:386:HIS:HB3	1.60	0.81
1:D:93:VAL:HG21	1:D:115:MET:HE3	1.63	0.78
1:B:171:MET:O	1:B:358:ARG:HD3	1.86	0.74
1:B:382:ASN:HB2	1:B:384:THR:HG22	1.70	0.73
1:C:223:TRP:CG	1:C:290:GLN:HE21	2.07	0.73
1:C:299:ARG:HH22	1:C:375:ARG:HH22	1.37	0.71
1:C:216:GLU:HB3	1:C:218:HIS:CE1	2.28	0.69
1:D:299:ARG:HH22	1:D:375:ARG:HH22	1.46	0.61
1:C:383:PRO:HA	1:C:386:HIS:CB	2.27	0.60
1:A:299:ARG:HH22	1:A:375:ARG:HH22	1.50	0.60
1:D:382:ASN:HB3	1:D:383:PRO:HD2	1.84	0.58
1:A:283:ARG:HH21	1:A:283:ARG:HG2	1.68	0.57
1:A:386:HIS:CE1	1:A:390:GLU:HG2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLN:OE1	1:C:199:LYS:HD3	2.06	0.55
1:D:202:LEU:C	1:D:202:LEU:HD13	2.32	0.55
1:C:223:TRP:CD1	1:C:290:GLN:HE21	2.25	0.55
1:D:383:PRO:HA	1:D:386:HIS:HB3	1.89	0.55
1:B:375:ARG:HH12	1:D:138:LEU:HD21	1.72	0.55
1:C:246:GLU:HA	1:C:250:LYS:HD3	1.89	0.54
1:B:387:LYS:HA	1:B:390:GLU:HG3	1.90	0.54
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.37	0.54
1:B:381:MET:HG3	1:B:385:ILE:HG23	1.90	0.54
2:A:401:HEM:HBB2	2:A:401:HEM:HMB2	1.89	0.53
1:C:331:MET:HE3	2:C:401:HEM:HAB	1.89	0.53
1:C:381:MET:SD	1:C:389:LEU:HD12	2.49	0.53
1:D:303:ARG:HD3	1:D:389:LEU:HA	1.90	0.53
1:A:383:PRO:HA	1:A:386:HIS:CB	2.31	0.53
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.39	0.52
1:A:381:MET:SD	1:A:389:LEU:HD12	2.50	0.52
1:A:283:ARG:HH21	1:A:283:ARG:CG	2.23	0.52
1:A:322:THR:HG22	1:C:326:TYR:OH	2.10	0.52
1:C:115:MET:HE3	1:C:317:ILE:CD1	2.39	0.52
1:C:303:ARG:HD3	1:C:389:LEU:HA	1.91	0.51
1:B:202:LEU:CD2	1:B:283:ARG:NH1	2.74	0.51
1:B:381:MET:SD	1:B:389:LEU:HD12	2.51	0.51
1:D:246:GLU:HA	1:D:250:LYS:HD2	1.94	0.50
1:B:326:TYR:OH	1:D:322:THR:HG22	2.11	0.50
1:A:106:ARG:HD2	1:D:386:HIS:NE2	2.26	0.50
1:C:40:LEU:HD13	1:C:44:ASN:HB3	1.94	0.50
1:D:95:GLU:OE2	1:D:99:ASN:ND2	2.44	0.50
1:B:303:ARG:HD3	1:B:389:LEU:HA	1.93	0.50
1:C:223:TRP:CG	1:C:290:GLN:NE2	2.78	0.49
1:A:283:ARG:CG	1:A:283:ARG:NH2	2.73	0.49
1:D:381:MET:SD	1:D:389:LEU:HD12	2.52	0.48
1:C:383:PRO:CA	1:C:386:HIS:HB3	2.29	0.48
1:A:169:GLN:HG3	1:A:179:HIS:NE2	2.29	0.48
1:C:329:VAL:HG22	1:C:351:LEU:HB3	1.96	0.48
1:C:202:LEU:CD2	1:C:283:ARG:NH2	2.78	0.47
1:B:332:VAL:HG22	2:B:401:HEM:C1B	2.50	0.47
1:B:385:ILE:HG13	1:B:388:PHE:CD1	2.50	0.46
1:B:149:PRO:HA	4:B:403:A1ADX:C12	2.45	0.46
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	1.98	0.46
1:C:40:LEU:O	1:D:150:ALA:HB2	2.15	0.45
1:B:176:ASN:O	1:B:178:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ILE:O	1:C:386:HIS:C	2.59	0.45
1:C:245:GLU:HG2	1:C:247:SER:HB3	1.99	0.45
1:C:187:GLU:HG3	1:C:190:GLU:OE2	2.17	0.45
1:C:41:ILE:HG12	1:C:44:ASN:OD1	2.17	0.45
1:B:329:VAL:HG22	1:B:351:LEU:HB3	2.00	0.44
1:C:104:ASP:CG	1:C:106:ARG:HG2	2.43	0.44
1:C:331:MET:HE2	1:C:331:MET:HB3	1.80	0.44
1:C:386:HIS:O	1:C:388:PHE:N	2.50	0.44
1:D:329:VAL:HG22	1:D:351:LEU:HB3	2.00	0.43
1:A:329:VAL:HG22	1:A:351:LEU:HB3	2.01	0.43
1:D:115:MET:HA	1:D:115:MET:HE2	2.01	0.43
1:C:232:ARG:NH2	1:C:236:GLU:OE2	2.52	0.43
1:A:249:GLU:HG2	1:A:253:GLN:HE21	1.83	0.42
1:C:329:VAL:HG22	1:C:351:LEU:CB	2.49	0.42
1:D:259:LYS:HA	1:D:259:LYS:HD3	1.75	0.42
1:B:115:MET:HE3	1:B:317:ILE:HD12	2.02	0.42
1:A:149:PRO:HD2	1:B:40:LEU:O	2.20	0.42
1:C:332:VAL:HG22	2:C:401:HEM:C1B	2.54	0.41
1:A:152:GLY:HA3	2:A:401:HEM:C1D	2.55	0.41
1:A:382:ASN:O	1:A:386:HIS:N	2.53	0.41
1:B:328:HIS:CE1	2:B:401:HEM:C4D	3.08	0.41
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.97	0.41
1:D:301:GLU:OE2	1:D:386:HIS:NE2	2.53	0.41
1:C:115:MET:HE3	1:C:317:ILE:HD12	2.02	0.41
1:B:375:ARG:NH1	1:D:138:LEU:HD21	2.35	0.41
1:B:360:LYS:O	1:B:363:VAL:HG13	2.21	0.41
1:C:223:TRP:CD1	1:C:290:GLN:NE2	2.89	0.41
1:C:386:HIS:O	1:C:387:LYS:C	2.64	0.41
1:D:132:LEU:HD12	1:D:132:LEU:HA	1.97	0.41
1:D:348:TYR:O	1:D:352:ARG:HG3	2.22	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	343/380 (90%)	340 (99%)	3 (1%)	0	100	100
1	B	343/380 (90%)	337 (98%)	6 (2%)	0	100	100
1	C	338/380 (89%)	333 (98%)	5 (2%)	0	100	100
1	D	337/380 (89%)	331 (98%)	6 (2%)	0	100	100
All	All	1361/1520 (90%)	1341 (98%)	20 (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	324/348 (93%)	321 (99%)	3 (1%)	70	75
1	B	323/348 (93%)	320 (99%)	3 (1%)	70	75
1	C	320/348 (92%)	318 (99%)	2 (1%)	78	83
1	D	320/348 (92%)	320 (100%)	0	100	100
All	All	1287/1392 (92%)	1279 (99%)	8 (1%)	78	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	283	ARG
1	A	386	HIS
1	B	149	PRO
1	B	382	ASN
1	B	391	HIS
1	C	149	PRO
1	C	385	ILE

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	58	GLN
1	A	107	ASN
1	A	169	GLN
1	A	170	ASN
1	A	176	ASN
1	A	253	GLN
1	A	275	HIS
1	A	309	GLN
1	A	376	HIS
1	B	242	GLN
1	B	376	HIS
1	B	386	HIS
1	C	183	ASN
1	C	242	GLN
1	C	376	HIS
1	C	386	HIS
1	D	44	ASN
1	D	101	HIS
1	D	169	GLN
1	D	189	ASN
1	D	260	GLN
1	D	309	GLN
1	D	376	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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
2	HEM	A	401	1	50,50,50	1.62	8 (16%)	67,82,82	1.84	17 (25%)
4	A1ADX	C	403	-	29,29,29	0.65	1 (3%)	41,41,41	0.84	1 (2%)
2	HEM	B	401	1	50,50,50	1.69	10 (20%)	67,82,82	1.84	20 (29%)
3	ZIQ	B	402	-	14,17,17	0.70	0	20,25,25	0.90	1 (5%)
4	A1ADX	B	403	-	29,29,29	0.74	1 (3%)	41,41,41	0.80	0
3	ZIQ	D	402	-	14,17,17	0.69	0	20,25,25	1.19	1 (5%)
2	HEM	D	401	1	50,50,50	1.84	14 (28%)	67,82,82	1.69	14 (20%)
2	HEM	C	401	1	50,50,50	1.63	7 (14%)	67,82,82	1.66	13 (19%)
3	ZIQ	C	402	-	14,17,17	0.67	0	20,25,25	0.90	1 (5%)
3	ZIQ	A	402	-	14,17,17	0.56	0	20,25,25	1.26	1 (5%)
4	A1ADX	A	403	-	29,29,29	0.88	1 (3%)	41,41,41	0.90	2 (4%)
4	A1ADX	D	403	-	29,29,29	0.66	1 (3%)	41,41,41	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	401	1	-	2/14/54/54	-
4	A1ADX	C	403	-	-	2/8/16/16	1/5/5/5
2	HEM	B	401	1	-	3/14/54/54	-
3	ZIQ	B	402	-	-	1/11/11/11	0/2/2/2
4	A1ADX	B	403	-	-	0/8/16/16	1/5/5/5
3	ZIQ	D	402	-	-	4/11/11/11	0/2/2/2
2	HEM	D	401	1	-	2/14/54/54	-
2	HEM	C	401	1	-	3/14/54/54	-
3	ZIQ	C	402	-	-	2/11/11/11	0/2/2/2
3	ZIQ	A	402	-	-	4/11/11/11	0/2/2/2
4	A1ADX	A	403	-	-	1/8/16/16	1/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1ADX	D	403	-	-	2/8/16/16	0/5/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	FE-NB	5.46	2.11	1.94
2	C	401	HEM	FE-NB	5.13	2.10	1.94
2	D	401	HEM	FE-NB	4.87	2.09	1.94
2	A	401	HEM	FE-NB	4.75	2.09	1.94
2	D	401	HEM	C1B-NB	-4.67	1.32	1.40
2	D	401	HEM	FE-NC	4.41	2.09	1.95
2	B	401	HEM	FE-NC	4.39	2.09	1.95
2	B	401	HEM	C1B-NB	-4.20	1.33	1.40
2	C	401	HEM	C4D-ND	-4.13	1.33	1.40
2	C	401	HEM	FE-NC	3.92	2.08	1.95
2	C	401	HEM	C1B-NB	-3.71	1.33	1.40
2	A	401	HEM	C1D-ND	-3.69	1.31	1.38
2	A	401	HEM	C4B-NB	-3.64	1.31	1.38
2	D	401	HEM	C4B-NB	-3.49	1.32	1.38
2	A	401	HEM	C1B-NB	-3.42	1.34	1.40
2	A	401	HEM	C1C-C2C	-3.37	1.38	1.45
4	A	403	A1ADX	C17-C6	-3.27	1.34	1.39
2	C	401	HEM	C1C-C2C	-3.04	1.39	1.45
2	D	401	HEM	O1D-CGD	3.02	1.32	1.22
2	B	401	HEM	C4D-ND	-2.87	1.35	1.40
2	D	401	HEM	C1C-C2C	-2.87	1.39	1.45
2	A	401	HEM	FE-NC	2.80	2.04	1.95
2	D	401	HEM	FE-NA	2.79	2.04	1.95
2	D	401	HEM	C4C-NC	-2.60	1.34	1.39
2	D	401	HEM	C1C-NC	-2.58	1.34	1.39
2	D	401	HEM	C4A-NA	-2.53	1.34	1.39
2	C	401	HEM	C3C-C4C	-2.53	1.41	1.46
2	B	401	HEM	C4B-NB	-2.51	1.33	1.38
4	B	403	A1ADX	C17-C6	-2.51	1.35	1.39
2	C	401	HEM	C4B-NB	-2.32	1.34	1.38
2	B	401	HEM	C4A-NA	-2.31	1.35	1.39
2	B	401	HEM	C1C-C2C	-2.31	1.40	1.45
2	A	401	HEM	FE-NA	2.28	2.02	1.95
2	B	401	HEM	C3C-C4C	-2.27	1.42	1.46
2	B	401	HEM	C1D-ND	-2.26	1.34	1.38
4	D	403	A1ADX	C17-C6	-2.24	1.36	1.39
2	D	401	HEM	C3C-C4C	-2.15	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	CHB-C1B	2.14	1.42	1.38
2	D	401	HEM	C4D-ND	-2.13	1.36	1.40
4	C	403	A1ADX	C17-C6	-2.13	1.36	1.39
2	D	401	HEM	C1D-ND	-2.07	1.34	1.38
2	D	401	HEM	C1A-C2A	-2.03	1.40	1.44
2	B	401	HEM	C1A-C2A	-2.03	1.40	1.44

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	CHD-C1D-ND	4.63	129.40	124.42
2	A	401	HEM	CHC-C4B-NB	4.60	129.38	124.42
2	C	401	HEM	CHC-C4B-NB	4.58	129.35	124.42
2	B	401	HEM	C1B-NB-C4B	4.46	110.48	105.21
2	A	401	HEM	CHA-C4D-ND	4.42	129.83	124.37
2	A	401	HEM	C1B-NB-C4B	4.41	110.43	105.21
3	D	402	ZIQ	O-C-CA	-4.36	114.96	122.78
2	D	401	HEM	CHD-C1D-ND	4.30	129.05	124.42
3	A	402	ZIQ	O-C-CA	-4.30	115.08	122.78
2	A	401	HEM	CHB-C1B-NB	4.25	129.63	124.37
2	D	401	HEM	C1B-NB-C4B	4.25	110.24	105.21
2	D	401	HEM	CHC-C4B-NB	4.15	128.89	124.42
2	B	401	HEM	CHC-C4B-NB	3.99	128.72	124.42
2	A	401	HEM	CHD-C4C-NC	3.96	128.76	124.45
2	C	401	HEM	C1B-NB-C4B	3.85	109.76	105.21
2	D	401	HEM	CHB-C1B-NB	3.84	129.11	124.37
2	A	401	HEM	CHD-C1D-ND	3.69	128.40	124.42
2	B	401	HEM	CHA-C4D-ND	3.57	128.78	124.37
2	C	401	HEM	CHB-C1B-NB	3.38	128.54	124.37
2	C	401	HEM	CHD-C1D-ND	3.35	128.03	124.42
2	D	401	HEM	CHA-C4D-ND	3.30	128.45	124.37
2	C	401	HEM	CHA-C4D-ND	3.18	128.30	124.37
2	B	401	HEM	CHB-C1B-NB	3.17	128.29	124.37
2	B	401	HEM	O2A-CGA-CBA	3.16	123.99	114.00
2	D	401	HEM	CBD-CAD-C3D	-3.07	104.03	112.53
2	B	401	HEM	C3B-C4B-NB	-3.06	107.27	109.47
2	A	401	HEM	CBD-CAD-C3D	-3.06	104.07	112.53
2	B	401	HEM	CAD-C3D-C4D	2.93	129.81	124.70
2	D	401	HEM	C4C-NC-C1C	2.91	110.56	105.82
2	C	401	HEM	CHD-C4C-NC	2.89	127.60	124.45
3	C	402	ZIQ	O-C-CA	-2.85	117.66	122.78
2	B	401	HEM	CBD-CAD-C3D	-2.85	104.65	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	CHD-C1D-C2D	-2.81	120.60	125.03
2	B	401	HEM	CHD-C4C-NC	2.79	127.49	124.45
2	D	401	HEM	C3B-C4B-NB	-2.77	107.48	109.47
3	B	402	ZIQ	O-C-CA	-2.76	117.83	122.78
2	B	401	HEM	O2A-CGA-O1A	-2.73	116.31	123.33
2	C	401	HEM	C4C-NC-C1C	2.69	110.20	105.82
2	C	401	HEM	CAC-C3C-C4C	2.64	131.12	124.82
2	B	401	HEM	C4C-NC-C1C	2.61	110.07	105.82
2	D	401	HEM	CHD-C4C-NC	2.60	127.28	124.45
2	C	401	HEM	C4B-C3B-C2B	-2.57	104.92	107.28
2	D	401	HEM	CHD-C1D-C2D	-2.57	120.97	125.03
2	A	401	HEM	CHD-C1D-C2D	-2.55	121.00	125.03
2	B	401	HEM	CAC-C3C-C4C	2.52	130.84	124.82
2	A	401	HEM	C3B-C4B-NB	-2.50	107.67	109.47
2	D	401	HEM	CMD-C2D-C1D	2.49	128.92	125.03
2	D	401	HEM	CAD-C3D-C4D	2.45	128.97	124.70
4	A	403	A1ADX	C10-N3-N2	2.42	121.27	119.67
2	A	401	HEM	C4C-NC-C1C	2.40	109.74	105.82
2	A	401	HEM	C1A-CHA-C4D	-2.33	120.77	126.25
4	C	403	A1ADX	C17-C16-N3	2.33	133.84	131.30
2	C	401	HEM	CAC-C3C-C2C	-2.32	120.89	128.43
2	A	401	HEM	CHA-C4D-C3D	-2.30	120.99	125.23
2	A	401	HEM	O2D-CGD-O1D	-2.27	117.49	123.33
2	C	401	HEM	CBD-CAD-C3D	-2.25	106.30	112.53
2	A	401	HEM	C4C-CHD-C1D	-2.23	121.28	126.02
2	B	401	HEM	CHA-C1A-NA	2.21	127.86	123.86
2	C	401	HEM	CHD-C1D-C2D	-2.17	121.60	125.03
2	A	401	HEM	C4B-C3B-C2B	-2.17	105.28	107.28
2	B	401	HEM	CAD-C3D-C2D	-2.17	123.81	127.87
2	A	401	HEM	O2A-CGA-O1A	-2.16	117.78	123.33
4	A	403	A1ADX	C17-C16-N3	2.16	133.65	131.30
2	D	401	HEM	CAD-C3D-C2D	-2.13	123.88	127.87
2	D	401	HEM	CHB-C1B-C2B	-2.12	120.92	126.95
2	B	401	HEM	C4D-ND-C1D	2.10	107.70	105.21
2	B	401	HEM	C1A-CHA-C4D	-2.09	121.33	126.25
2	B	401	HEM	C2A-C1A-NA	-2.06	107.87	110.15
2	A	401	HEM	O2D-CGD-CBD	2.03	120.42	114.00
2	B	401	HEM	CAC-C3C-C2C	-2.03	121.84	128.43
2	C	401	HEM	CHA-C1A-NA	2.02	127.53	123.86

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
3	D	402	ZIQ	O-C-CA-C1
3	A	402	ZIQ	O-C-CA-C1
4	C	403	A1ADX	N3-C10-C11-C15
3	D	402	ZIQ	OXT-C-CA-CB
4	C	403	A1ADX	N3-C10-C11-C12
4	D	403	A1ADX	N3-C10-C11-C12
4	D	403	A1ADX	N3-C10-C11-C15
2	C	401	HEM	C3D-CAD-CBD-CGD
3	C	402	ZIQ	O-C-CA-C1
3	A	402	ZIQ	O-C-CA-CB
3	A	402	ZIQ	OXT-C-CA-CB
3	D	402	ZIQ	O-C-CA-CB
4	A	403	A1ADX	N3-C10-C11-C15
2	D	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
3	B	402	ZIQ	O-C-CA-C1
3	C	402	ZIQ	OXT-C-CA-C1
2	B	401	HEM	C3D-CAD-CBD-CGD

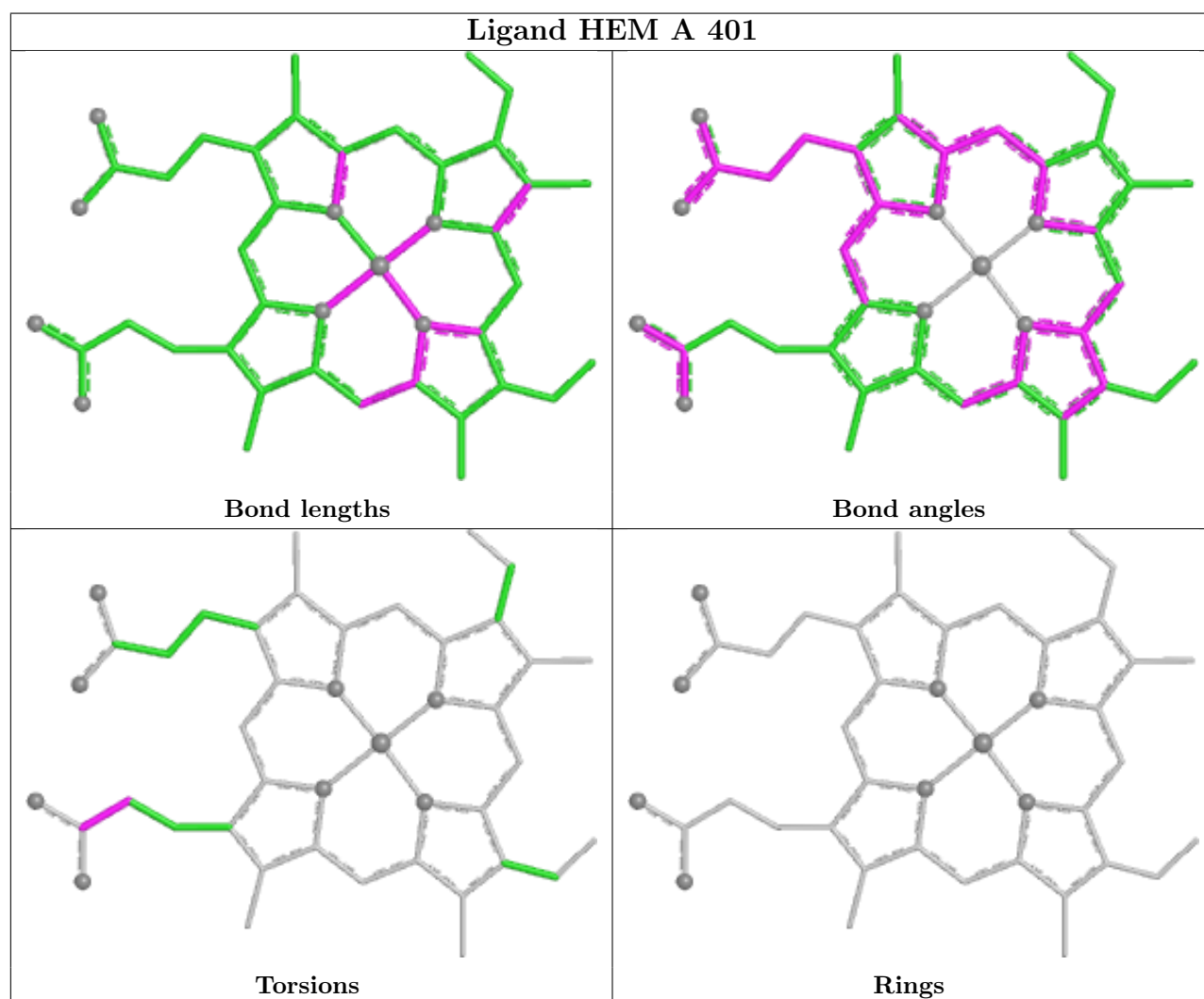
All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	A1ADX	C11-C12-C13-C14-C15-N4
4	A	403	A1ADX	C11-C12-C13-C14-C15-N4
4	C	403	A1ADX	C11-C12-C13-C14-C15-N4

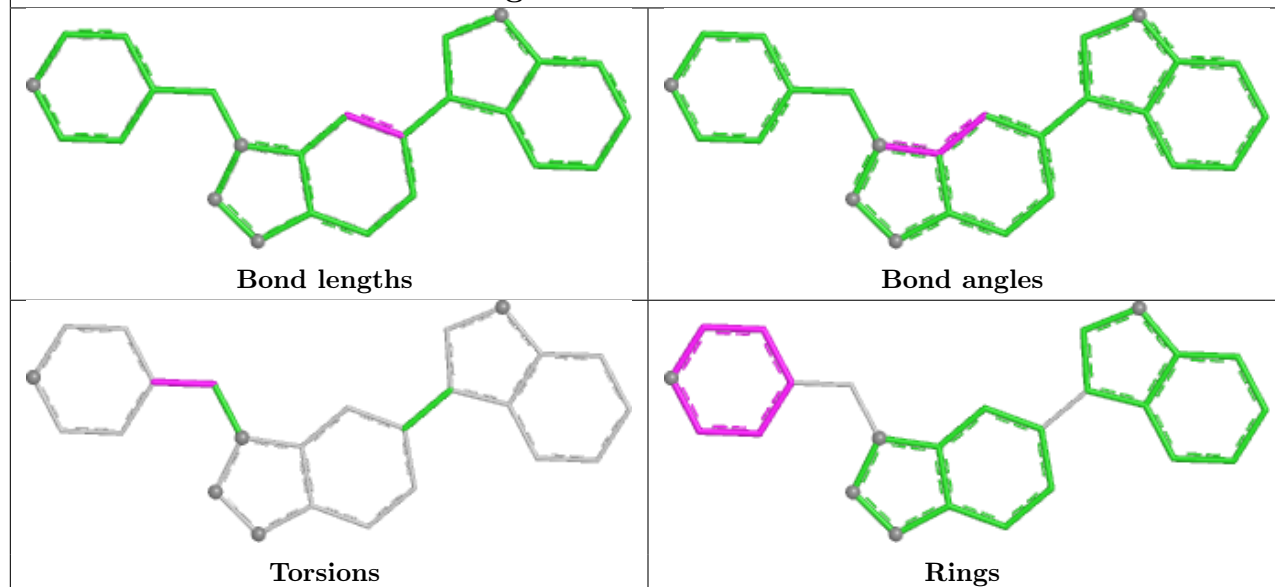
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	2	0
2	B	401	HEM	2	0
4	B	403	A1ADX	1	0
2	D	401	HEM	1	0
2	C	401	HEM	2	0

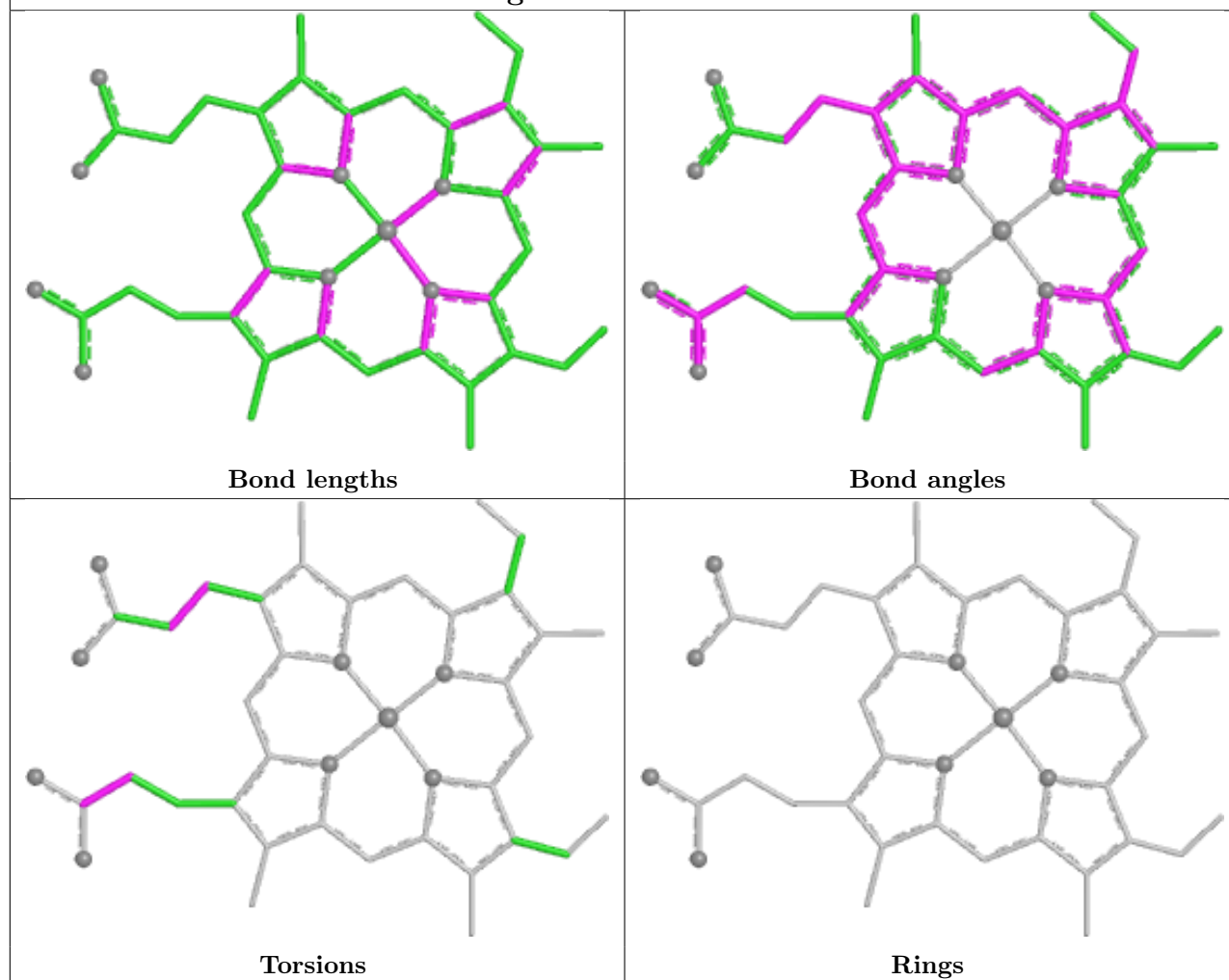
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



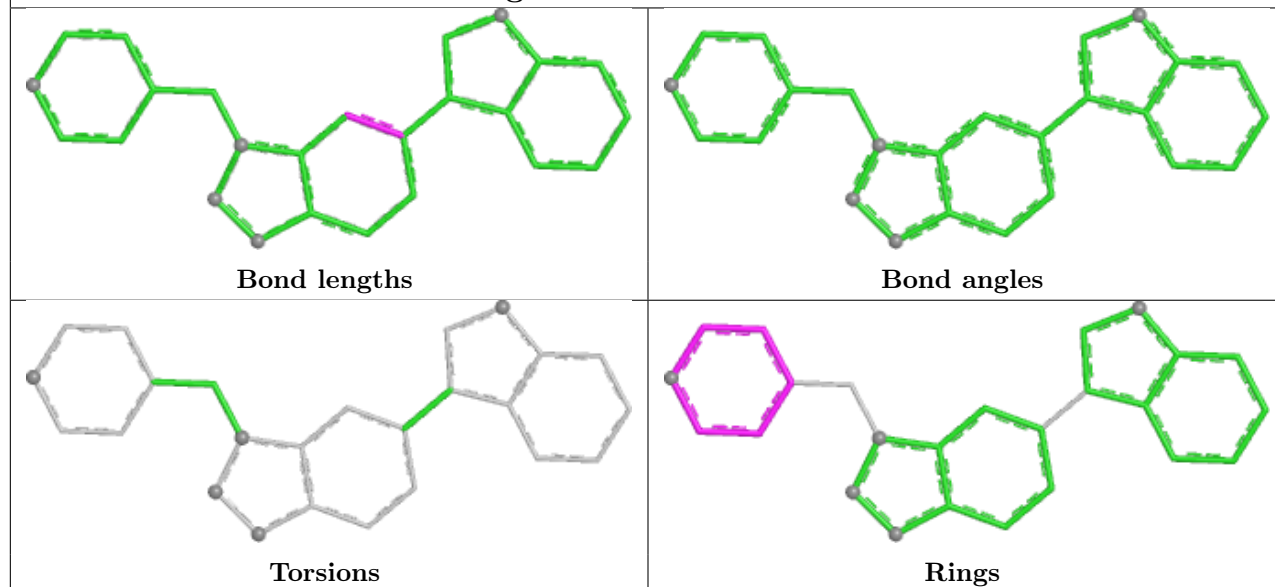
Ligand A1ADX C 403



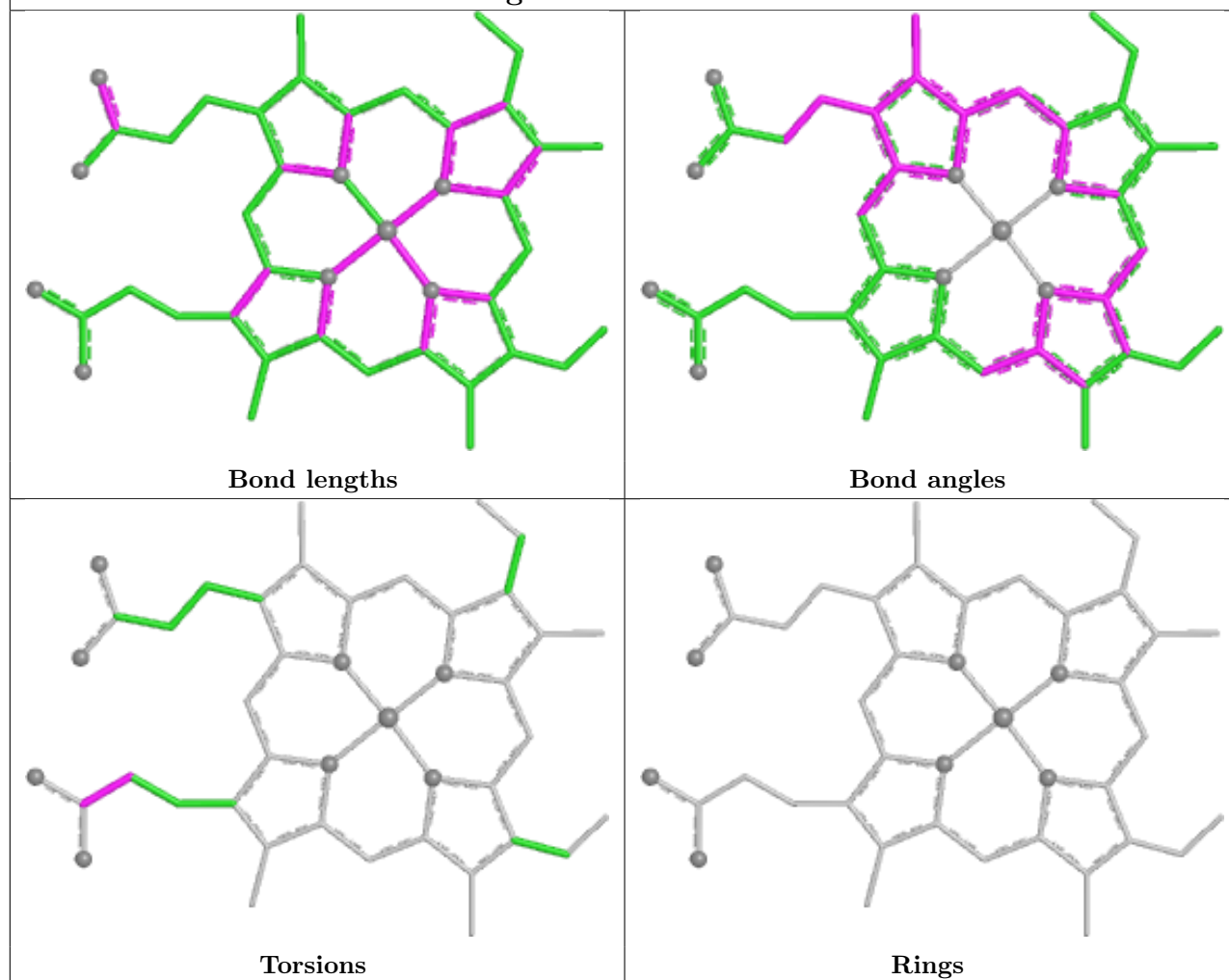
Ligand HEM B 401

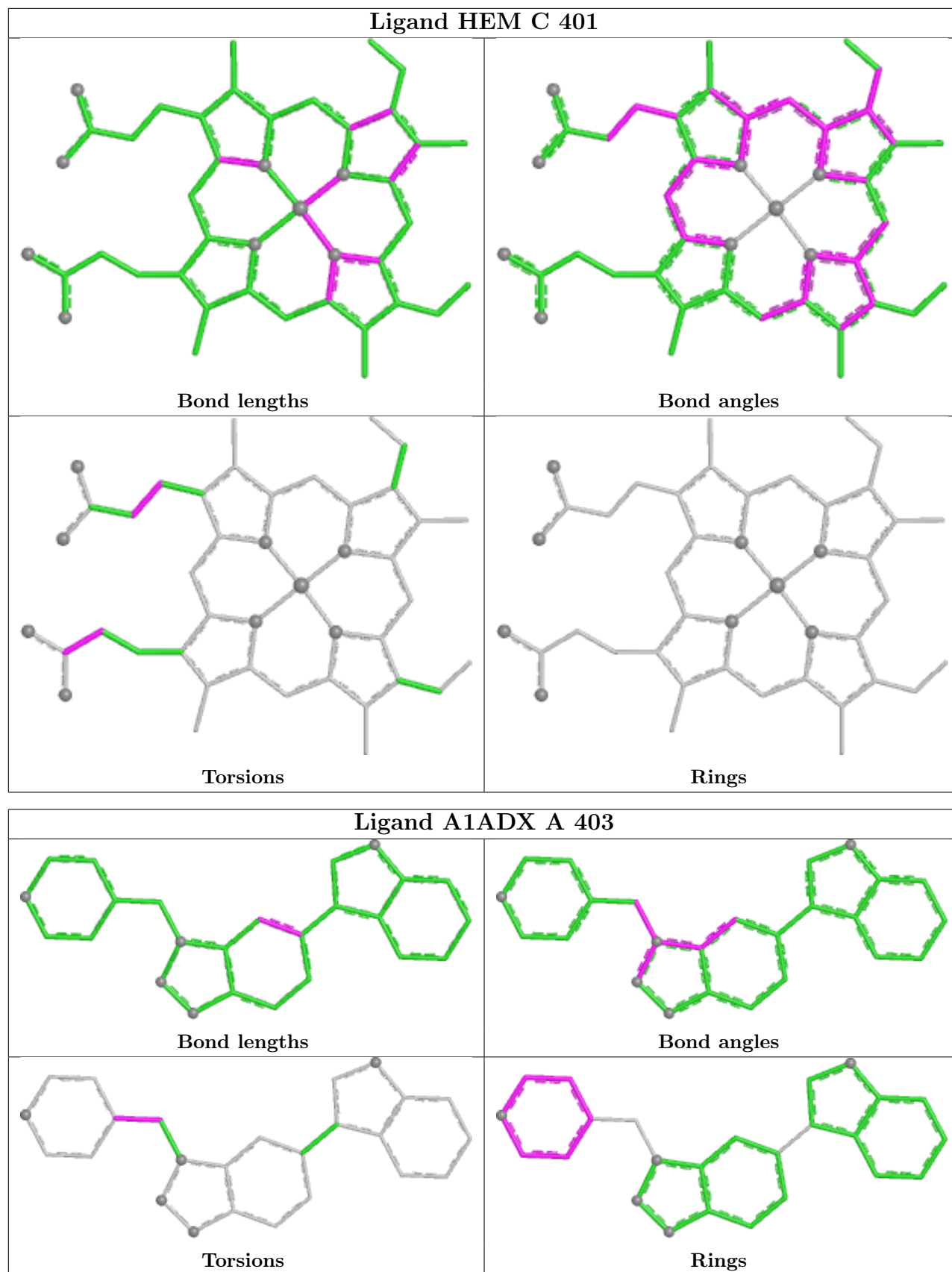


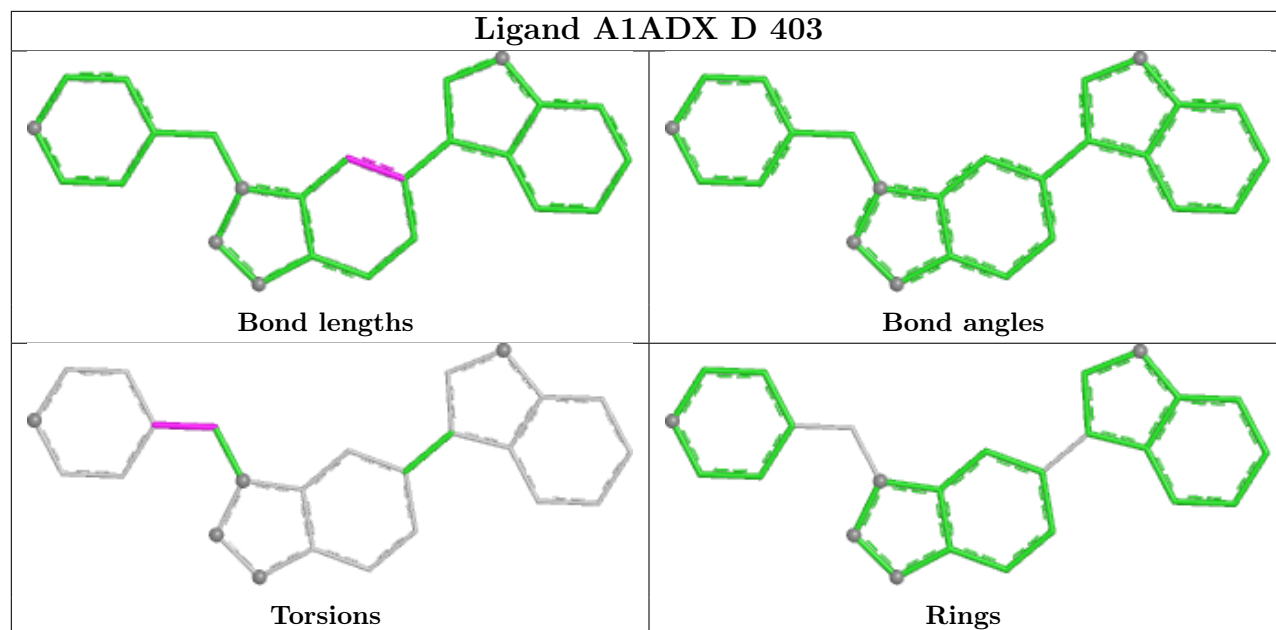
Ligand A1ADX B 403



Ligand HEM D 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	347/380 (91%)	0.18	10 (2%) 53 55	44, 63, 125, 180	0
1	B	347/380 (91%)	0.26	10 (2%) 53 55	45, 69, 126, 185	0
1	C	344/380 (90%)	0.40	11 (3%) 50 50	49, 88, 171, 246	0
1	D	343/380 (90%)	0.25	13 (3%) 44 44	45, 70, 128, 180	0
All	All	1381/1520 (90%)	0.27	44 (3%) 50 50	44, 71, 139, 246	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	385	ILE	4.7
1	C	340	ALA	4.6
1	D	389	LEU	4.2
1	C	389	LEU	4.0
1	C	385	ILE	3.8
1	B	40	LEU	3.8
1	A	40	LEU	3.7
1	A	385	ILE	3.5
1	D	386	HIS	3.3
1	C	296	TYR	3.3
1	A	138	LEU	3.3
1	D	348	TYR	3.2
1	C	40	LEU	3.1
1	B	385	ILE	3.0
1	D	243	ALA	2.9
1	A	386	HIS	2.9
1	B	348	TYR	2.9
1	B	296	TYR	2.8
1	C	243	ALA	2.7
1	C	386	HIS	2.7
1	D	138	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	347	GLY	2.7
1	D	40	LEU	2.6
1	D	339	LYS	2.6
1	A	389	LEU	2.6
1	D	384	THR	2.6
1	B	386	HIS	2.5
1	C	348	TYR	2.5
1	D	388	PHE	2.5
1	C	339	LYS	2.5
1	A	339	LYS	2.4
1	C	326	TYR	2.4
1	B	347	GLY	2.3
1	B	247	SER	2.3
1	B	340	ALA	2.3
1	A	383	PRO	2.3
1	B	383	PRO	2.3
1	A	183	ASN	2.3
1	A	254	VAL	2.2
1	D	353	SER	2.1
1	D	346	SER	2.1
1	A	384	THR	2.1
1	B	138	LEU	2.0
1	C	368	LEU	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.

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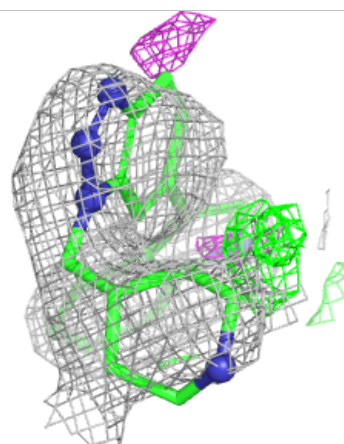
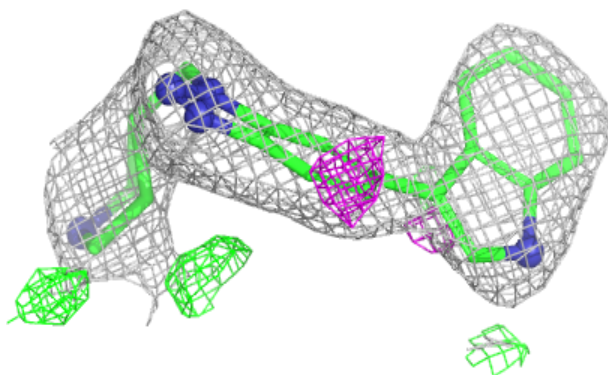
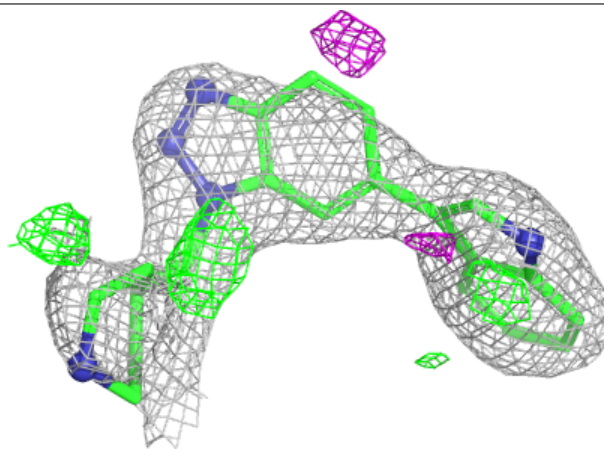
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1ADX	C	403	25/25	0.86	0.15	87,99,144,148	0
4	A1ADX	A	403	25/25	0.87	0.16	64,89,140,143	0
4	A1ADX	B	403	25/25	0.90	0.13	71,82,110,117	0
4	A1ADX	D	403	25/25	0.92	0.12	56,63,100,101	0
2	HEM	C	401	43/43	0.95	0.11	69,82,105,122	0
3	ZIQ	C	402	16/16	0.96	0.08	69,79,86,92	0
3	ZIQ	D	402	16/16	0.96	0.07	56,62,66,71	0
3	ZIQ	A	402	16/16	0.97	0.06	44,52,59,60	0
3	ZIQ	B	402	16/16	0.97	0.07	58,65,69,71	0
2	HEM	B	401	43/43	0.97	0.09	58,68,82,90	0
2	HEM	A	401	43/43	0.97	0.09	51,60,74,88	0
2	HEM	D	401	43/43	0.98	0.08	50,57,75,87	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.

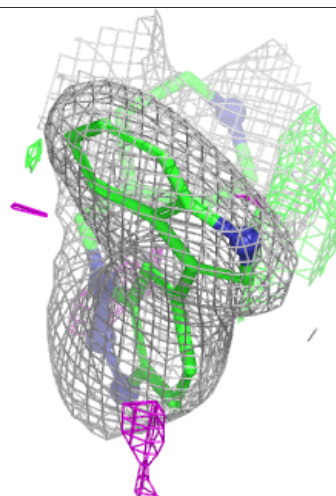
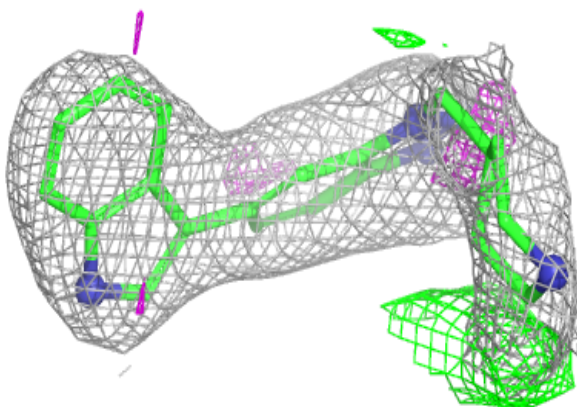
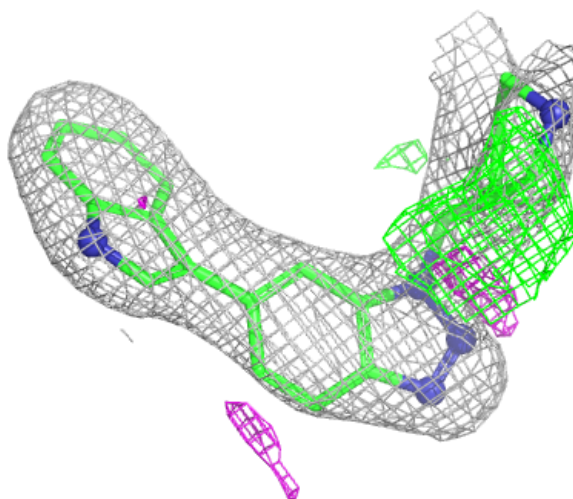
Electron density around A1ADX C 403:

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



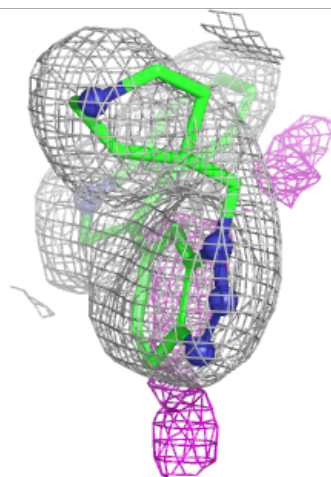
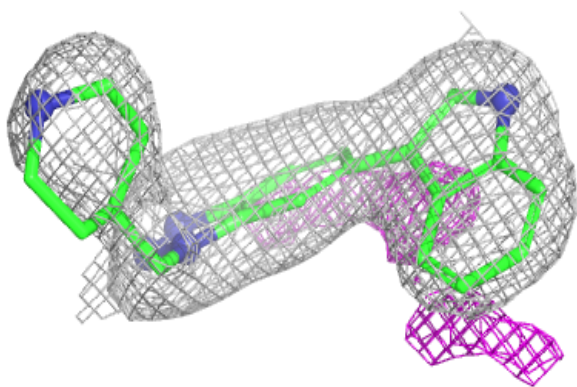
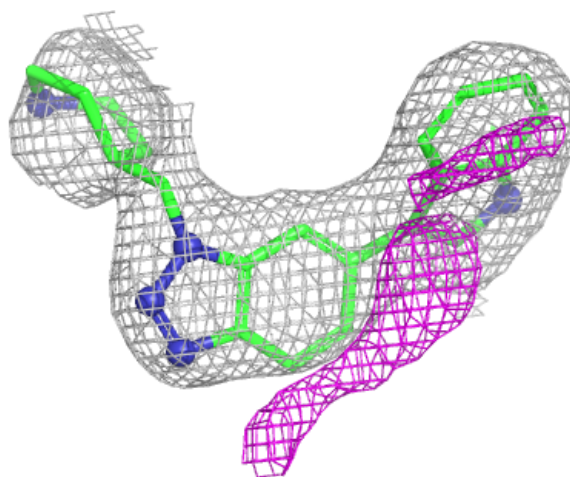
Electron density around A1ADX A 403:

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



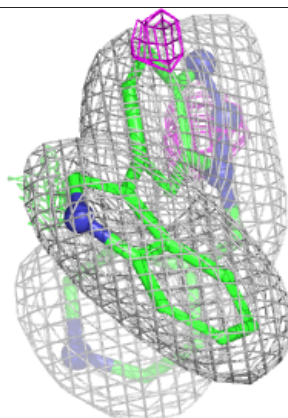
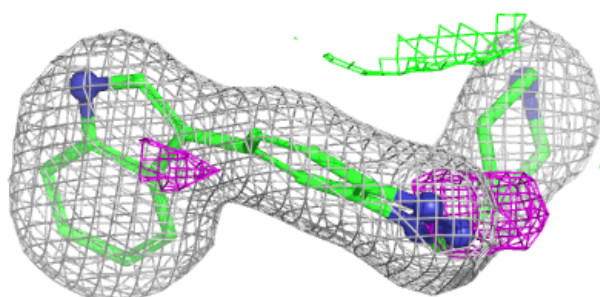
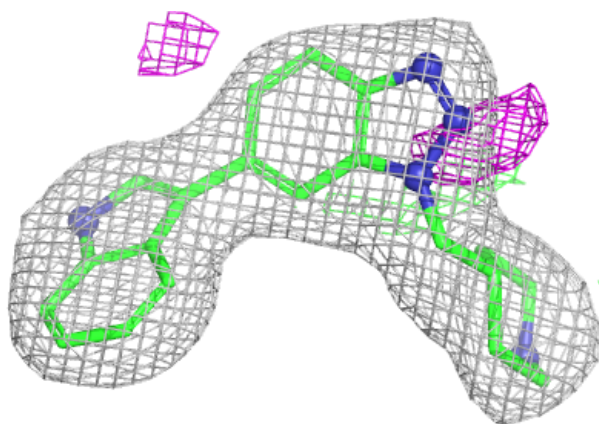
Electron density around A1ADX B 403:

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



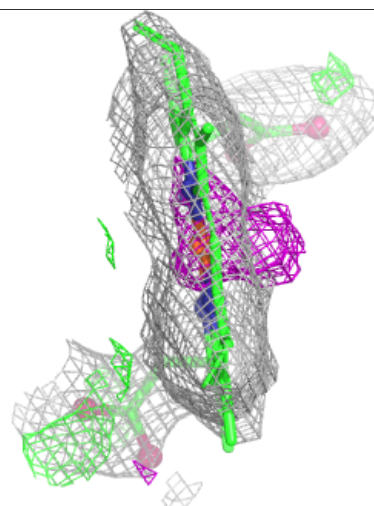
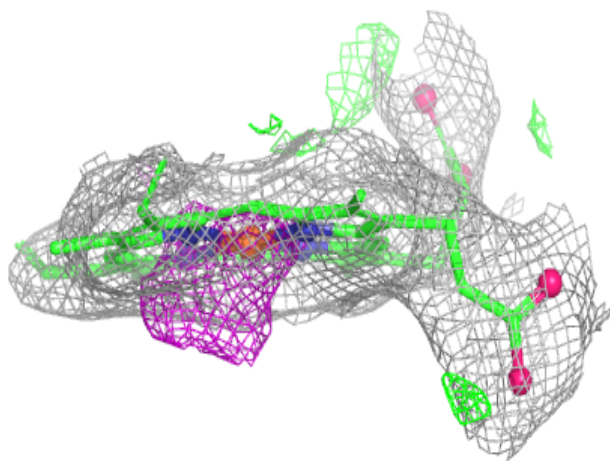
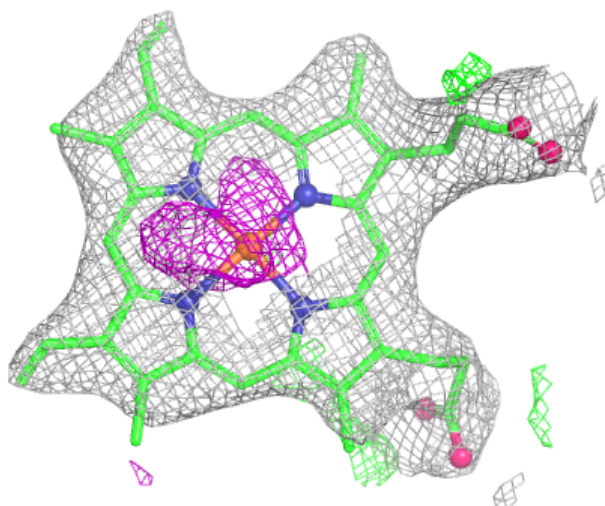
Electron density around A1ADX D 403:

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



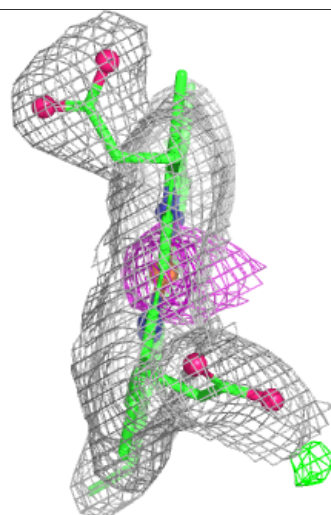
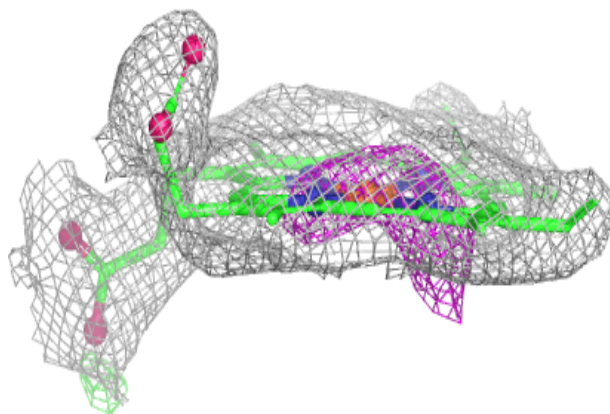
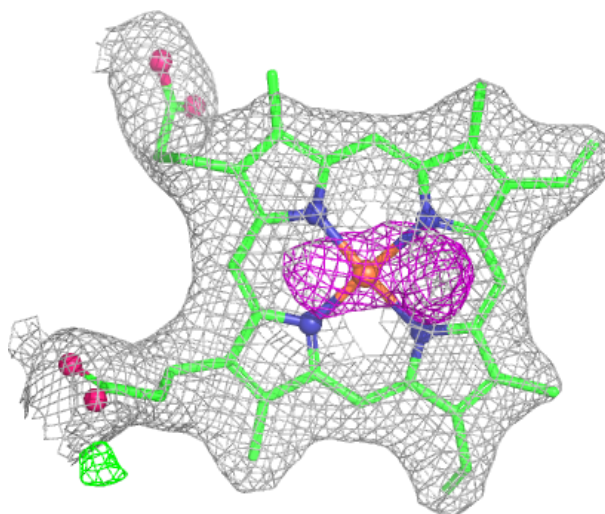
Electron density around HEM C 401:

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



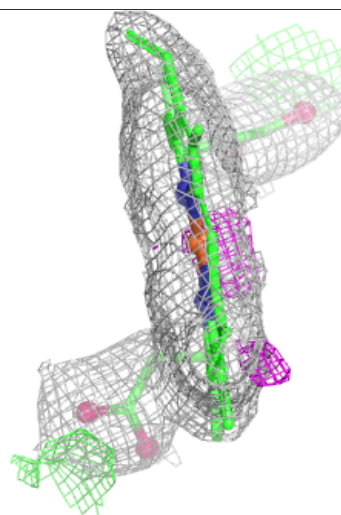
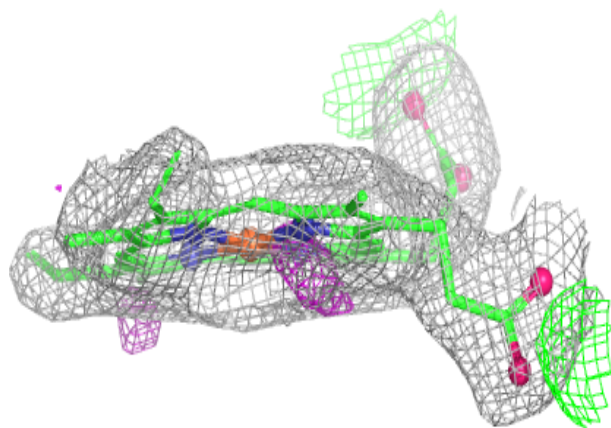
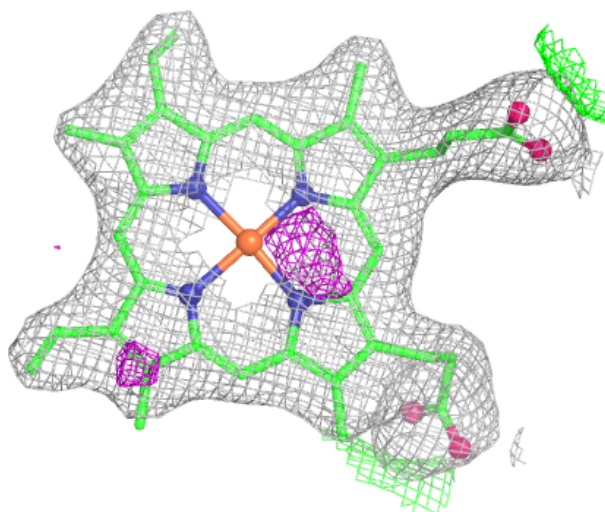
Electron density around HEM B 401:

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



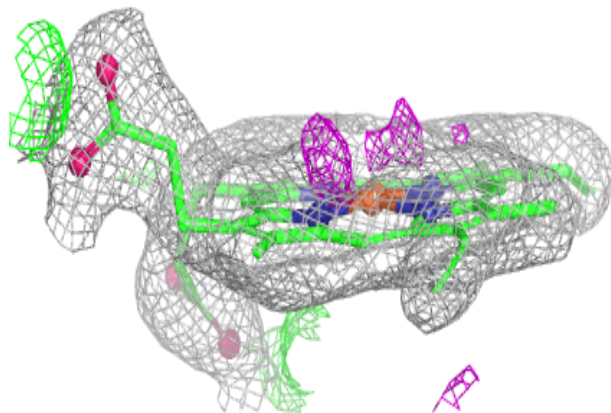
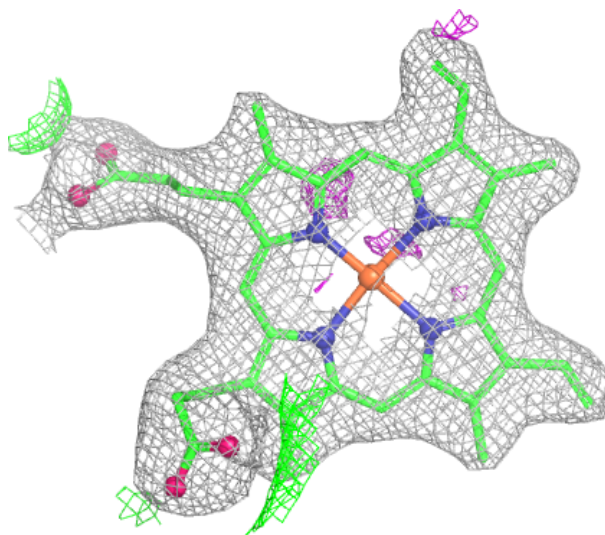
Electron density around HEM A 401:

$2mF_o-DF_c$ (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.