



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2025 – 03:23 pm GMT

PDB ID : 9ESD
Title : Holo TDO with a bound inhibitor
Authors : Wicki, M.; Mac Sweeney, A.
Deposited on : 2024-03-26
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

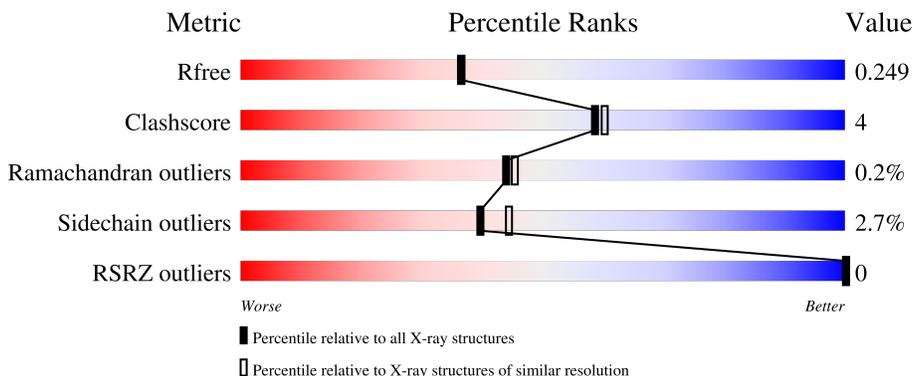
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	 81% 7% • 10%
1	B	365	 83% 6% • 11%
1	C	365	 82% 11% • 6%
1	D	365	 80% 9% • 9%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11368 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	328	Total 2735	C 1753	N 468	O 502	S 12	0	1	0
1	B	326	Total 2715	C 1740	N 469	O 494	S 12	0	1	0
1	C	344	Total 2849	C 1820	N 493	O 524	S 12	0	1	0
1	D	331	Total 2755	C 1763	N 475	O 505	S 12	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

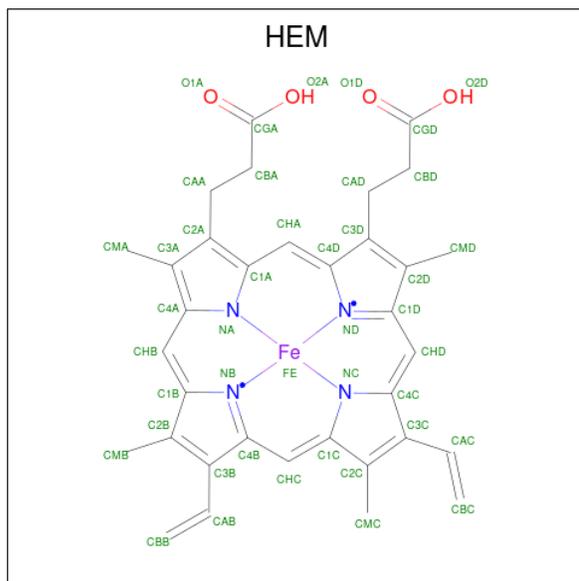
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P20351
A	380	LEU	-	expression tag	UNP P20351
A	381	GLU	-	expression tag	UNP P20351
A	382	HIS	-	expression tag	UNP P20351
A	383	HIS	-	expression tag	UNP P20351
A	384	HIS	-	expression tag	UNP P20351
A	385	HIS	-	expression tag	UNP P20351
A	386	HIS	-	expression tag	UNP P20351
A	387	HIS	-	expression tag	UNP P20351
B	23	MET	-	initiating methionine	UNP P20351
B	380	LEU	-	expression tag	UNP P20351
B	381	GLU	-	expression tag	UNP P20351
B	382	HIS	-	expression tag	UNP P20351
B	383	HIS	-	expression tag	UNP P20351
B	384	HIS	-	expression tag	UNP P20351
B	385	HIS	-	expression tag	UNP P20351
B	386	HIS	-	expression tag	UNP P20351
B	387	HIS	-	expression tag	UNP P20351
C	23	MET	-	initiating methionine	UNP P20351
C	380	LEU	-	expression tag	UNP P20351
C	381	GLU	-	expression tag	UNP P20351

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Chain	Residue	Modelled	Actual	Comment	Reference
C	382	HIS	-	expression tag	UNP P20351
C	383	HIS	-	expression tag	UNP P20351
C	384	HIS	-	expression tag	UNP P20351
C	385	HIS	-	expression tag	UNP P20351
C	386	HIS	-	expression tag	UNP P20351
C	387	HIS	-	expression tag	UNP P20351
D	23	MET	-	initiating methionine	UNP P20351
D	380	LEU	-	expression tag	UNP P20351
D	381	GLU	-	expression tag	UNP P20351
D	382	HIS	-	expression tag	UNP P20351
D	383	HIS	-	expression tag	UNP P20351
D	384	HIS	-	expression tag	UNP P20351
D	385	HIS	-	expression tag	UNP P20351
D	386	HIS	-	expression tag	UNP P20351
D	387	HIS	-	expression tag	UNP P20351

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



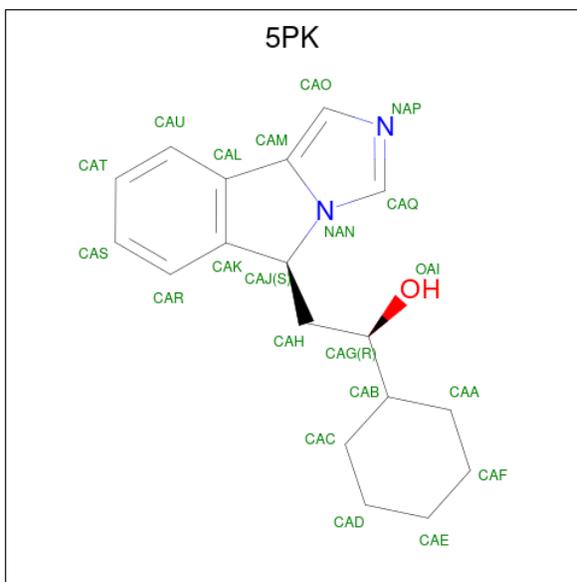
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is (1 {R})-1-cyclohexyl-2-[(5 {S})-5 {H}-imidazo[1,5-b]isoindol-5-yl]ethanol (three-letter code: 5PK) (formula: C₁₈H₂₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	21	18	2	1	0	0
3	B	1	21	18	2	1	0	0
3	C	1	21	18	2	1	0	0
3	D	1	21	18	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total 12 O	0	0
4	B	13	Total 13 O	0	0
4	C	17	Total 17 O	0	0

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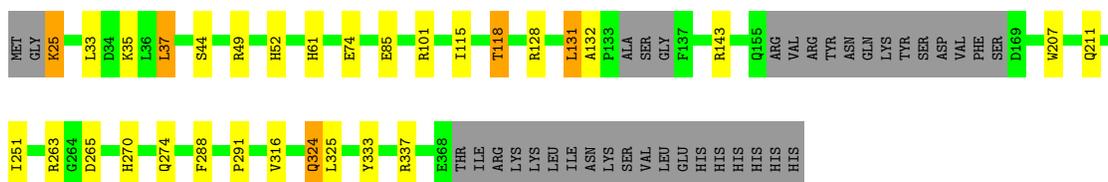
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	16	Total	O	0	0
			16	16		

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.

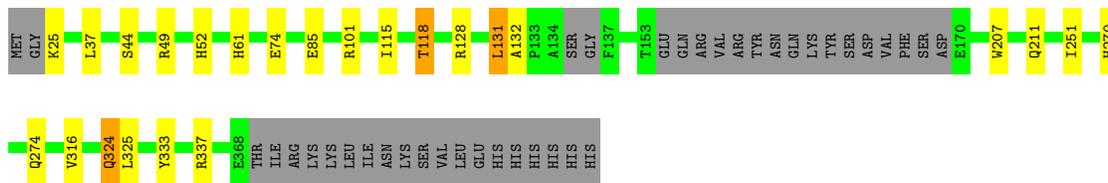
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain A: 



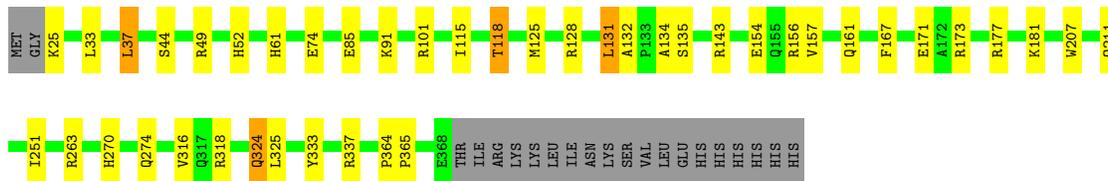
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain B: 



- Molecule 1: Tryptophan 2,3-dioxygenase

Chain C: 



- Molecule 1: Tryptophan 2,3-dioxygenase

Chain D: 



A233	M239	I251	R263	R267	H270	Q274	F288	P291	D300	V316	Q324	L325	Y333	R337	R343	E368	THR	ILE	ARG	LYS	LYS	LEU	ILE	ASN	LYS	SER	SER	VAL	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	143.74Å 143.74Å 141.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.05 – 2.10 47.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.05-2.10) 100.0 (47.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.10Å)	Xtrriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.233 , 0.255 0.223 , 0.249	Depositor DCC
R_{free} test set	4795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtrriage
Anisotropy	0.007	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.124 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11368	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 5PK

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	0.39	0/2793	0.51	0/3766
1	B	0.38	0/2773	0.50	0/3738
1	C	0.41	0/2910	0.52	0/3927
1	D	0.39	0/2811	0.49	0/3790
All	All	0.39	0/11287	0.51	0/15221

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2735	0	2734	26	0
1	B	2715	0	2718	22	0
1	C	2849	0	2838	35	0
1	D	2755	0	2761	35	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	21	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	22	2	0
3	C	21	0	22	5	0
3	D	21	0	22	2	0
4	A	12	0	0	0	0
4	B	13	0	0	0	0
4	C	17	0	0	0	0
4	D	16	0	0	0	0
All	All	11368	0	11259	97	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 (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:HIS:NE2	3:D:402:5PK:H22	1.87	0.89
1:B:101:ARG:HE	1:C:118:THR:CG2	1.87	0.88
1:A:101:ARG:HE	1:D:118:THR:CG2	1.88	0.87
1:A:118:THR:CG2	1:D:101:ARG:HE	1.89	0.86
1:B:118:THR:CG2	1:C:101:ARG:HE	1.90	0.84
1:A:132:ALA:HB2	1:D:25:LYS:HG3	1.64	0.79
1:C:61:HIS:NE2	3:C:402:5PK:H22	1.99	0.77
1:B:61:HIS:NE2	3:B:402:5PK:H22	2.01	0.75
1:D:152:LEU:CD2	1:D:267:ARG:HE	2.00	0.75
1:A:101:ARG:HE	1:D:118:THR:HG21	1.53	0.74
1:B:132:ALA:HB2	1:C:25:LYS:HG3	1.70	0.73
2:C:401:HEM:NA	3:C:402:5PK:H21	2.03	0.72
1:C:251:ILE:O	1:C:270:HIS:HE1	1.78	0.67
1:A:118:THR:HG22	1:D:101:ARG:HE	1.63	0.64
1:C:324:GLN:HE21	1:C:325:LEU:H	1.46	0.64
1:A:25:LYS:HG3	1:D:132:ALA:HB2	1.79	0.64
1:A:251:ILE:O	1:A:270:HIS:HE1	1.81	0.64
2:B:401:HEM:NA	3:B:402:5PK:H21	2.13	0.63
1:C:270:HIS:CD2	1:C:274:GLN:HE21	2.16	0.63
1:A:270:HIS:CD2	1:A:274:GLN:HE21	2.17	0.63
1:B:251:ILE:O	1:B:270:HIS:HE1	1.80	0.63
1:D:270:HIS:CD2	1:D:274:GLN:HE21	2.17	0.62
1:D:251:ILE:O	1:D:270:HIS:HE1	1.82	0.62
1:B:101:ARG:HE	1:C:118:THR:HG21	1.64	0.62
1:A:52:HIS:HE1	1:D:74:GLU:OE1	1.82	0.61
1:A:118:THR:HG21	1:D:101:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:OE1	1:D:52:HIS:HE1	1.83	0.60
1:C:161:GLN:HG2	1:D:233:ALA:HA	1.84	0.60
1:B:270:HIS:CD2	1:B:274:GLN:HE21	2.19	0.59
1:B:74:GLU:OE1	1:C:52:HIS:HE1	1.87	0.58
1:D:49:ARG:NH1	1:D:130:TYR:OH	2.35	0.57
2:D:401:HEM:NA	3:D:402:5PK:H21	2.19	0.57
1:B:324:GLN:HE21	1:B:325:LEU:H	1.52	0.56
1:B:25:LYS:HD2	1:C:132:ALA:HB2	1.87	0.56
1:B:118:THR:HG21	1:C:101:ARG:HE	1.68	0.55
1:B:118:THR:HG22	1:C:101:ARG:HE	1.70	0.55
1:C:115:ILE:O	1:C:118:THR:HB	2.08	0.54
1:B:115:ILE:O	1:B:118:THR:HB	2.07	0.53
1:B:324:GLN:NE2	1:B:325:LEU:H	2.06	0.53
1:A:324:GLN:NE2	1:A:325:LEU:H	2.06	0.53
1:D:324:GLN:NE2	1:D:325:LEU:H	2.07	0.53
1:A:324:GLN:HE21	1:A:325:LEU:H	1.54	0.52
1:A:61:HIS:NE2	3:A:402:5PK:H22	2.24	0.52
1:C:128[A]:ARG:HB2	3:C:402:5PK:H4	1.91	0.52
1:C:324:GLN:NE2	1:C:325:LEU:H	2.06	0.52
1:C:125:MET:HA	1:C:128[A]:ARG:HG2	1.91	0.51
1:B:52:HIS:HE1	1:C:74:GLU:OE1	1.92	0.51
1:D:153:THR:HA	1:D:156:ARG:HD2	1.93	0.50
1:D:115:ILE:O	1:D:118:THR:HB	2.13	0.49
1:A:115:ILE:O	1:A:118:THR:HB	2.12	0.49
1:B:333:TYR:CZ	1:B:337:ARG:HD2	2.49	0.48
1:A:333:TYR:CZ	1:A:337:ARG:HD2	2.47	0.48
1:C:333:TYR:CZ	1:C:337:ARG:HD2	2.50	0.47
1:B:101:ARG:HE	1:C:118:THR:HG22	1.74	0.47
1:D:333:TYR:CZ	1:D:337:ARG:HD2	2.49	0.47
1:A:132:ALA:CB	1:D:25:LYS:HG3	2.40	0.46
1:C:161:GLN:HG2	1:D:233:ALA:CA	2.45	0.46
2:C:401:HEM:C4A	3:C:402:5PK:H21	2.50	0.46
1:D:324:GLN:HE21	1:D:325:LEU:H	1.62	0.46
1:C:33:LEU:HB3	1:C:37:LEU:HD22	1.99	0.45
1:A:316:VAL:HG22	2:A:401:HEM:C1B	2.52	0.45
1:D:33:LEU:HB3	1:D:37:LEU:HD22	1.97	0.45
1:D:207:TRP:O	1:D:211:GLN:HG3	2.17	0.45
1:D:81:MET:HG2	1:D:91:LYS:NZ	2.32	0.44
1:D:44:SER:HB2	1:D:49:ARG:O	2.18	0.44
1:C:44:SER:HB2	1:C:49:ARG:O	2.17	0.44
1:C:128[A]:ARG:HA	1:C:131:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:VAL:HG22	2:C:401:HEM:C1B	2.53	0.43
1:B:316:VAL:HG22	2:B:401:HEM:C1B	2.53	0.43
1:A:44:SER:HB2	1:A:49:ARG:O	2.18	0.43
1:D:155:GLN:HB3	1:D:343:ARG:HB3	2.00	0.43
1:A:128:ARG:HA	1:A:131:LEU:HD22	2.01	0.42
3:A:402:5PK:OAI	3:A:402:5PK:H21	2.19	0.42
1:C:364:PRO:HA	1:C:365:PRO:HD3	1.93	0.42
1:D:316:VAL:HG22	2:D:401:HEM:C1B	2.54	0.42
1:A:101:ARG:HE	1:D:118:THR:HG22	1.78	0.42
1:C:167:PHE:CE2	1:C:173:ARG:HG3	2.55	0.42
1:C:177:ARG:O	1:C:181:LYS:HG2	2.20	0.42
1:A:33:LEU:HB3	1:A:37:LEU:HD22	2.02	0.42
1:C:161:GLN:HG2	1:D:233:ALA:CB	2.50	0.42
1:C:207:TRP:O	1:C:211:GLN:HG3	2.20	0.42
1:D:288:PHE:C	1:D:291:PRO:HD2	2.40	0.42
1:D:270:HIS:CD2	1:D:274:GLN:NE2	2.86	0.41
1:B:207:TRP:O	1:B:211:GLN:HG3	2.20	0.41
1:C:270:HIS:CD2	1:C:274:GLN:NE2	2.84	0.41
1:B:44:SER:HB2	1:B:49:ARG:O	2.20	0.41
1:A:288:PHE:C	1:A:291:PRO:HD2	2.40	0.41
1:B:128:ARG:HA	1:B:131:LEU:HD22	2.02	0.41
1:A:35:LYS:HG3	1:D:35:LYS:HG3	2.02	0.41
1:C:251:ILE:O	1:C:270:HIS:CE1	2.66	0.41
1:D:128:ARG:HA	1:D:131:LEU:HD22	2.03	0.41
1:A:207:TRP:O	1:A:211:GLN:HG3	2.20	0.41
1:C:128[B]:ARG:HB2	3:C:402:5PK:H4	2.03	0.41
1:B:270:HIS:CD2	1:B:274:GLN:NE2	2.87	0.40
1:A:251:ILE:O	1:A:270:HIS:CE1	2.68	0.40
1:C:128[B]:ARG:HA	1:C:131:LEU:HD22	2.03	0.40
1:C:318:ARG:NH2	1:D:300:ASP:OD1	2.54	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	323/365 (88%)	318 (98%)	5 (2%)	0	100	100
1	B	321/365 (88%)	316 (98%)	5 (2%)	0	100	100
1	C	343/365 (94%)	333 (97%)	7 (2%)	3 (1%)	14	11
1	D	327/365 (90%)	322 (98%)	5 (2%)	0	100	100
All	All	1314/1460 (90%)	1289 (98%)	22 (2%)	3 (0%)	44	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	134	ALA
1	C	154	GLU
1	C	157	VAL

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	302/337 (90%)	293 (97%)	9 (3%)	36	40
1	B	298/337 (88%)	293 (98%)	5 (2%)	56	63
1	C	313/337 (93%)	302 (96%)	11 (4%)	31	34
1	D	304/337 (90%)	296 (97%)	8 (3%)	41	46
All	All	1217/1348 (90%)	1184 (97%)	33 (3%)	40	44

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	37	LEU
1	A	85	GLU
1	A	118	THR
1	A	131	LEU

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Mol	Chain	Res	Type
1	A	143	ARG
1	A	263	ARG
1	A	265	ASP
1	A	324	GLN
1	B	37	LEU
1	B	85	GLU
1	B	118	THR
1	B	131	LEU
1	B	324	GLN
1	C	37	LEU
1	C	85	GLU
1	C	91	LYS
1	C	118	THR
1	C	131	LEU
1	C	135	SER
1	C	143	ARG
1	C	156	ARG
1	C	171	GLU
1	C	263	ARG
1	C	324	GLN
1	D	37	LEU
1	D	118	THR
1	D	131	LEU
1	D	152	LEU
1	D	155	GLN
1	D	239	MET
1	D	263	ARG
1	D	324	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	112	GLN
1	A	141	GLN
1	A	190	GLN
1	A	221	GLN
1	A	270	HIS
1	A	290	GLN
1	A	324	GLN
1	B	52	HIS
1	B	112	GLN

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	190	GLN
1	B	221	GLN
1	B	270	HIS
1	B	274	GLN
1	B	324	GLN
1	C	52	HIS
1	C	112	GLN
1	C	141	GLN
1	C	190	GLN
1	C	221	GLN
1	C	270	HIS
1	C	274	GLN
1	C	324	GLN
1	D	52	HIS
1	D	112	GLN
1	D	141	GLN
1	D	190	GLN
1	D	221	GLN
1	D	270	HIS
1	D	274	GLN
1	D	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	1,3	41,50,50	0.98	2 (4%)	45,82,82	1.17	5 (11%)
2	HEM	A	401	1,3	41,50,50	0.97	2 (4%)	45,82,82	1.18	4 (8%)
2	HEM	C	401	1,3	41,50,50	0.98	3 (7%)	45,82,82	1.05	3 (6%)
3	5PK	B	402	2	22,24,24	2.87	7 (31%)	26,34,34	1.80	4 (15%)
3	5PK	D	402	2	22,24,24	2.74	6 (27%)	26,34,34	1.60	4 (15%)
3	5PK	A	402	2	22,24,24	3.05	6 (27%)	26,34,34	1.22	3 (11%)
2	HEM	D	401	1,3	41,50,50	0.93	2 (4%)	45,82,82	1.20	5 (11%)
3	5PK	C	402	2	22,24,24	2.61	6 (27%)	26,34,34	1.35	3 (11%)

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	-	2/12/54/54	-
2	HEM	A	401	1,3	-	2/12/54/54	-
2	HEM	C	401	1,3	-	2/12/54/54	-
3	5PK	B	402	2	-	0/8/28/28	0/4/4/4
3	5PK	D	402	2	-	0/8/28/28	0/4/4/4
3	5PK	A	402	2	-	0/8/28/28	0/4/4/4
2	HEM	D	401	1,3	-	3/12/54/54	-
3	5PK	C	402	2	-	0/8/28/28	0/4/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	5PK	CAK-CAJ	-10.43	1.39	1.51
3	B	402	5PK	CAK-CAJ	-8.94	1.41	1.51
3	D	402	5PK	CAK-CAJ	-7.96	1.42	1.51
3	C	402	5PK	CAK-CAJ	-6.87	1.43	1.51
3	D	402	5PK	CAL-CAM	-6.47	1.33	1.46
3	C	402	5PK	CAL-CAM	-6.45	1.33	1.46
3	B	402	5PK	CAL-CAM	-6.29	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	5PK	CAL-CAM	-6.14	1.34	1.46
3	B	402	5PK	CAR-CAK	-4.25	1.34	1.39
3	D	402	5PK	CAR-CAK	-4.13	1.34	1.39
3	A	402	5PK	CAR-CAK	-3.98	1.34	1.39
3	C	402	5PK	CAR-CAK	-3.95	1.34	1.39
3	D	402	5PK	CAU-CAL	-3.91	1.33	1.40
3	A	402	5PK	CAU-CAL	-3.83	1.33	1.40
3	C	402	5PK	CAU-CAL	-3.63	1.34	1.40
3	B	402	5PK	CAU-CAL	-3.45	1.34	1.40
2	B	401	HEM	CHB-C1B	3.16	1.43	1.35
2	C	401	HEM	CHB-C1B	3.08	1.42	1.35
2	A	401	HEM	CHB-C1B	3.08	1.42	1.35
3	A	402	5PK	CAL-CAK	-3.04	1.35	1.40
3	B	402	5PK	CAO-CAM	-2.89	1.33	1.38
3	D	402	5PK	CAL-CAK	-2.89	1.35	1.40
3	D	402	5PK	CAO-CAM	-2.84	1.33	1.38
3	B	402	5PK	CAL-CAK	-2.82	1.35	1.40
2	D	401	HEM	CHB-C1B	2.75	1.42	1.35
3	C	402	5PK	CAO-CAM	-2.72	1.33	1.38
3	A	402	5PK	CAO-CAM	-2.65	1.33	1.38
3	C	402	5PK	CAL-CAK	-2.60	1.36	1.40
2	B	401	HEM	C1B-NB	-2.39	1.36	1.40
2	A	401	HEM	C1B-NB	-2.33	1.36	1.40
2	C	401	HEM	C1B-NB	-2.13	1.36	1.40
2	D	401	HEM	C1B-NB	-2.07	1.36	1.40
2	C	401	HEM	C3C-C2C	-2.05	1.37	1.40
3	B	402	5PK	CAM-NAN	-2.01	1.32	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	5PK	CAH-CAJ-NAN	-5.64	102.85	113.50
3	D	402	5PK	CAH-CAJ-NAN	-5.26	103.57	113.50
3	B	402	5PK	CAH-CAG-CAB	-4.26	105.79	114.41
2	D	401	HEM	C4C-CHD-C1D	4.12	128.00	122.56
2	A	401	HEM	C4C-CHD-C1D	4.01	127.85	122.56
2	B	401	HEM	C4C-CHD-C1D	3.90	127.71	122.56
2	C	401	HEM	C4C-CHD-C1D	3.46	127.13	122.56
2	B	401	HEM	C4B-CHC-C1C	3.15	126.72	122.56
3	C	402	5PK	NAP-CAQ-NAN	-3.12	107.63	112.26
3	A	402	5PK	OAI-CAG-CAH	3.10	115.33	109.11
3	D	402	5PK	NAP-CAQ-NAN	-3.09	107.67	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	5PK	CAH-CAJ-NAN	-3.05	107.74	113.50
3	B	402	5PK	NAP-CAQ-NAN	-3.04	107.75	112.26
2	A	401	HEM	C4B-CHC-C1C	2.88	126.36	122.56
2	D	401	HEM	C4B-CHC-C1C	2.86	126.33	122.56
3	A	402	5PK	CAU-CAL-CAM	2.83	128.91	123.45
3	B	402	5PK	CAU-CAL-CAM	2.74	128.74	123.45
2	B	401	HEM	CMC-C2C-C3C	2.65	129.63	124.68
2	A	401	HEM	CMC-C2C-C3C	2.63	129.59	124.68
2	C	401	HEM	C4B-CHC-C1C	2.60	125.98	122.56
3	D	402	5PK	CAH-CAG-CAB	-2.47	109.41	114.41
2	D	401	HEM	CMC-C2C-C3C	2.46	129.28	124.68
3	A	402	5PK	NAP-CAQ-NAN	-2.45	108.63	112.26
3	D	402	5PK	CAU-CAL-CAM	2.39	128.07	123.45
3	C	402	5PK	CAU-CAL-CAM	2.36	128.02	123.45
2	C	401	HEM	CMC-C2C-C3C	2.35	129.08	124.68
2	A	401	HEM	CAD-C3D-C4D	2.27	128.62	124.66
2	D	401	HEM	CAD-C3D-C4D	2.10	128.33	124.66
2	B	401	HEM	CAD-C3D-C4D	2.09	128.31	124.66
2	D	401	HEM	C3B-C2B-C1B	-2.07	104.95	106.49
2	B	401	HEM	CMA-C3A-C4A	-2.01	125.37	128.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

8 monomers are involved in 15 short contacts:

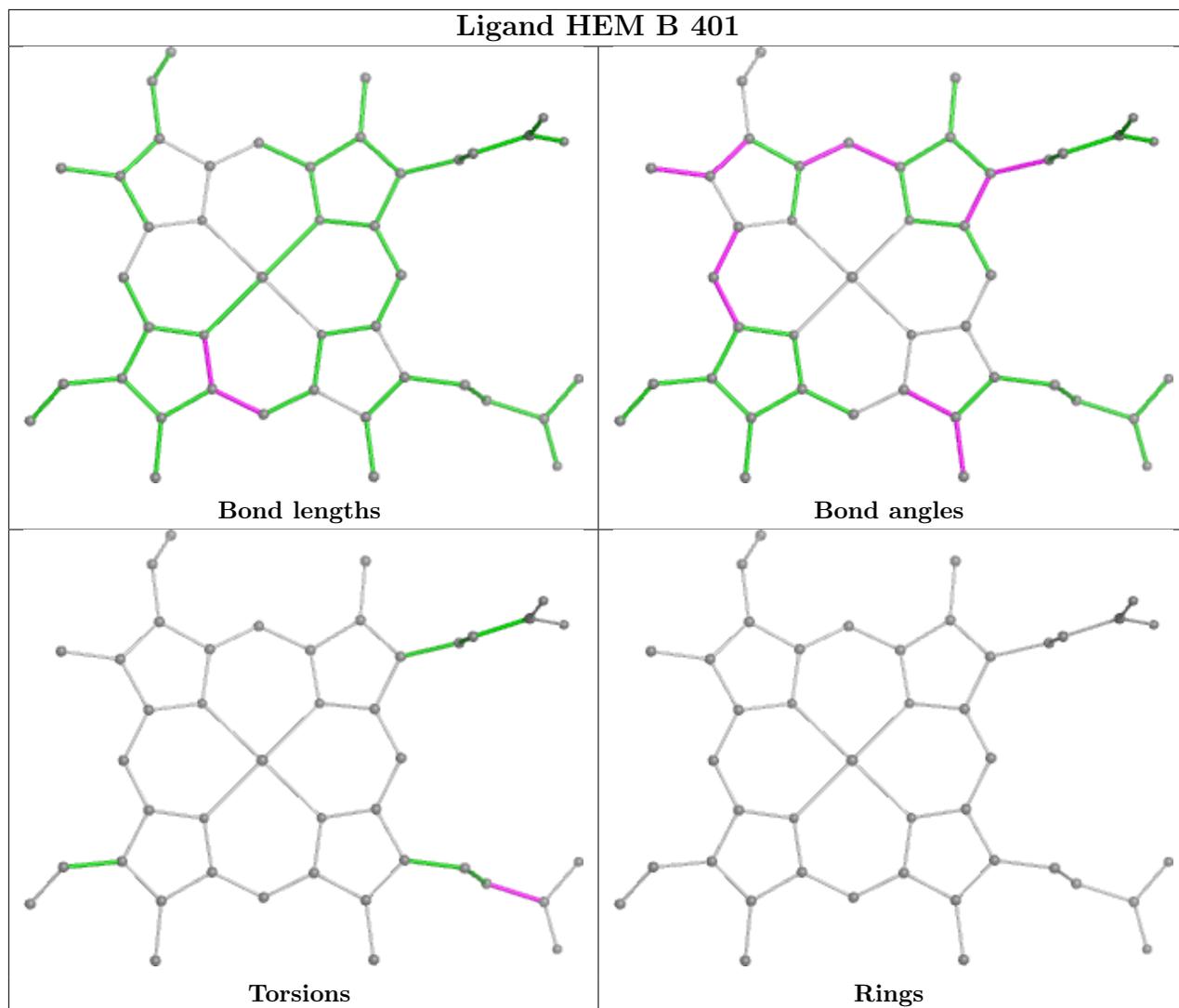
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	2	0
2	A	401	HEM	1	0

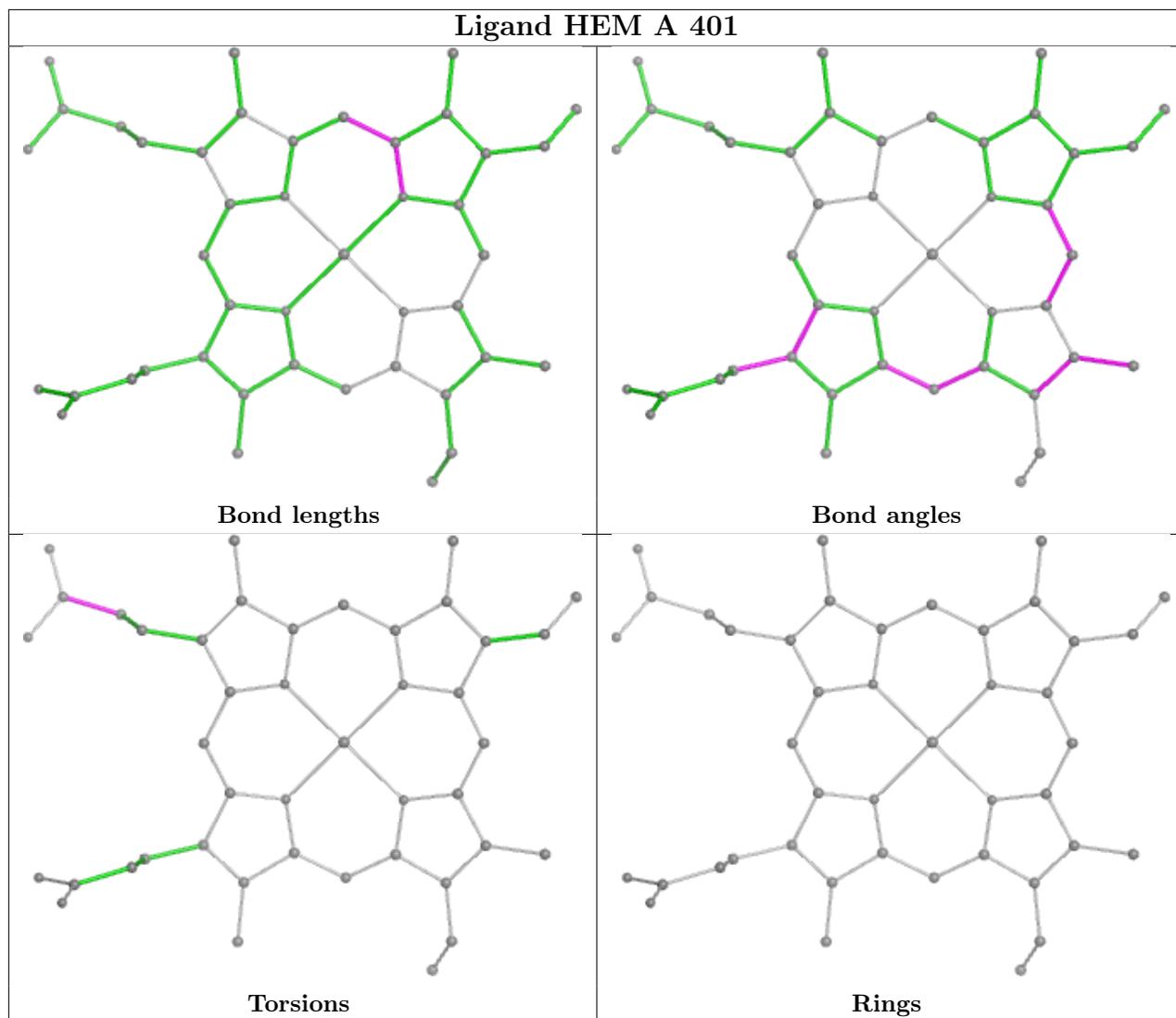
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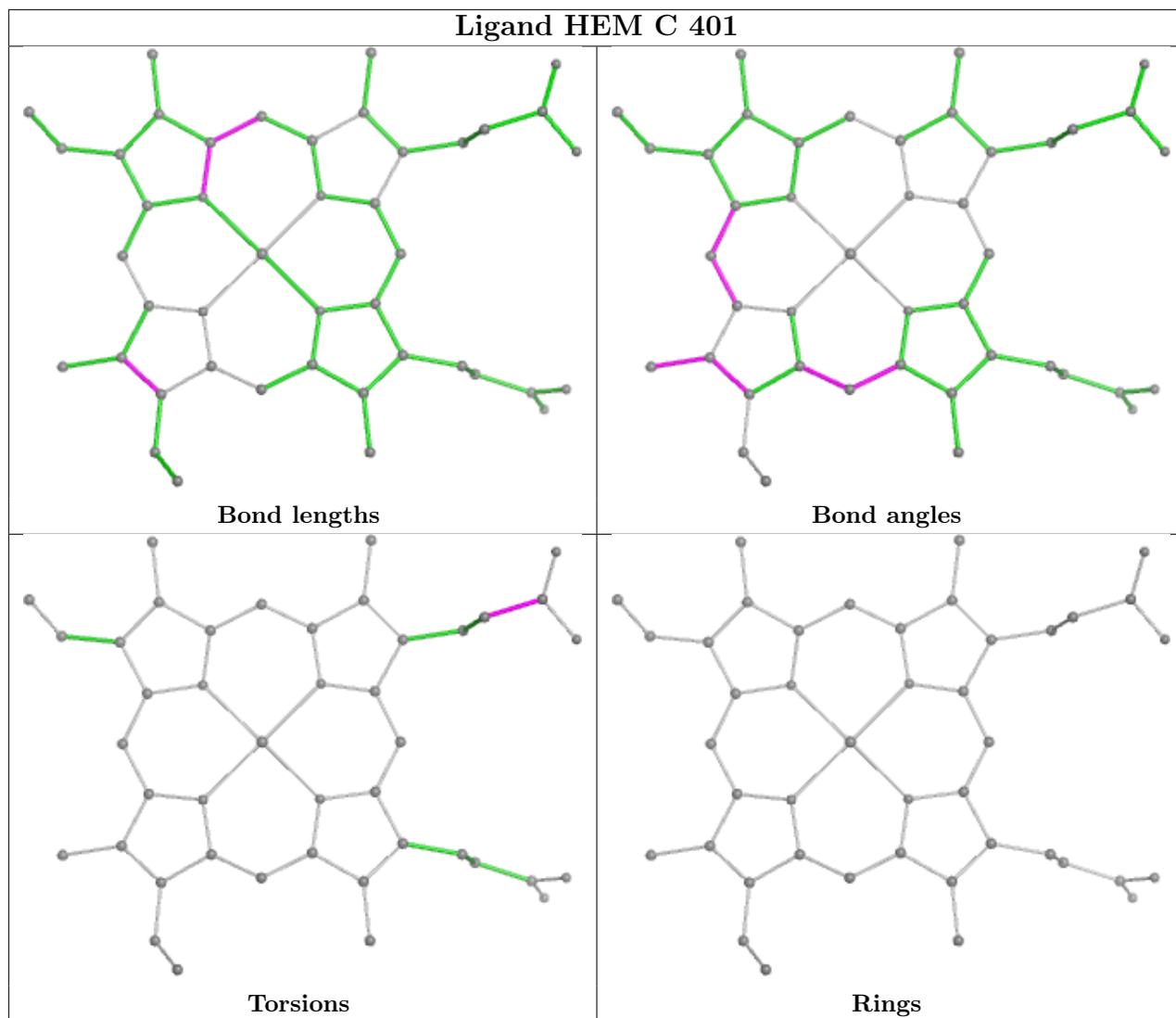
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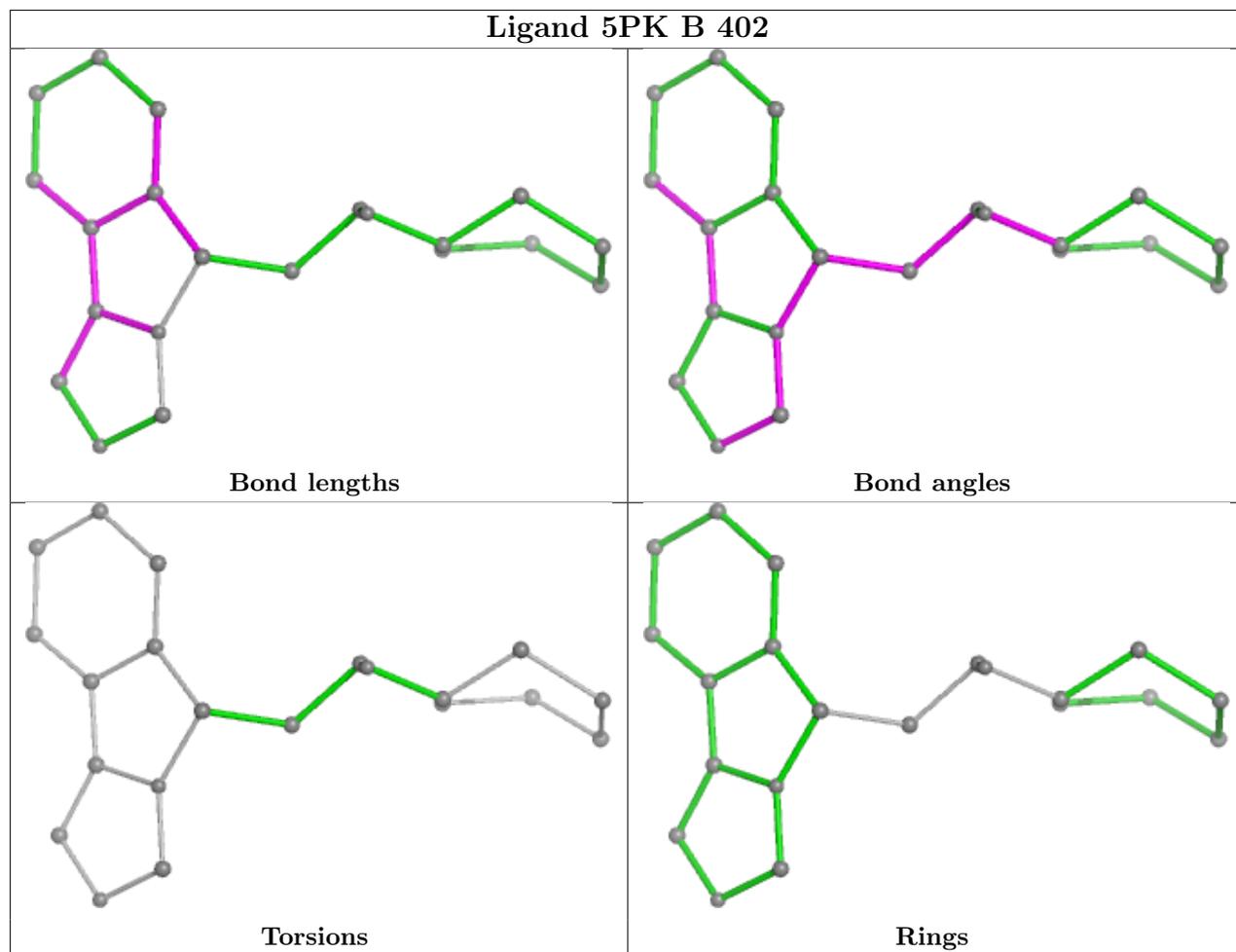
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	HEM	3	0
3	B	402	5PK	2	0
3	D	402	5PK	2	0
3	A	402	5PK	2	0
2	D	401	HEM	2	0
3	C	402	5PK	5	0

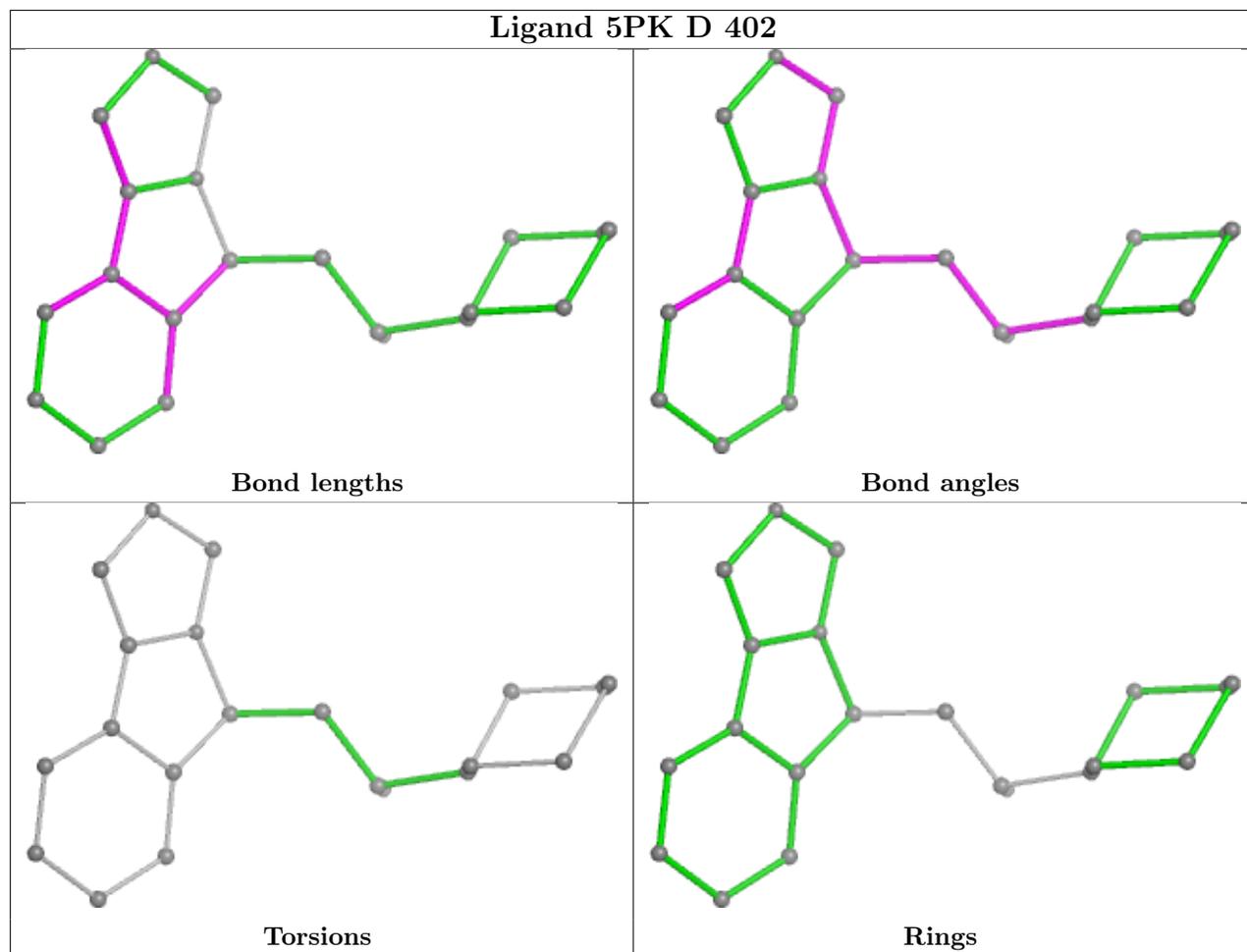
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

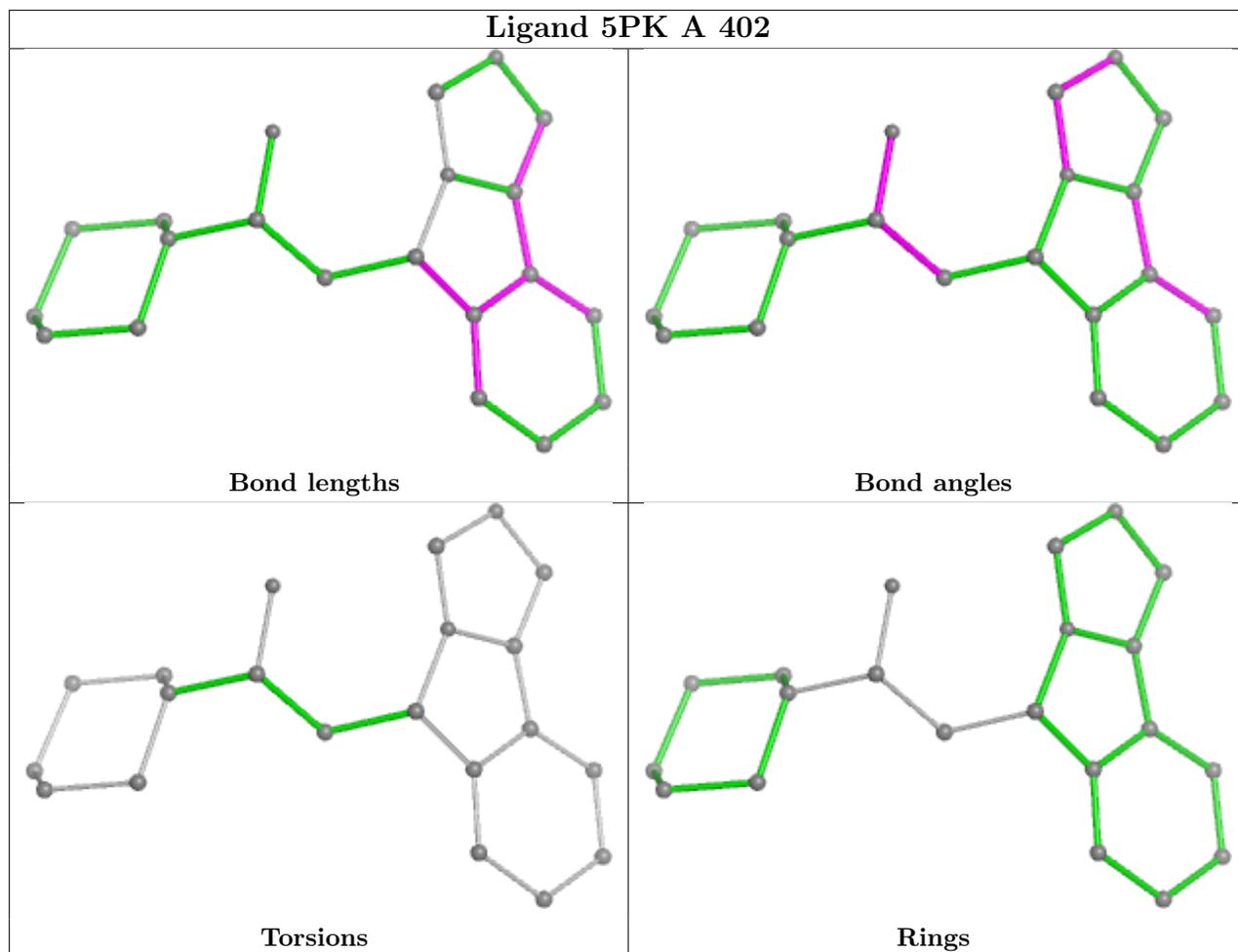


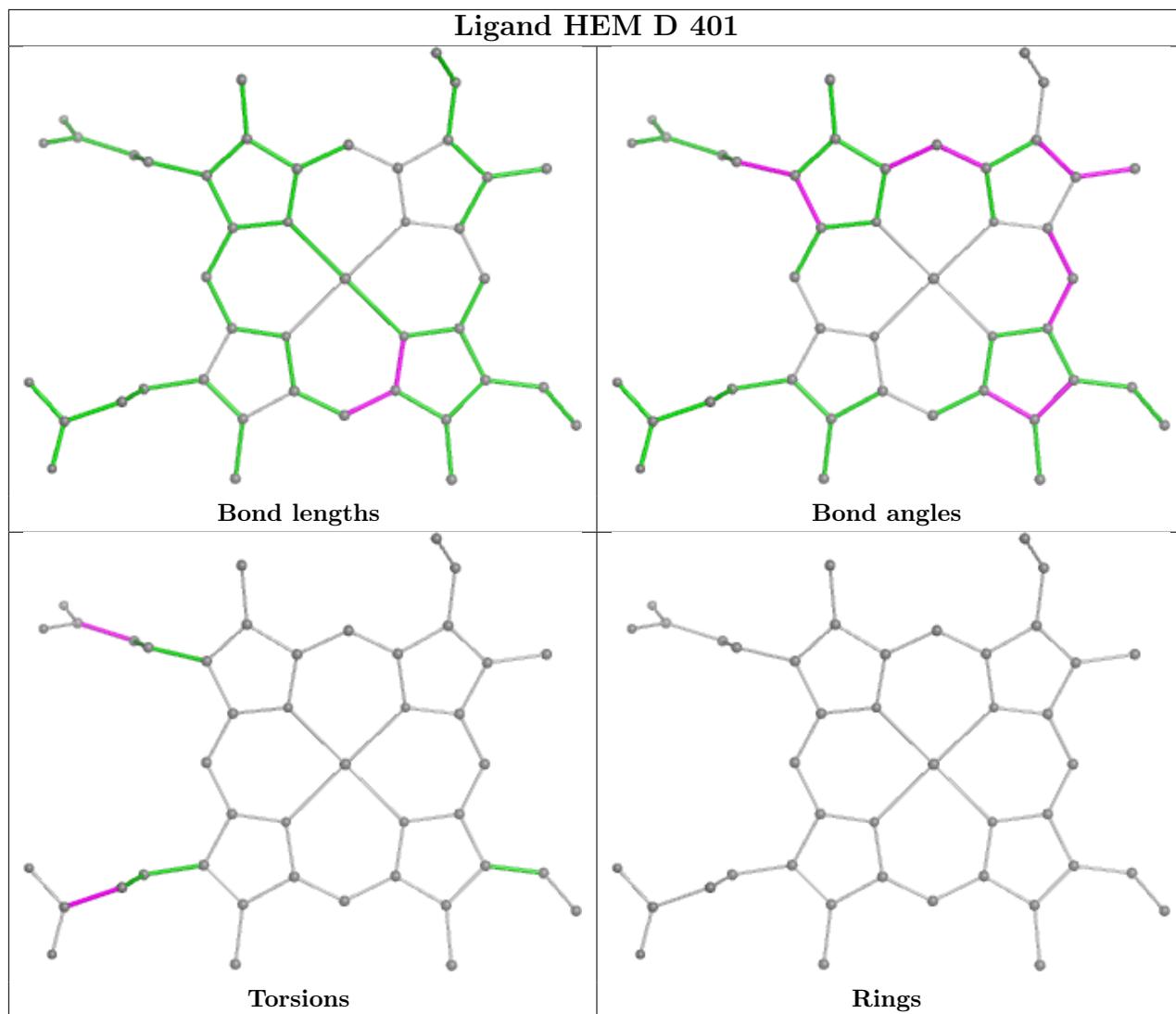


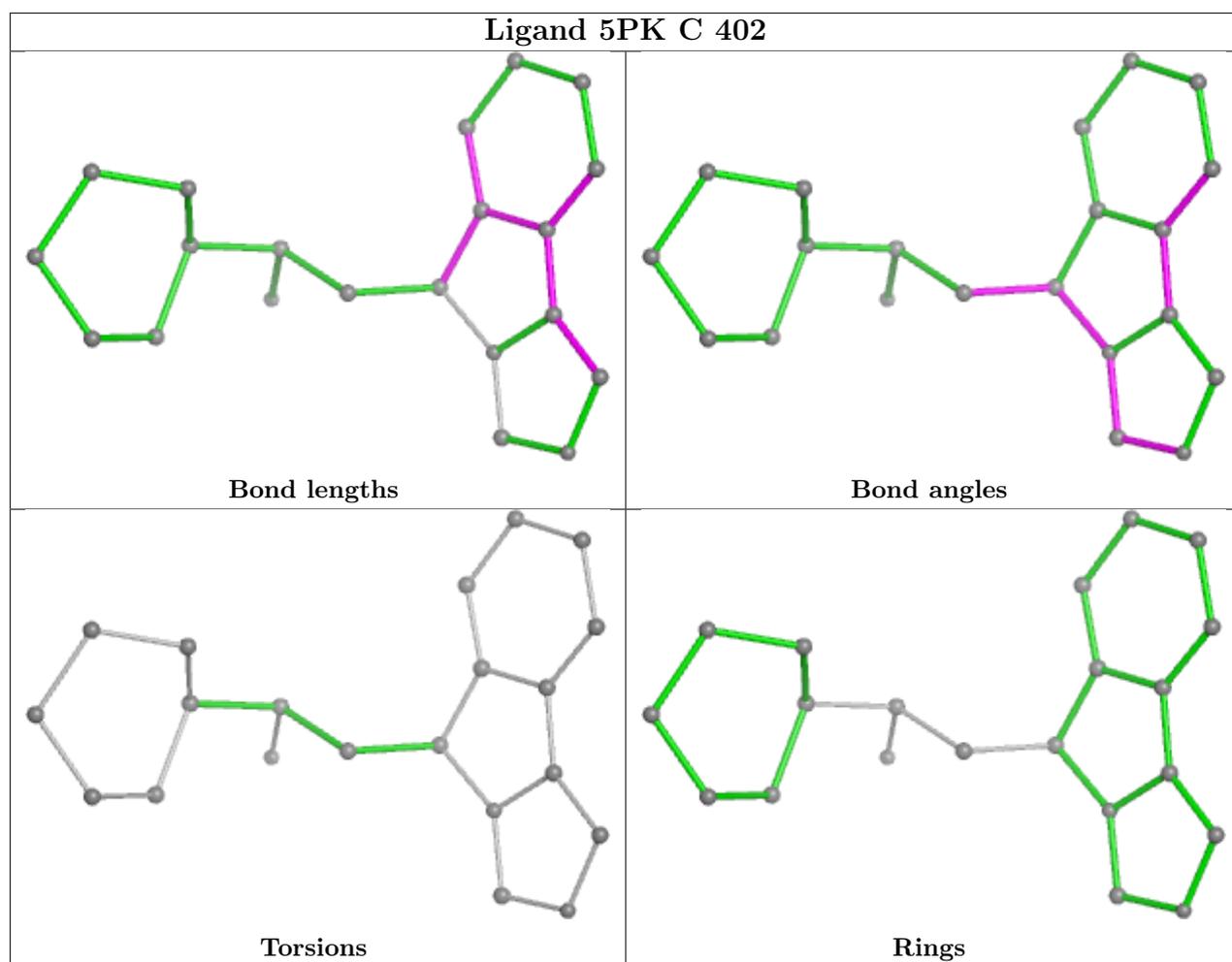












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	328/365 (89%)	-1.12	0 100 100	29, 48, 73, 89	1 (0%)
1	B	326/365 (89%)	-1.09	0 100 100	30, 49, 75, 94	1 (0%)
1	C	344/365 (94%)	-1.09	0 100 100	30, 47, 74, 92	1 (0%)
1	D	331/365 (90%)	-1.11	0 100 100	33, 48, 76, 91	0
All	All	1329/1460 (91%)	-1.10	0 100 100	29, 48, 75, 94	3 (0%)

There are no RSRZ outliers to report.

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 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.

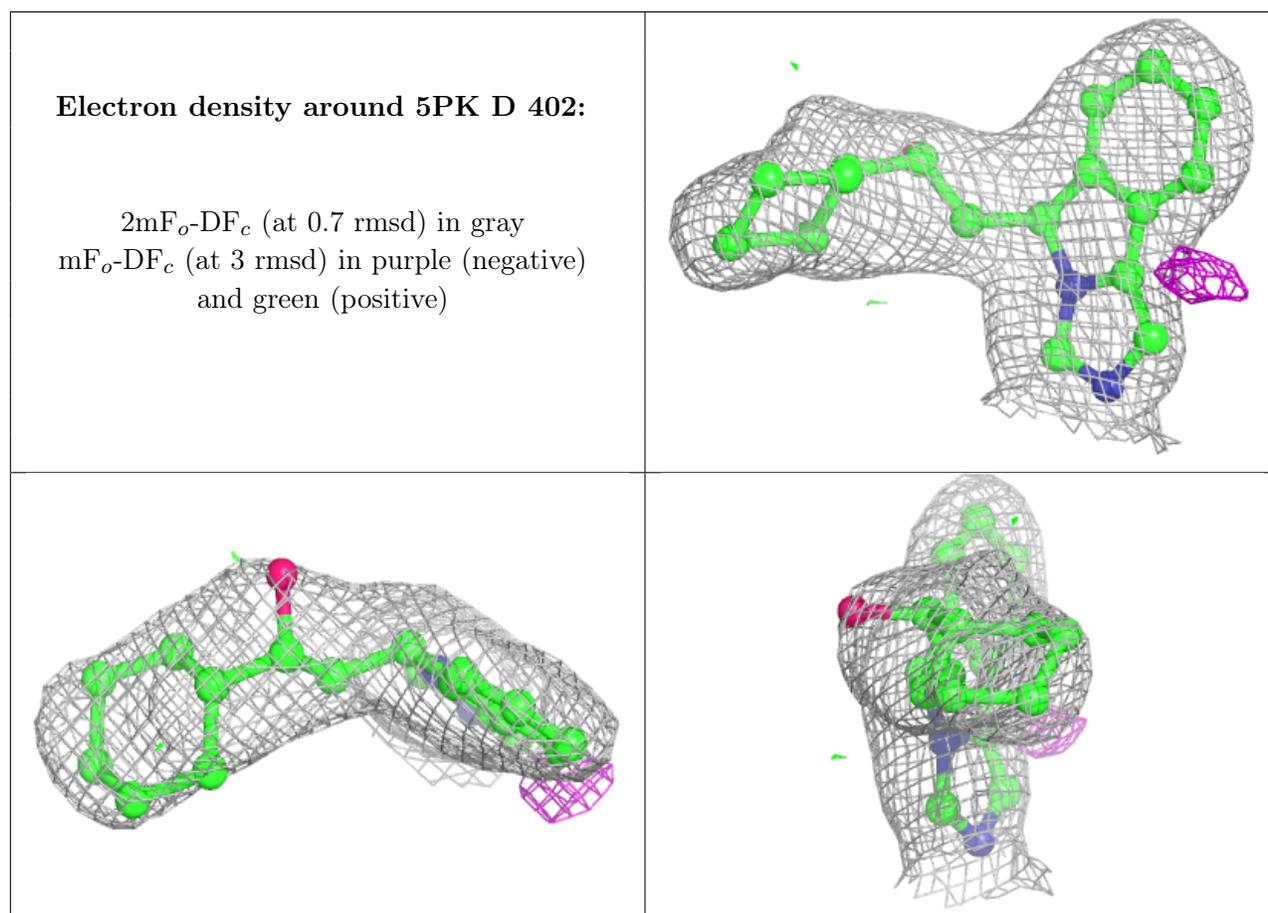
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	5PK	D	402	21/21	0.98	0.06	51,53,56,57	0
2	HEM	B	401	43/43	0.99	0.04	41,43,51,53	0
3	5PK	A	402	21/21	0.99	0.05	54,55,60,60	0
3	5PK	B	402	21/21	0.99	0.05	50,51,57,58	0

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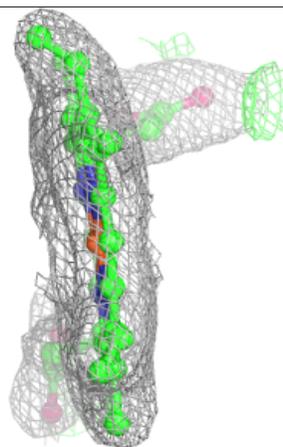
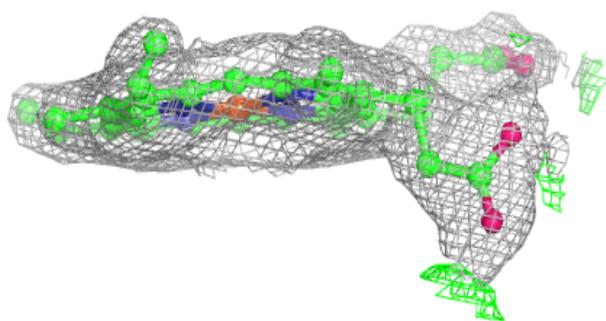
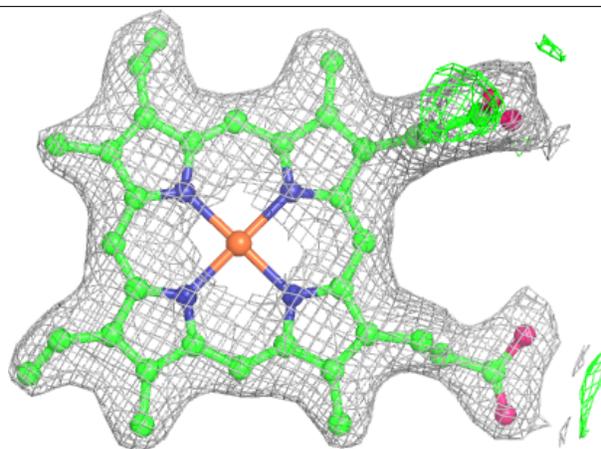
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	5PK	C	402	21/21	0.99	0.05	54,54,60,61	0
2	HEM	A	401	43/43	0.99	0.04	43,45,51,53	0
2	HEM	C	401	43/43	1.00	0.03	40,42,48,50	0
2	HEM	D	401	43/43	1.00	0.03	42,44,50,53	0

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.



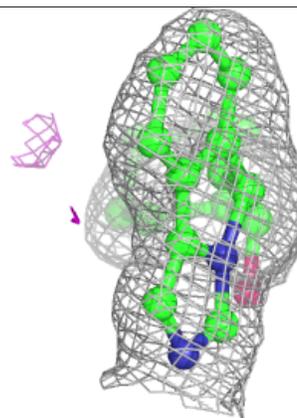
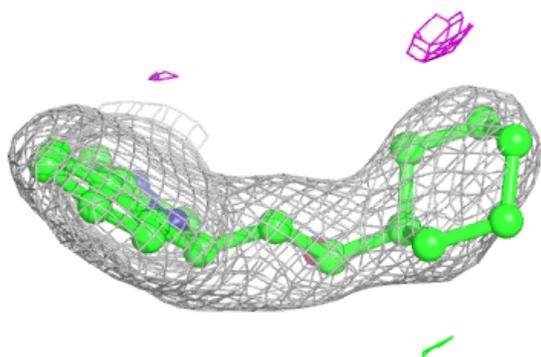
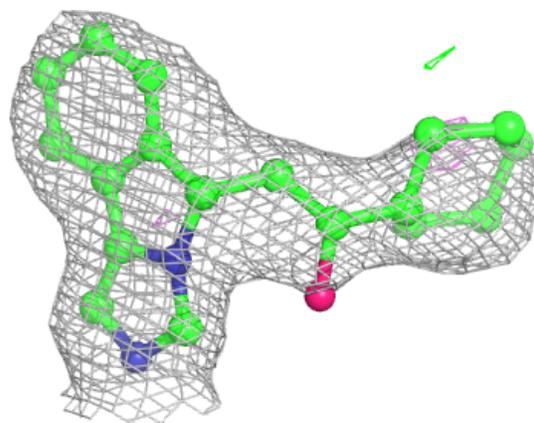
Electron density around HEM B 401:

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

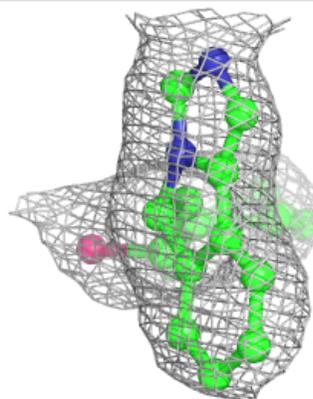
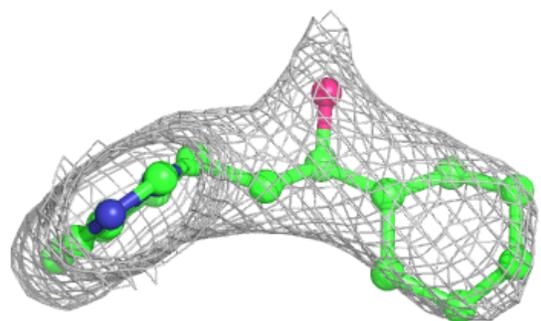
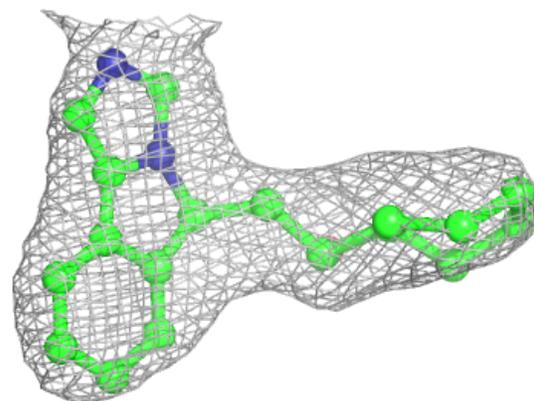


Electron density around 5PK A 402:

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

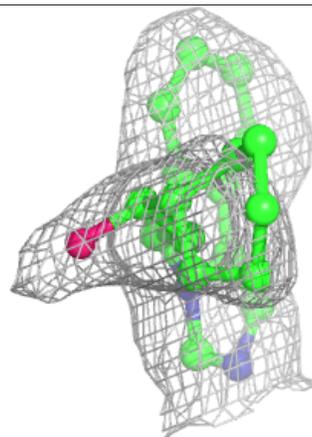
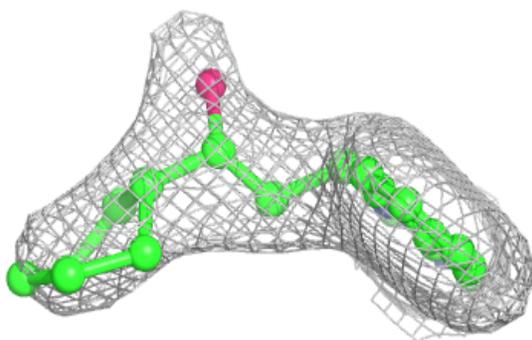
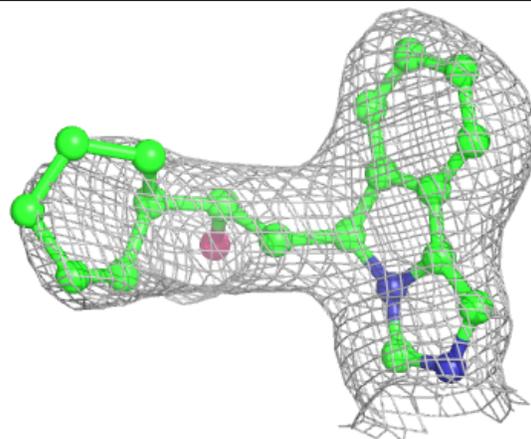
**Electron density around 5PK B 402:**

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



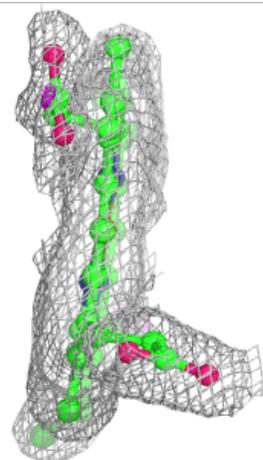
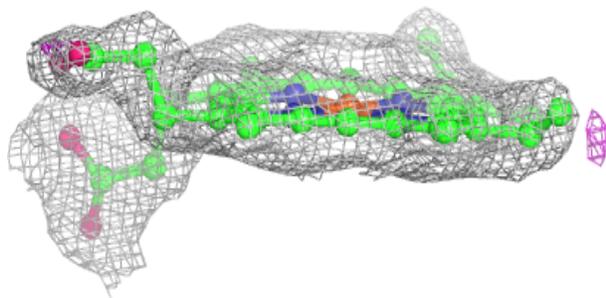
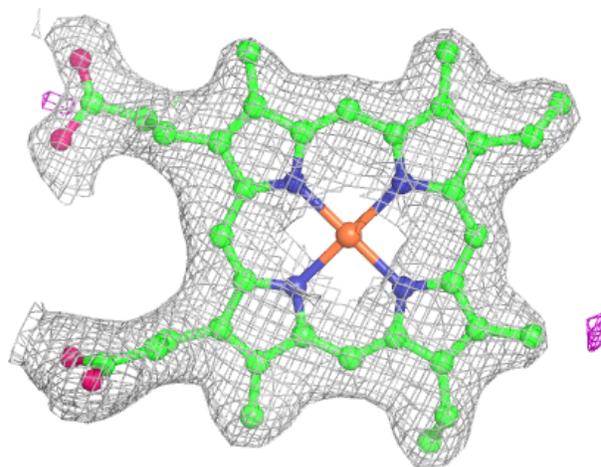
Electron density around 5PK C 402:

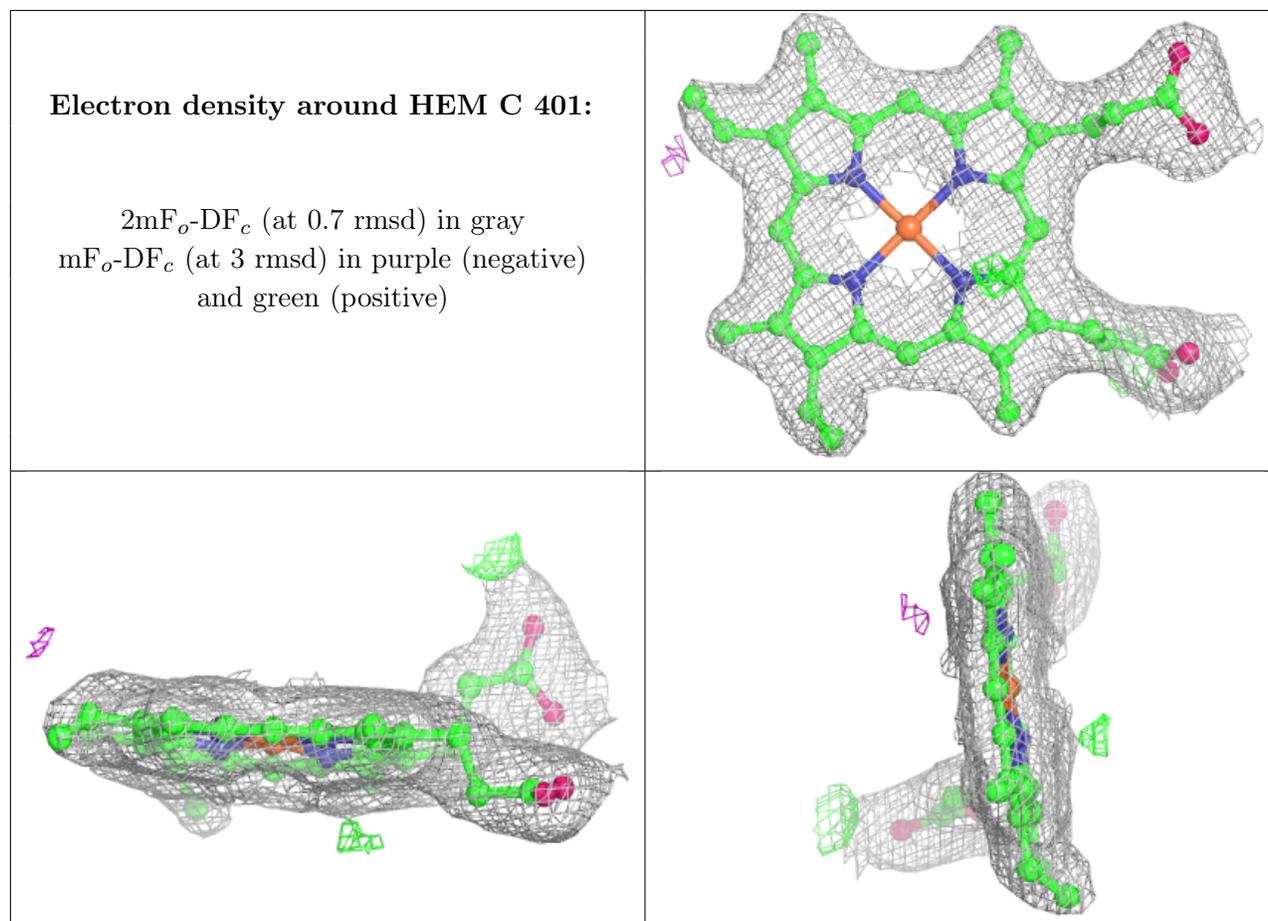
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

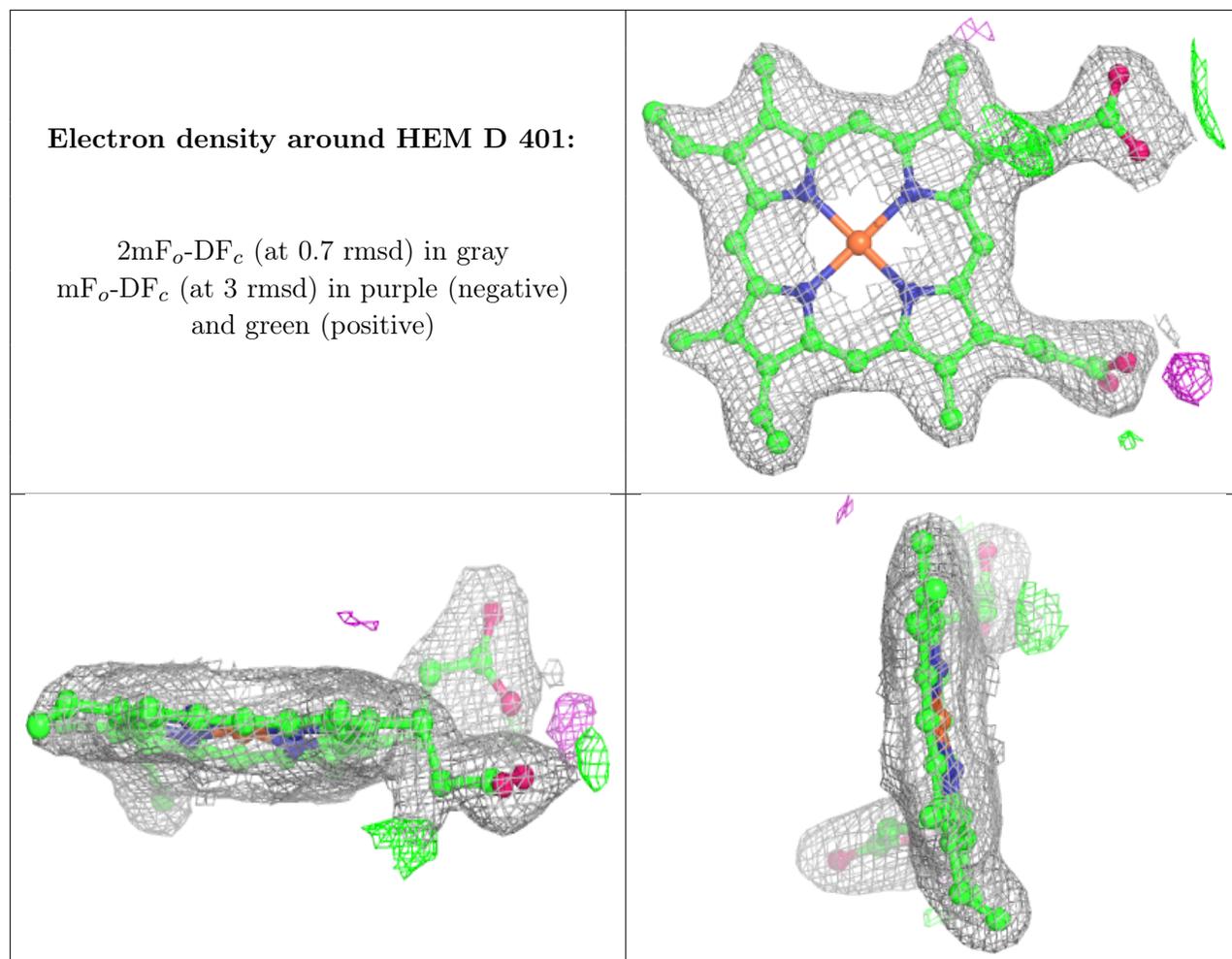


Electron density around HEM A 401:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.