



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2024 – 09:51 PM EDT

PDB ID : 8VTQ
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

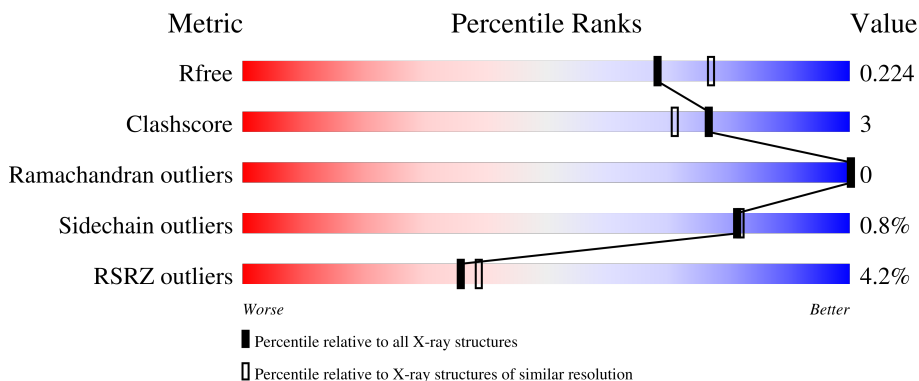
1 Overall quality at a glance

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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	 2% 85% 5% • 9%
1	B	380	 4% 82% 7% • 9%
1	C	380	 7% 81% 8% • 9%
1	D	380	 2% 83% 7% • 10%

2 Entry composition i

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
			Total	C	N	O	S			
1	A	347	2947	1893	517	526	11	0	0	0
1	B	347	2946	1893	517	525	11	0	0	0
1	C	344	2918	1876	511	520	11	0	0	0
1	D	343	2913	1873	510	519	11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

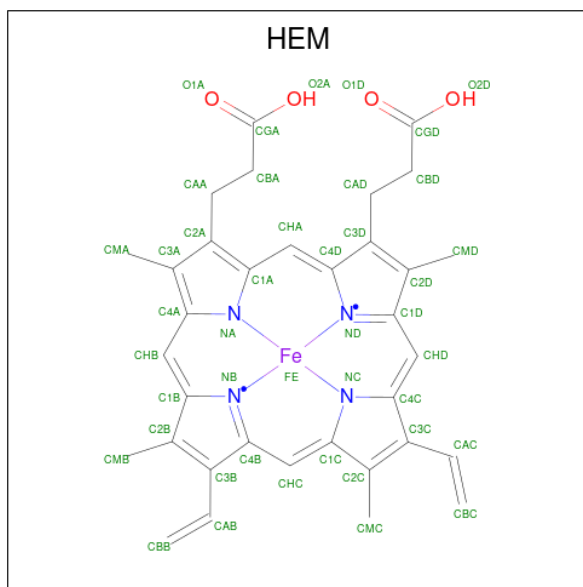
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	UNP P48775
B	17	MET	-	initiating methionine	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	HIS	-	expression tag	UNP P48775
C	17	MET	-	initiating methionine	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775

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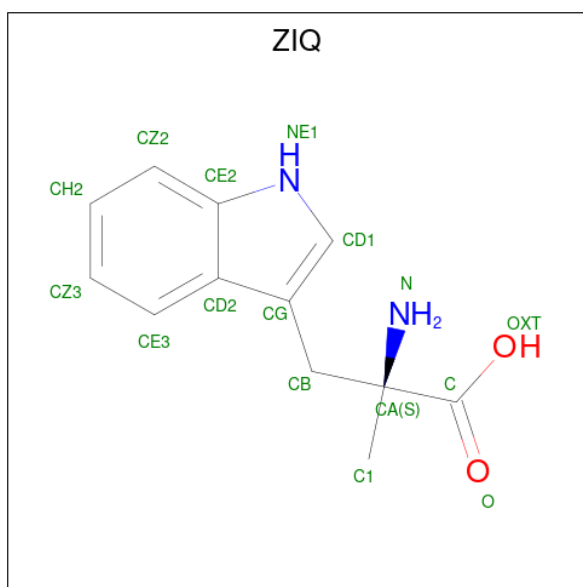
Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



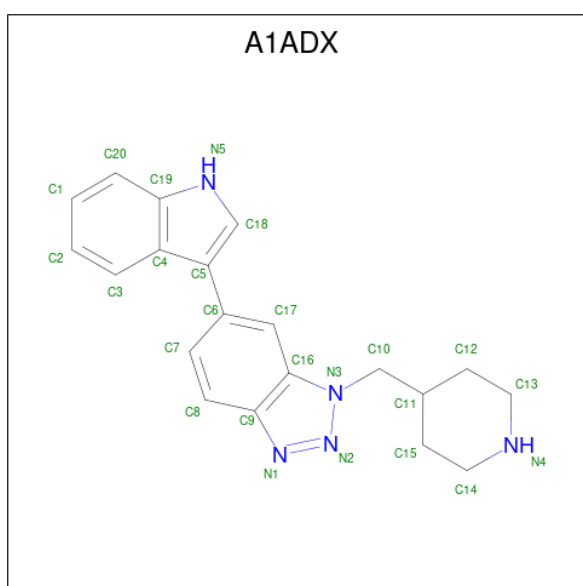
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is alpha-methyl-L-tryptophan (three-letter code: ZIQ) (formula: $C_{12}H_{14}N_2O_2$).



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

- Molecule 4 is (6M)-6-(1H-indol-3-yl)-1-[(piperidin-4-yl)methyl]-1H-benzotriazole (three-letter code: A1ADX) (formula: $C_{20}H_{21}N_5$) (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.

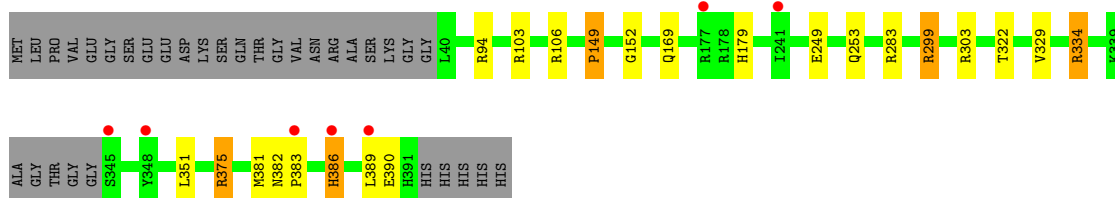
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	36	Total	O	0	0
			36	36		
5	C	20	Total	O	0	0
			20	20		
5	D	41	Total	O	0	0
			41	41		

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.

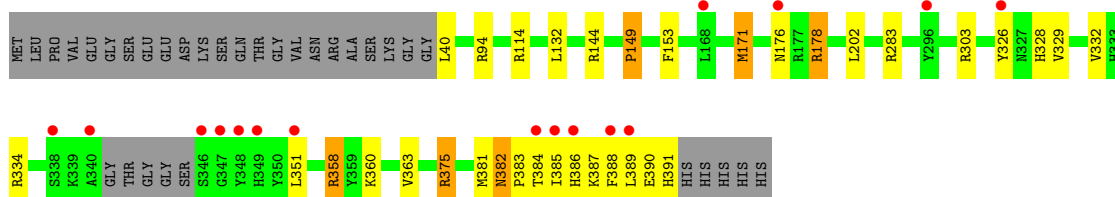
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain A: 




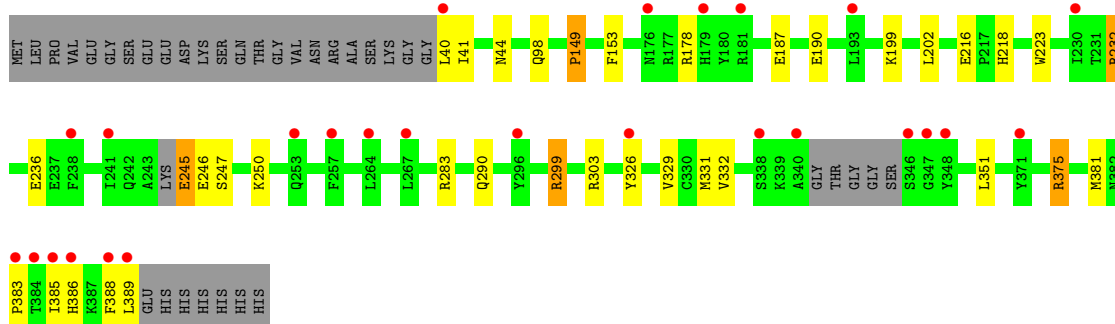
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain B: 




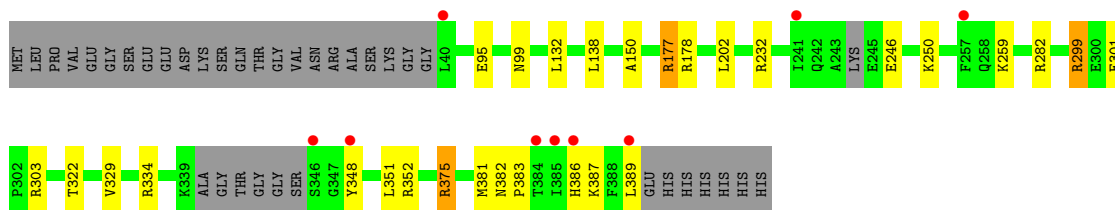
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain C: 



- Molecule 1: Tryptophan 2,3-dioxygenase

Chain D:  2% 83% 7% 10%



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)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.191 , 0.218 0.200 , 0.224	Depositor DCC
R_{free} test set	6043 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtrriage
Anisotropy	0.429	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: ZIQ, A1ADX, 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	0.51	0/3016	0.83	2/4058 (0.0%)
1	B	0.50	0/3015	0.84	4/4057 (0.1%)
1	C	0.46	0/2985	0.77	2/4016 (0.0%)
1	D	0.57	1/2980 (0.0%)	0.90	4/4009 (0.1%)
All	All	0.51	1/11996 (0.0%)	0.84	12/16140 (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	12.13	1.48	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	ARG	NE-CZ-NH2	16.25	128.43	120.30
1	D	177	ARG	NE-CZ-NH1	-12.85	113.88	120.30
1	D	178	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	B	375	ARG	NE-CZ-NH1	6.80	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	103	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	334	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	114	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	171	MET	CG-SD-CE	5.08	108.32	100.20
1	C	331	MET	CG-SD-CE	-5.05	92.12	100.20
1	C	149	PRO	N-CA-CB	-5.03	97.07	102.60
1	B	144	ARG	NE-CZ-NH1	-5.03	117.79	120.30

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 [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	2947	0	2932	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2946	0	2932	20	0
1	C	2918	0	2905	24	0
1	D	2913	0	2900	18	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	1	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	72	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 (72) 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: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: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
1:C:98:GLN:OE1	1:C:199:LYS:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:381:MET:HG3	1:B:385:ILE:HG23	1.90	0.54
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: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: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:202:LEU:C	1:D:202:LEU:HD13	2.32	0.50
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:132:LEU:HD12	1:D:132:LEU:HA	1.97	0.41
1:C:385:ILE:O	1:C:386:HIS:C	2.59	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 [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	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 [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	324/348 (93%)	322 (99%)	2 (1%)	86	87
1	B	323/348 (93%)	319 (99%)	4 (1%)	71	70
1	C	320/348 (92%)	317 (99%)	3 (1%)	78	79
1	D	320/348 (92%)	319 (100%)	1 (0%)	92	93
All	All	1287/1392 (92%)	1277 (99%)	10 (1%)	81	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	386	HIS
1	B	149	PRO
1	B	153	PHE
1	B	382	ASN
1	B	391	HIS
1	C	149	PRO
1	C	153	PHE
1	C	245	GLU
1	D	387	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	HIS
1	B	386	HIS
1	C	183	ASN
1	C	386	HIS
1	D	183	ASN
1	D	260	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	B	401	1	41,50,50	1.42	6 (14%)	45,82,82	1.97	13 (28%)
2	HEM	A	401	1	41,50,50	1.52	6 (14%)	45,82,82	2.01	13 (28%)
3	ZIQ	C	402	-	13,17,17	0.82	0	14,25,25	0.97	1 (7%)
3	ZIQ	D	402	-	13,17,17	0.79	0	14,25,25	0.91	0
4	A1ADX	D	403	-	26,29,29	0.83	0	27,41,41	1.10	3 (11%)
2	HEM	D	401	1	41,50,50	1.59	6 (14%)	45,82,82	1.92	12 (26%)
4	A1ADX	B	403	-	26,29,29	0.79	0	27,41,41	1.10	3 (11%)
4	A1ADX	A	403	-	26,29,29	0.88	0	27,41,41	1.17	3 (11%)
3	ZIQ	B	402	-	13,17,17	0.79	0	14,25,25	1.00	1 (7%)
4	A1ADX	C	403	-	26,29,29	0.76	0	27,41,41	1.07	3 (11%)
3	ZIQ	A	402	-	13,17,17	0.86	0	14,25,25	0.98	0
2	HEM	C	401	1	41,50,50	1.37	4 (9%)	45,82,82	1.77	11 (24%)

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	B	401	1	-	3/12/54/54	-
2	HEM	A	401	1	-	2/12/54/54	-
3	ZIQ	C	402	-	-	2/9/11/11	0/2/2/2
3	ZIQ	D	402	-	-	4/9/11/11	0/2/2/2
4	A1ADX	D	403	-	-	2/7/16/16	0/5/5/5
2	HEM	D	401	1	-	2/12/54/54	-
4	A1ADX	B	403	-	-	0/7/16/16	1/5/5/5
4	A1ADX	A	403	-	-	1/7/16/16	1/5/5/5
3	ZIQ	B	402	-	-	1/9/11/11	0/2/2/2
4	A1ADX	C	403	-	-	2/7/16/16	1/5/5/5
3	ZIQ	A	402	-	-	4/9/11/11	0/2/2/2
2	HEM	C	401	1	-	3/12/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEM	C1B-NB	-4.72	1.32	1.40
2	B	401	HEM	C1B-NB	-4.25	1.33	1.40
2	C	401	HEM	C4D-ND	-4.18	1.33	1.40
2	C	401	HEM	C1B-NB	-3.76	1.33	1.40
2	A	401	HEM	C1D-ND	-3.49	1.31	1.38
2	A	401	HEM	C1B-NB	-3.47	1.34	1.40
2	A	401	HEM	C4B-NB	-3.45	1.31	1.38
2	D	401	HEM	C4B-NB	-3.30	1.32	1.38
2	A	401	HEM	CHB-C1B	3.04	1.42	1.35
2	B	401	HEM	FE-NB	3.01	2.11	1.96
2	D	401	HEM	O1D-CGD	2.96	1.32	1.22
2	B	401	HEM	C4D-ND	-2.92	1.35	1.40
2	B	401	HEM	CHB-C1B	2.87	1.42	1.35
2	C	401	HEM	FE-NB	2.79	2.10	1.96
2	D	401	HEM	FE-NB	2.64	2.09	1.96
2	A	401	HEM	FE-NB	2.56	2.09	1.96
2	D	401	HEM	CHB-C1B	2.50	1.41	1.35
2	B	401	HEM	C4B-NB	-2.37	1.33	1.38
2	C	401	HEM	C4B-NB	-2.19	1.34	1.38
2	D	401	HEM	C4D-ND	-2.18	1.36	1.40
2	B	401	HEM	C1D-ND	-2.13	1.34	1.38
2	A	401	HEM	C1D-C2D	2.00	1.48	1.44

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	C1B-NB-C4B	5.24	110.48	105.07
2	A	401	HEM	C1B-NB-C4B	5.18	110.43	105.07
2	D	401	HEM	C1B-NB-C4B	5.00	110.24	105.07
2	B	401	HEM	CHD-C1D-ND	4.57	129.40	124.43
2	A	401	HEM	CHC-C4B-NB	4.55	129.38	124.43
2	C	401	HEM	C1B-NB-C4B	4.54	109.76	105.07
2	C	401	HEM	CHC-C4B-NB	4.53	129.35	124.43
2	A	401	HEM	CHA-C4D-ND	4.41	129.83	124.38
2	D	401	HEM	CHD-C1D-ND	4.26	129.05	124.43
2	A	401	HEM	CHB-C1B-NB	4.25	129.63	124.38
2	D	401	HEM	CHC-C4B-NB	4.11	128.89	124.43
2	B	401	HEM	CHC-C4B-NB	3.95	128.72	124.43
2	D	401	HEM	CHB-C1B-NB	3.83	129.11	124.38
2	A	401	HEM	CHD-C1D-ND	3.65	128.40	124.43
2	B	401	HEM	CHA-C4D-ND	3.56	128.78	124.38
2	C	401	HEM	CHB-C1B-NB	3.37	128.54	124.38
2	C	401	HEM	CHD-C1D-ND	3.31	128.03	124.43
2	D	401	HEM	CHA-C4D-ND	3.30	128.45	124.38
2	C	401	HEM	CHA-C4D-ND	3.17	128.30	124.38
2	B	401	HEM	CHB-C1B-NB	3.17	128.29	124.38
4	A	403	A1ADX	C10-N3-N2	3.13	121.27	116.67
2	B	401	HEM	O2A-CGA-CBA	3.10	123.99	114.03
2	D	401	HEM	CBD-CAD-C3D	-3.09	104.03	112.63
2	A	401	HEM	CBD-CAD-C3D	-3.08	104.07	112.63
4	B	403	A1ADX	C7-C8-C9	-2.95	117.12	120.84
2	B	401	HEM	CAD-C3D-C4D	2.95	129.81	124.66
4	D	403	A1ADX	C10-N3-N2	2.93	120.96	116.67
2	B	401	HEM	CBD-CAD-C3D	-2.87	104.65	112.63
2	B	401	HEM	CHD-C1D-C2D	-2.81	120.60	124.98
2	B	401	HEM	O2A-CGA-O1A	-2.80	116.31	123.30
2	C	401	HEM	C4B-C3B-C2B	-2.77	104.92	107.11
4	C	403	A1ADX	C10-N3-N2	2.75	120.70	116.67
4	B	403	A1ADX	C10-N3-N2	2.69	120.61	116.67
4	A	403	A1ADX	C7-C8-C9	-2.61	117.56	120.84
4	B	403	A1ADX	C6-C17-C16	-2.57	119.12	121.87
2	D	401	HEM	CHD-C1D-C2D	-2.56	120.97	124.98
2	A	401	HEM	CHD-C1D-C2D	-2.55	121.00	124.98
2	D	401	HEM	CMD-C2D-C1D	2.55	128.92	125.04
4	D	403	A1ADX	C6-C17-C16	-2.55	119.15	121.87
2	B	401	HEM	C4D-ND-C1D	2.54	107.70	105.07
4	C	403	A1ADX	C6-C17-C16	-2.48	119.22	121.87
2	D	401	HEM	CAD-C3D-C4D	2.47	128.97	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	A1ADX	C6-C17-C16	-2.44	119.26	121.87
4	C	403	A1ADX	C7-C8-C9	-2.41	117.81	120.84
4	D	403	A1ADX	C7-C8-C9	-2.41	117.81	120.84
2	A	401	HEM	O2D-CGD-O1D	-2.33	117.49	123.30
2	A	401	HEM	CHA-C4D-C3D	-2.31	120.99	125.33
2	A	401	HEM	C4B-C3B-C2B	-2.30	105.28	107.11
2	C	401	HEM	CBD-CAD-C3D	-2.28	106.30	112.63
3	B	402	ZIQ	CH2-CZ2-CE2	-2.26	116.83	120.08
2	C	401	HEM	C3C-C4C-NC	-2.26	106.68	110.94
2	D	401	HEM	CBA-CAA-C2A	-2.26	108.77	112.62
2	C	401	HEM	C4D-ND-C1D	2.22	107.37	105.07
2	A	401	HEM	O2A-CGA-O1A	-2.21	117.78	123.30
2	B	401	HEM	CBA-CAA-C2A	-2.19	108.88	112.62
2	B	401	HEM	CAD-C3D-C2D	-2.19	123.81	127.88
2	A	401	HEM	C3C-C4C-NC	-2.19	106.82	110.94
2	C	401	HEM	CHD-C1D-C2D	-2.17	121.60	124.98
2	C	401	HEM	CBA-CAA-C2A	-2.15	108.96	112.62
2	D	401	HEM	CAD-C3D-C2D	-2.15	123.88	127.88
3	C	402	ZIQ	CH2-CZ2-CE2	-2.14	117.00	120.08
2	D	401	HEM	CHB-C1B-C2B	-2.10	120.92	126.72
2	A	401	HEM	C4D-ND-C1D	2.07	107.21	105.07

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

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Mol	Chain	Res	Type	Atoms
2	D	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
3	C	402	ZIQ	O-C-CA-C1
2	A	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O2A
3	B	402	ZIQ	O-C-CA-C1
2	B	401	HEM	C3D-CAD-CBD-CGD
3	C	402	ZIQ	OXT-C-CA-C1

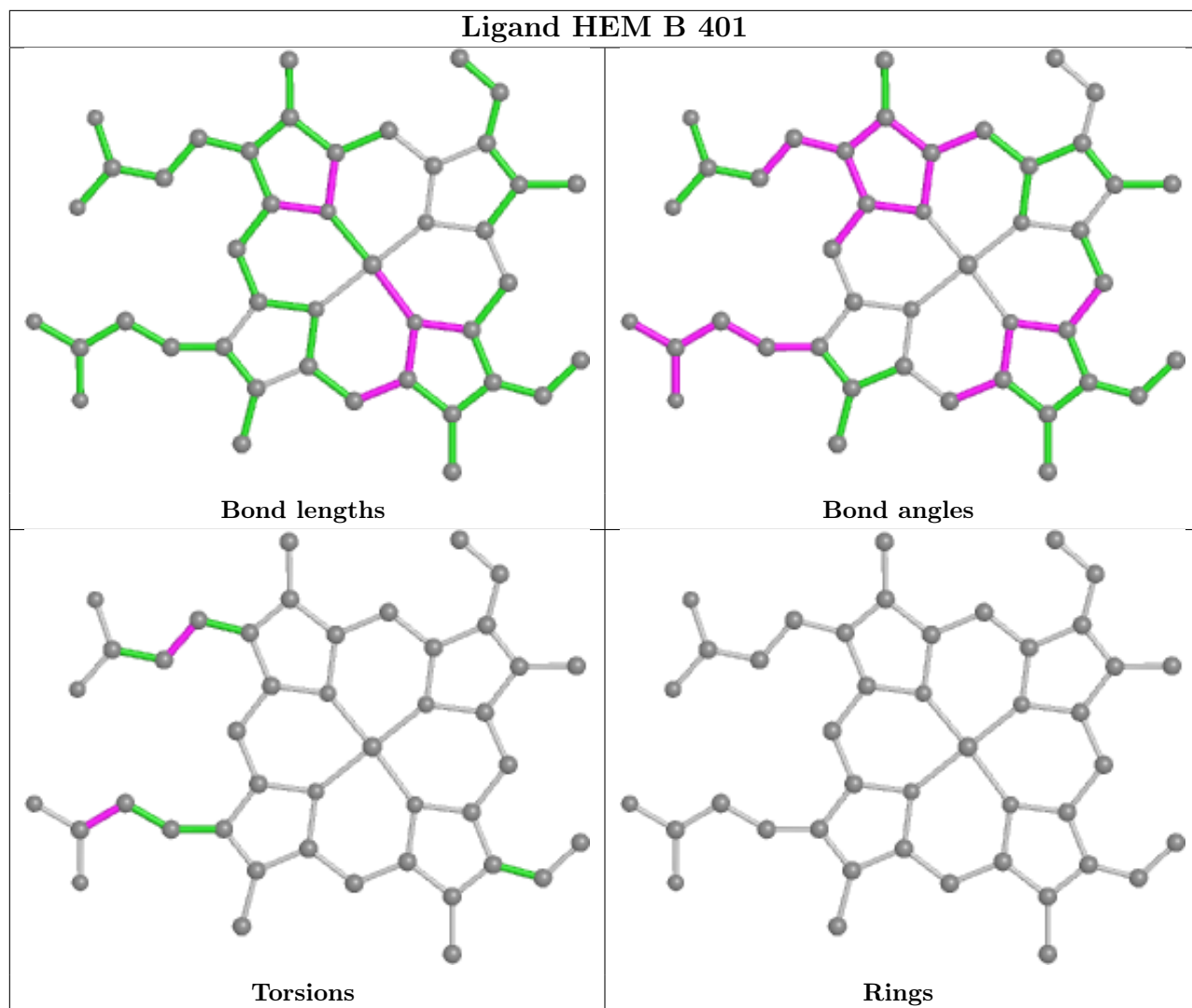
All (3) ring outliers are listed below:

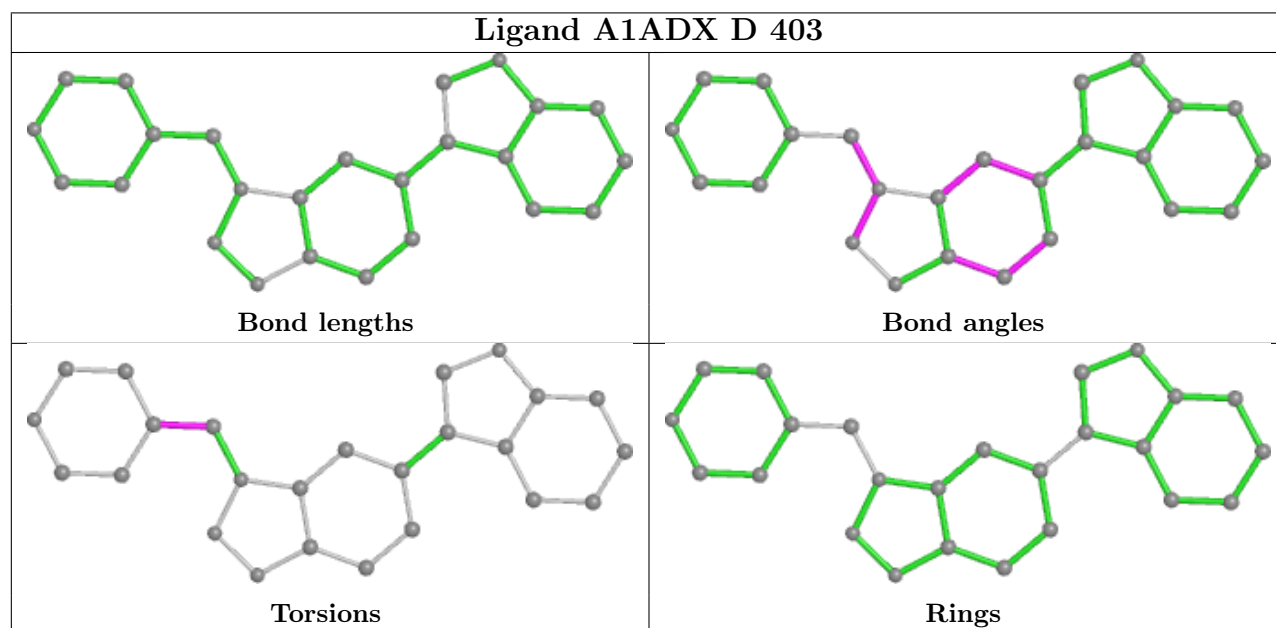
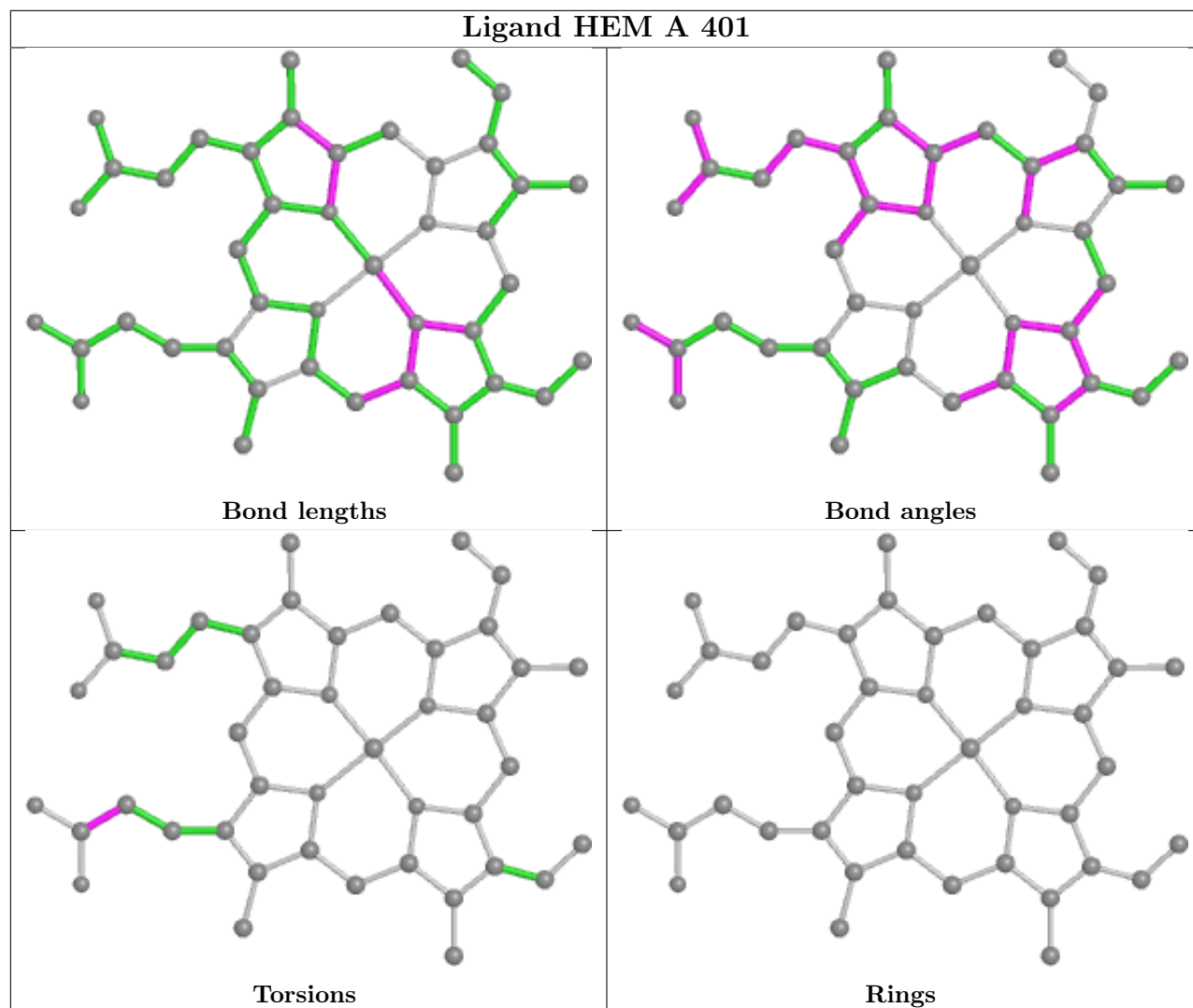
Mol	Chain	Res	Type	Atoms
4	B	403	A1ADX	C11-C12-C13-C14-C15-N4
4	A	403	A1ADX	C11-C12-C13-C14-C15-N4
4	C	403	A1ADX	C11-C12-C13-C14-C15-N4

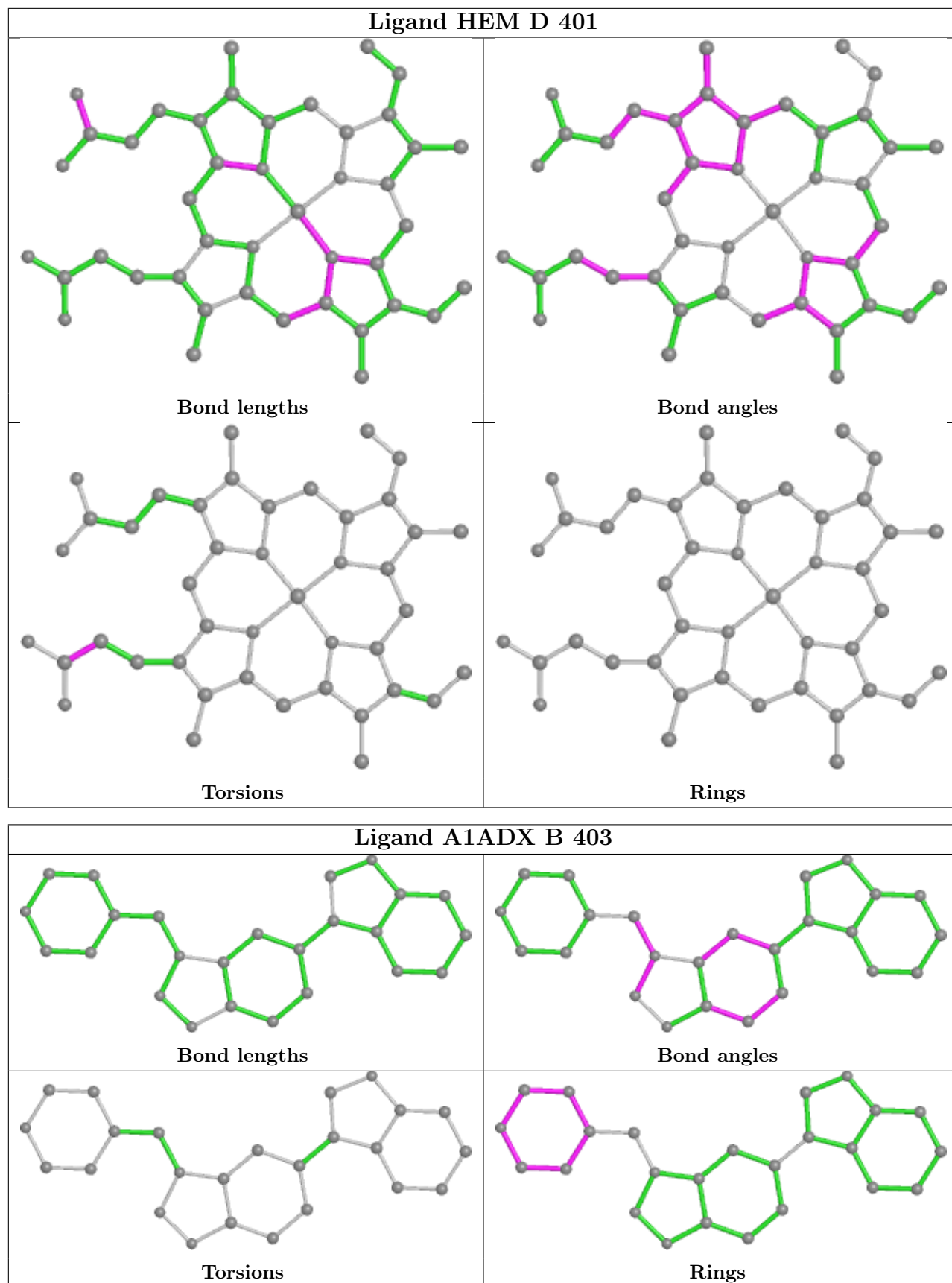
5 monomers are involved in 6 short contacts:

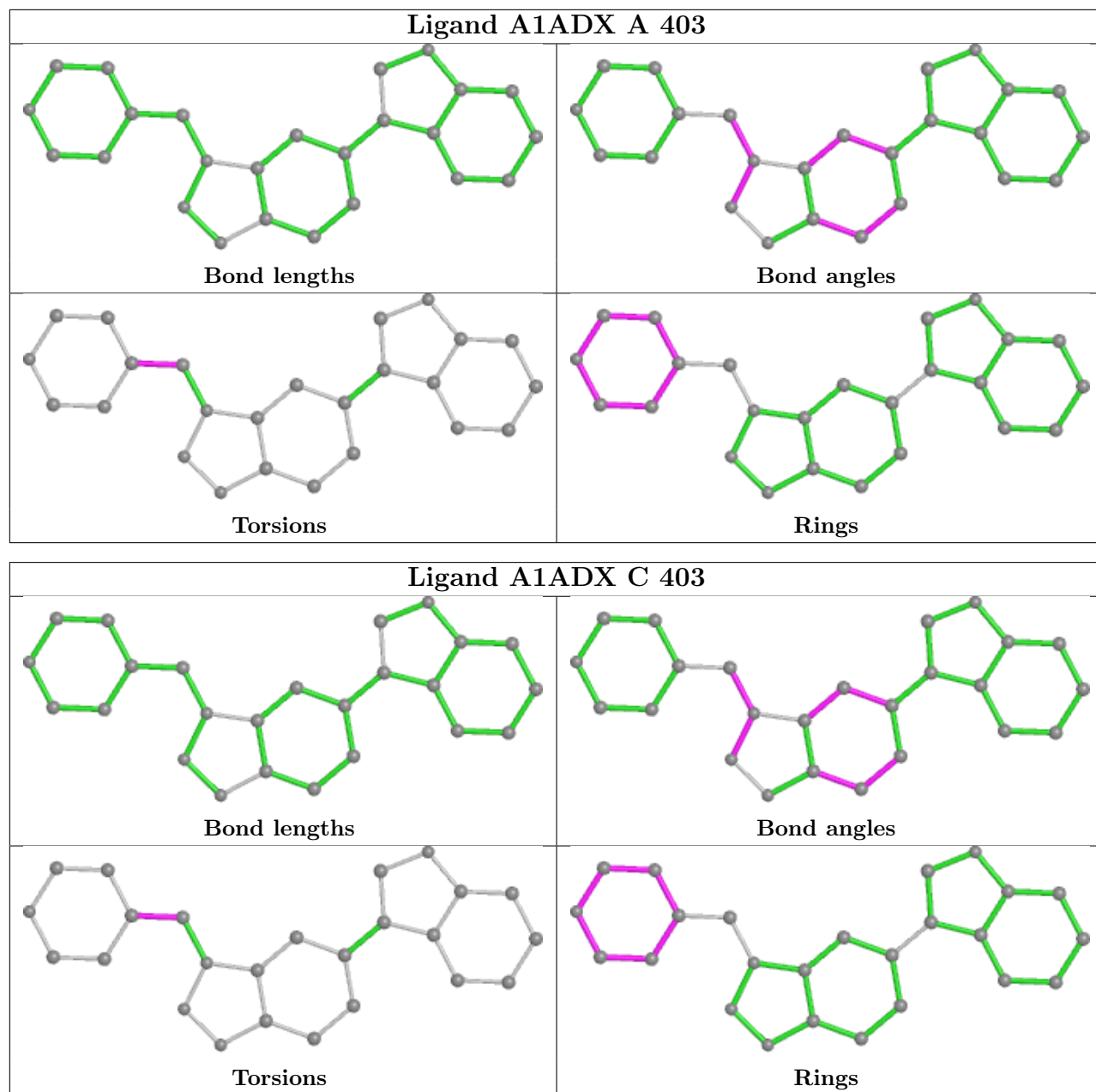
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	2	0
2	A	401	HEM	1	0
2	D	401	HEM	1	0
4	B	403	A1ADX	1	0
2	C	401	HEM	1	0

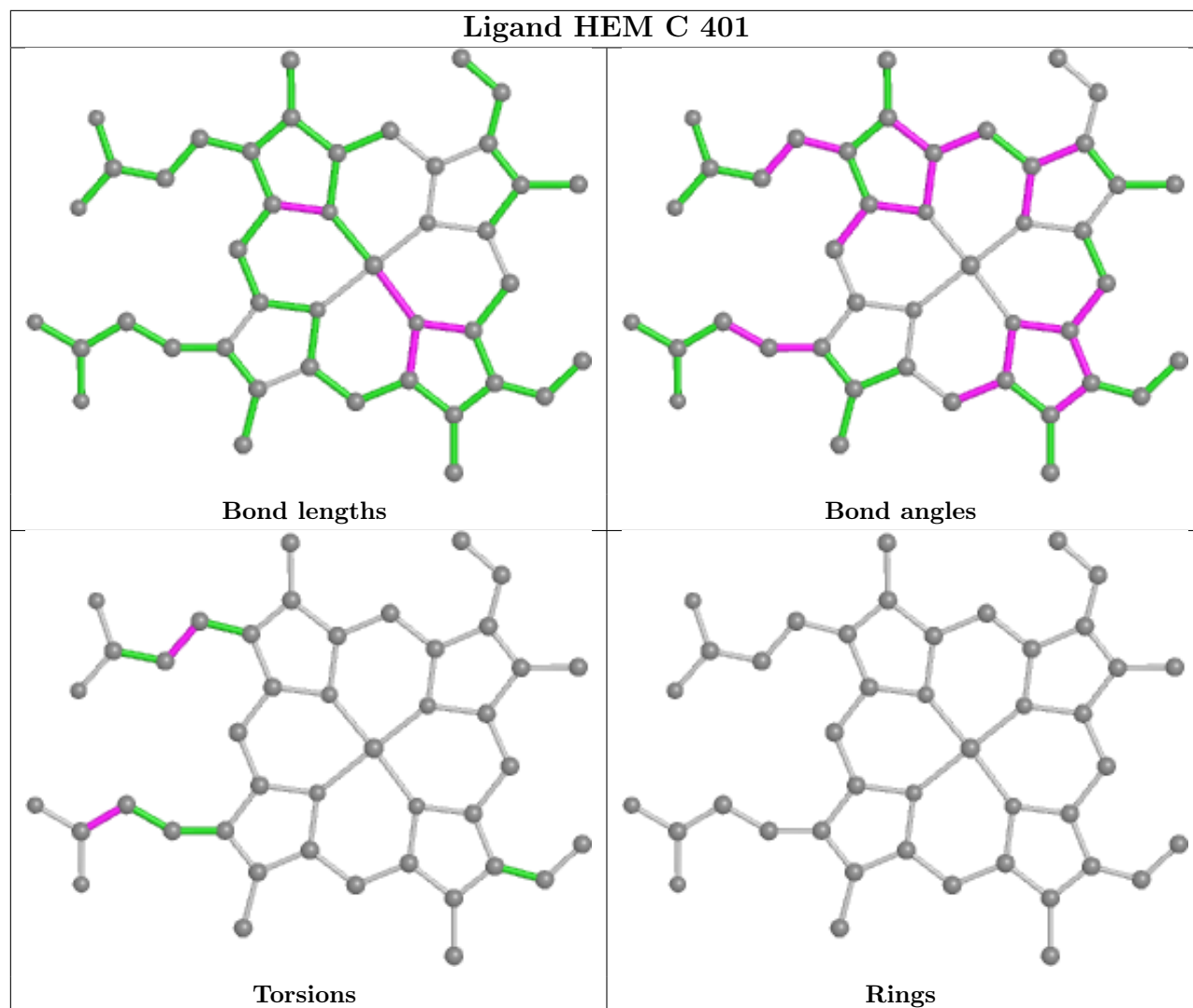
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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%)	0.42	7 (2%) 65 69	44, 63, 125, 180	0
1	B	347/380 (91%)	0.51	16 (4%) 32 35	45, 69, 126, 185	0
1	C	344/380 (90%)	0.62	26 (7%) 13 14	49, 88, 171, 246	0
1	D	343/380 (90%)	0.42	9 (2%) 56 60	45, 70, 128, 180	0
All	All	1381/1520 (90%)	0.49	58 (4%) 36 39	44, 71, 139, 246	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	HIS	11.9
1	A	386	HIS	6.0
1	C	389	LEU	5.9
1	C	383	PRO	5.7
1	B	386	HIS	5.3
1	C	384	THR	5.2
1	A	383	PRO	4.7
1	D	386	HIS	4.5
1	B	389	LEU	4.4
1	D	346	SER	4.3
1	C	179	HIS	4.3
1	B	348	TYR	4.3
1	C	238	PHE	3.9
1	C	371	TYR	3.7
1	C	348	TYR	3.7
1	C	264	LEU	3.6
1	D	384	THR	3.6
1	A	389	LEU	3.6
1	D	389	LEU	3.4
1	A	177	ARG	3.4
1	B	296	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	347	GLY	3.4
1	C	296	TYR	3.3
1	B	346	SER	3.2
1	C	193	LEU	3.1
1	D	348	TYR	3.1
1	D	241	ILE	3.1
1	D	40	LEU	2.9
1	C	176	ASN	2.8
1	B	340	ALA	2.8
1	B	384	THR	2.7
1	B	388	PHE	2.7
1	C	388	PHE	2.7
1	B	168	LEU	2.6
1	C	230	ILE	2.5
1	D	385	ILE	2.5
1	C	257	PHE	2.5
1	C	338	SER	2.5
1	A	345	SER	2.5
1	B	176	ASN	2.5
1	B	338	SER	2.5
1	B	351	LEU	2.4
1	C	267	LEU	2.4
1	C	253	GLN	2.4
1	C	241	ILE	2.4
1	C	340	ALA	2.4
1	C	40	LEU	2.3
1	D	257	PHE	2.3
1	C	346	SER	2.2
1	C	347	GLY	2.2
1	C	385	ILE	2.2
1	A	348	TYR	2.2
1	B	326	TYR	2.2
1	C	326	TYR	2.1
1	B	349	HIS	2.1
1	C	181	ARG	2.0
1	B	385	ILE	2.0
1	A	241	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

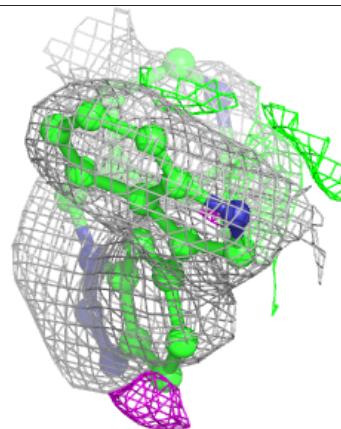
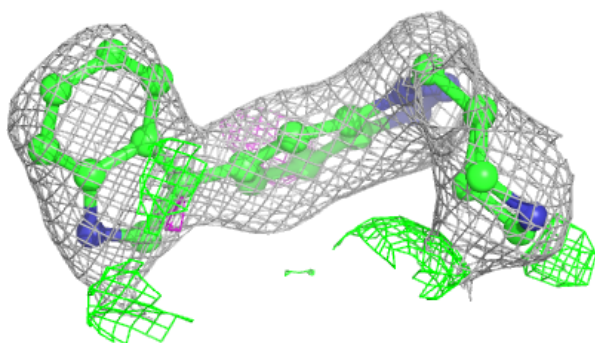
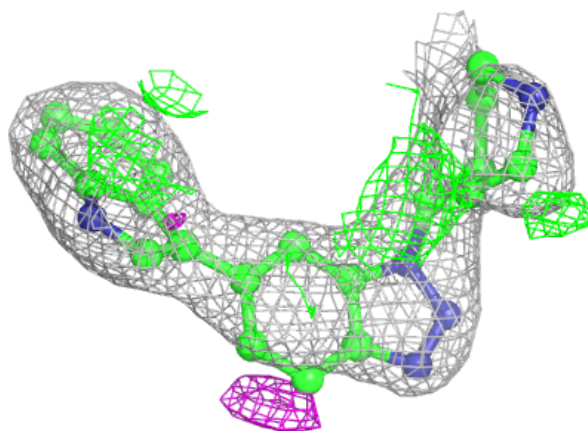
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1ADX	C	403	25/25	0.83	0.23	87,99,144,148	0
4	A1ADX	A	403	25/25	0.86	0.21	64,89,140,143	0
4	A1ADX	B	403	25/25	0.89	0.22	71,82,110,117	0
4	A1ADX	D	403	25/25	0.92	0.15	56,63,100,101	0
2	HEM	C	401	43/43	0.95	0.18	69,82,105,122	0
2	HEM	B	401	43/43	0.96	0.15	58,68,82,90	0
3	ZIQ	C	402	16/16	0.96	0.13	69,79,86,92	0
2	HEM	D	401	43/43	0.97	0.14	50,57,75,87	0
3	ZIQ	B	402	16/16	0.97	0.16	58,65,69,71	0
2	HEM	A	401	43/43	0.97	0.15	51,60,74,88	0
3	ZIQ	D	402	16/16	0.97	0.15	56,62,66,71	0
3	ZIQ	A	402	16/16	0.98	0.15	44,52,59,60	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.

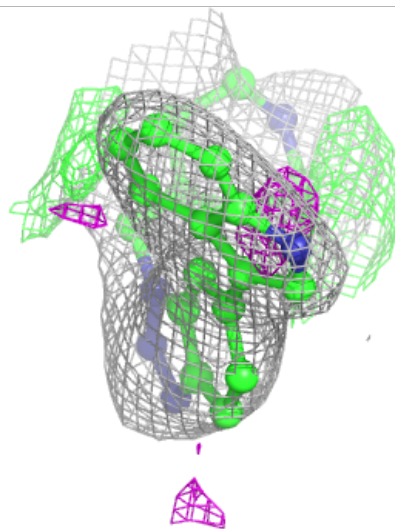
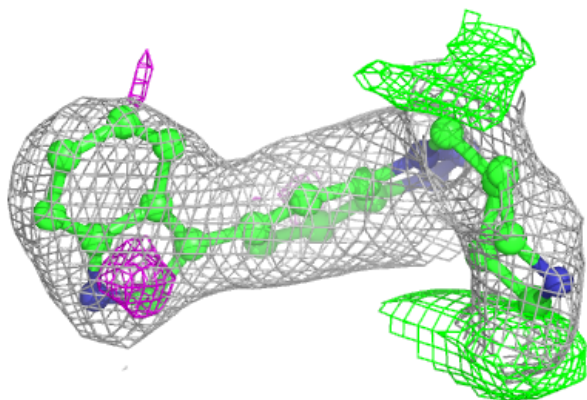
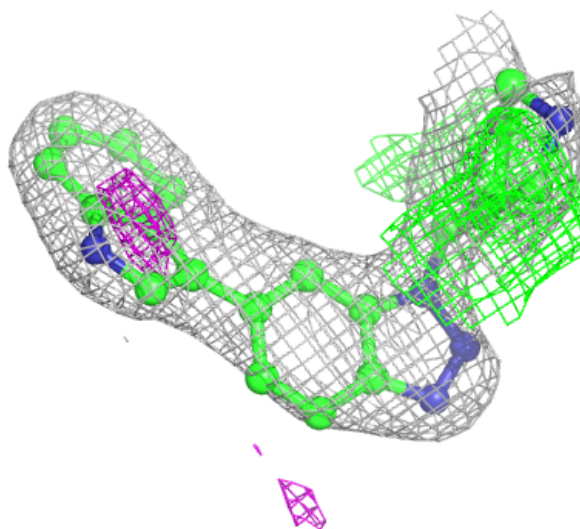
Electron density around A1ADX C 403:

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



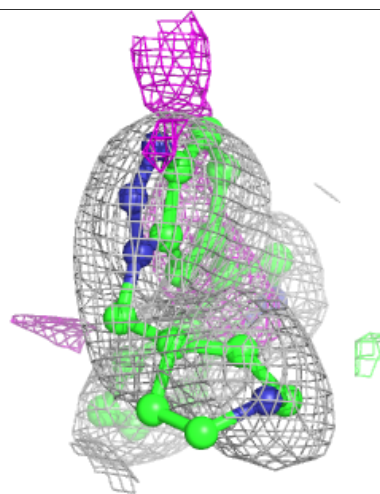
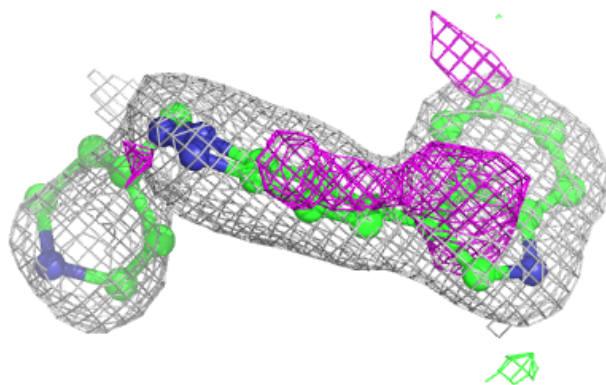
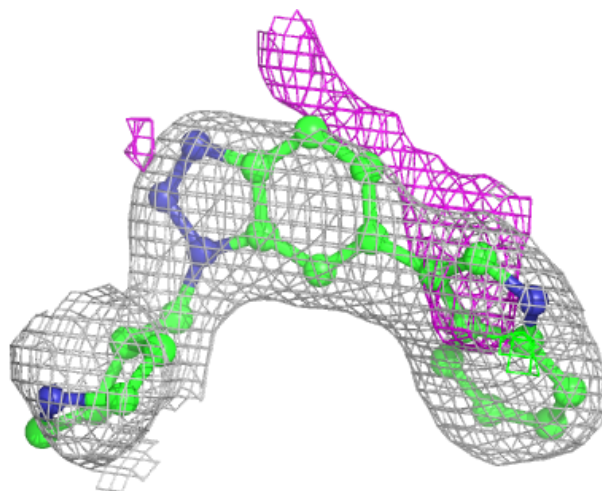
Electron density around A1ADX A 403:

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



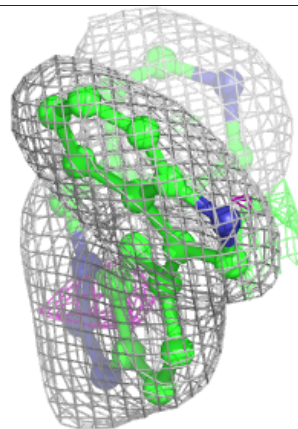
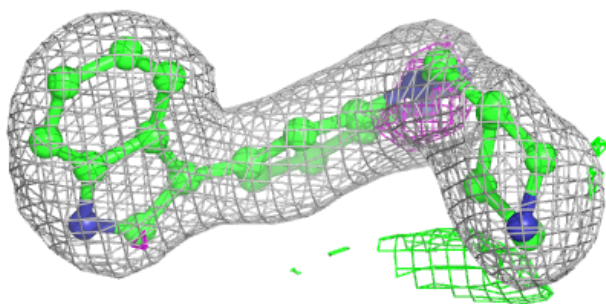
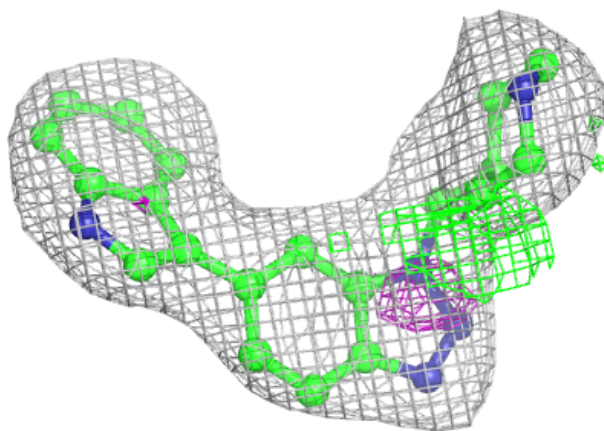
Electron density around A1ADX B 403:

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



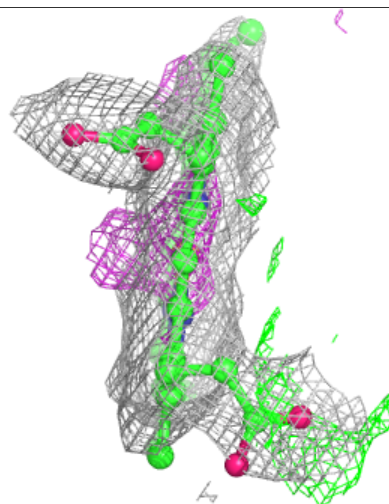
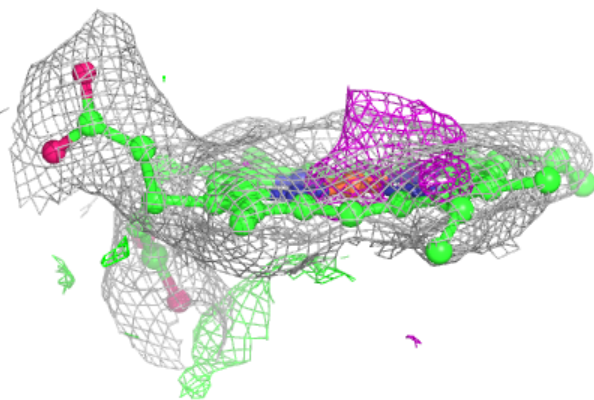
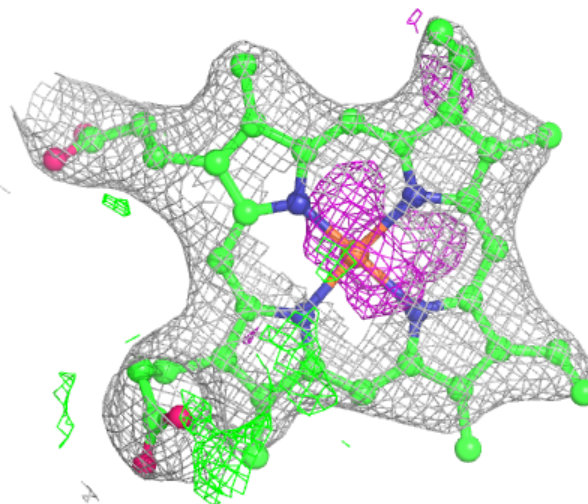
Electron density around A1ADX D 403:

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



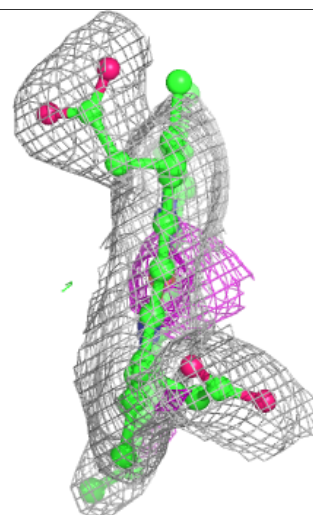
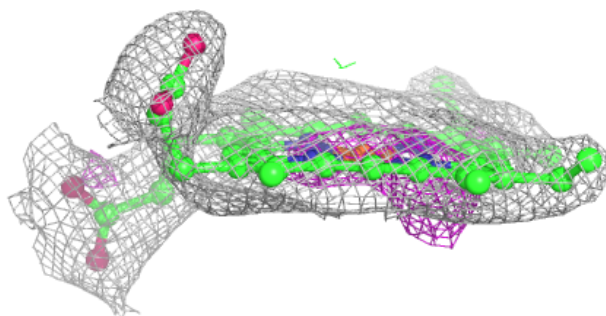
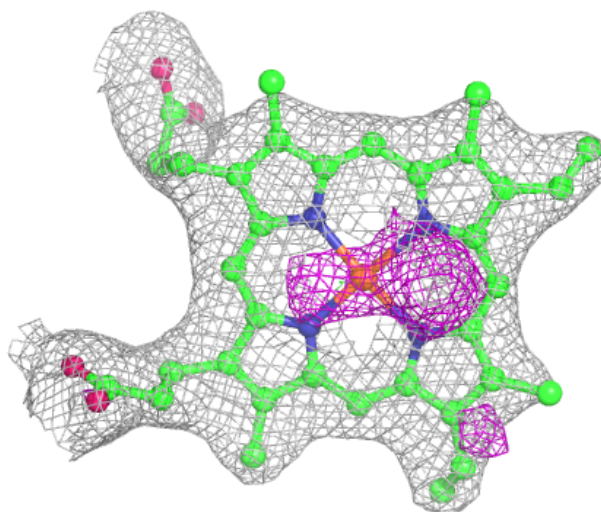
Electron density around HEM C 401:

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



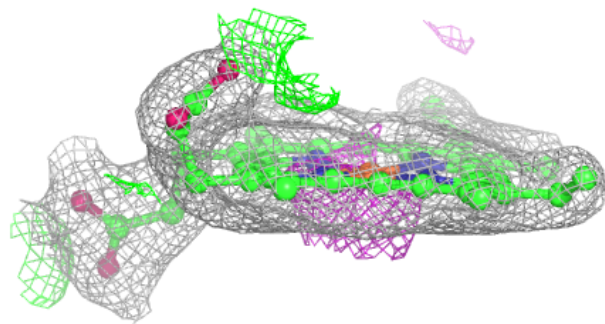
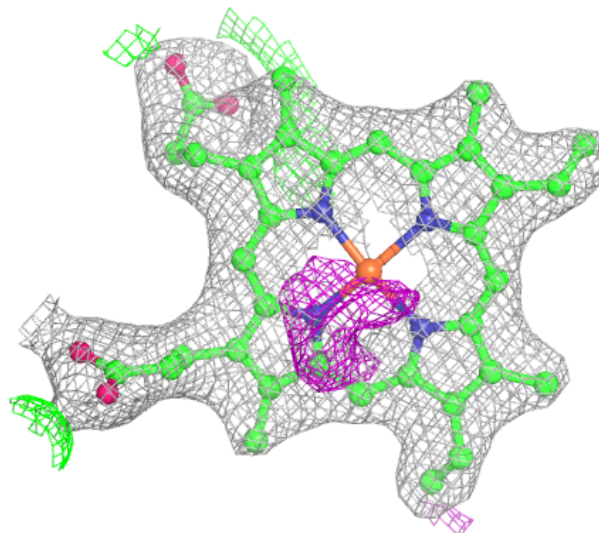
Electron density around HEM B 401:

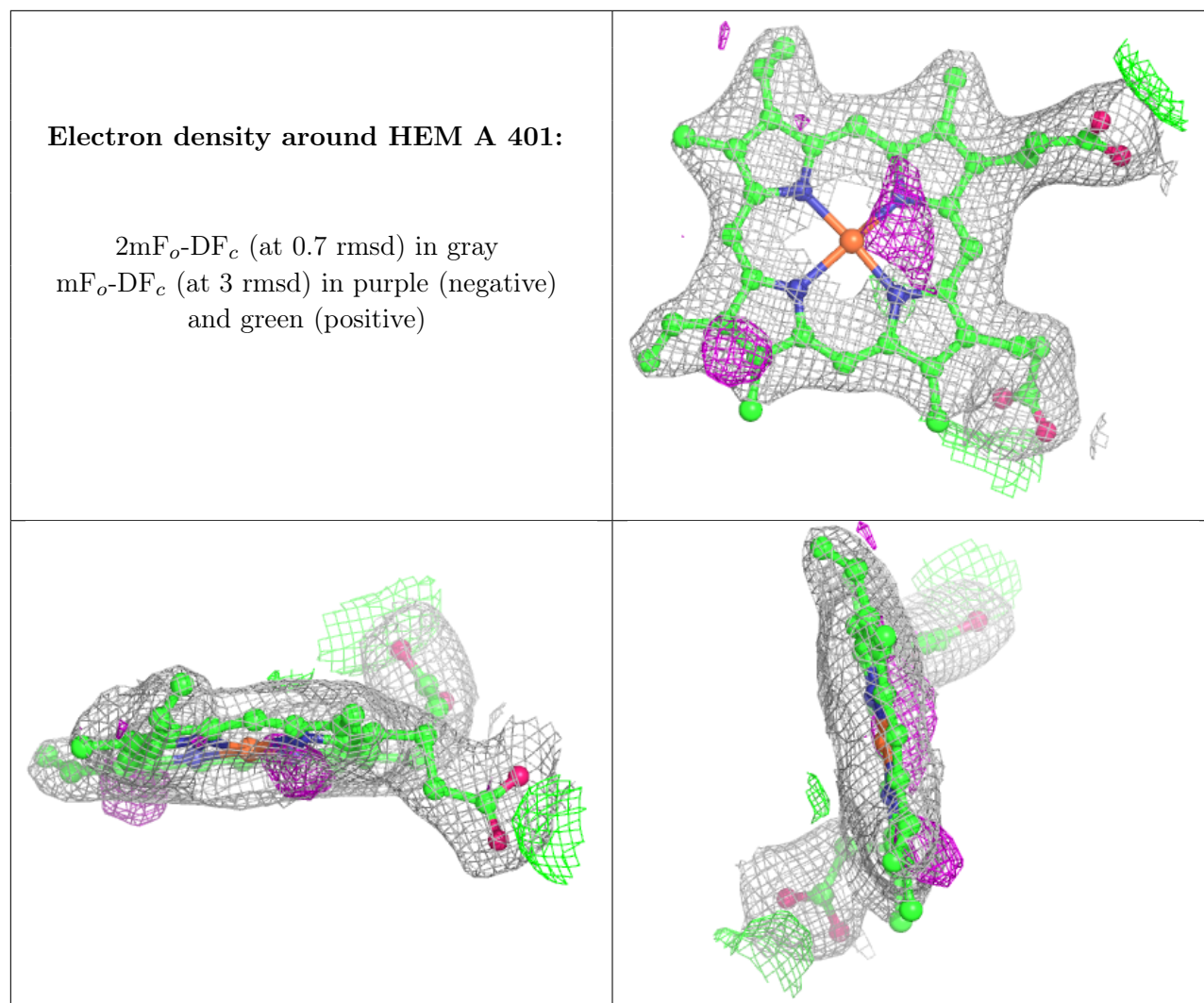
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.