



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2025 – 04:09 pm BST

PDB ID : 9FB7 / pdb\_00009fb7  
Title : Dye-decolourising peroxidase DtpB (280 kGy)  
Authors : Lucic, M.; Worrall, J.A.R.; Hough, M.A.; Strange, R.W.; Owen, R.L.  
Deposited on : 2024-05-12  
Resolution : 2.02 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](mailto: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>.

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

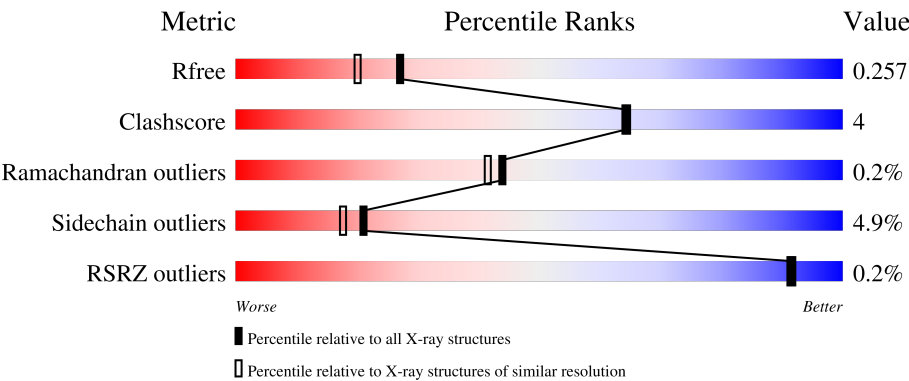
MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

# 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 2.02 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 <sub>free</sub>	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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  $\geq 3$ , 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	313	<div><div></div><div>85%9%...</div></div>
1	B	313	<div><div></div><div>87%9%...</div></div>
1	C	313	<div><div></div><div>84%12%...</div></div>
1	D	313	<div><div>%</div><div>82%12%...</div></div>
1	E	313	<div><div></div><div>87%7%...</div></div>

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Mol	Chain	Length	Quality of chain
1	F	313	<div><div><div>%</div><div><div></div></div><div>82%</div><div>14%</div><div><div></div><div></div></div></div></div>

## 2 Entry composition [i](#)

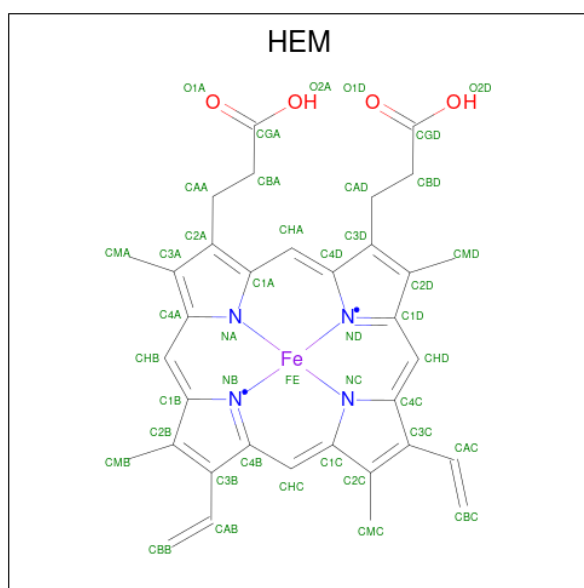
There are 5 unique types of molecules in this entry. The entry contains 14157 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2313	1458	396	450	9			
1	B	305	Total	C	N	O	S	0	0	0
			2284	1443	386	446	9			
1	C	306	Total	C	N	O	S	0	0	0
			2300	1455	392	444	9			
1	D	306	Total	C	N	O	S	0	0	0
			2301	1452	396	444	9			
1	E	306	Total	C	N	O	S	0	0	0
			2305	1456	396	444	9			
1	F	305	Total	C	N	O	S	0	1	0
			2309	1457	395	448	9			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).

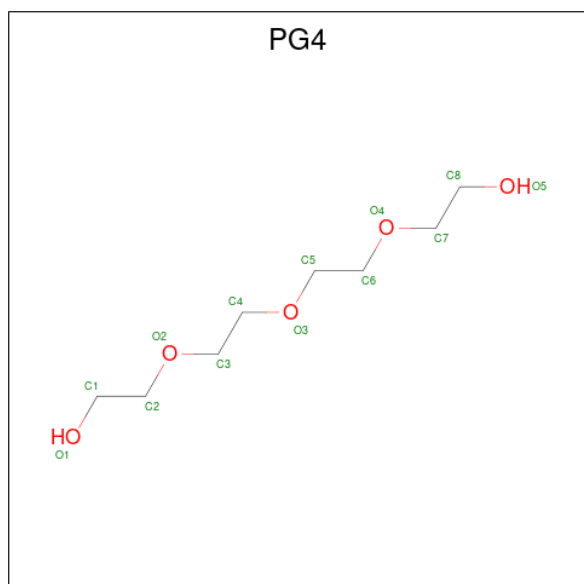


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			13	8	5		

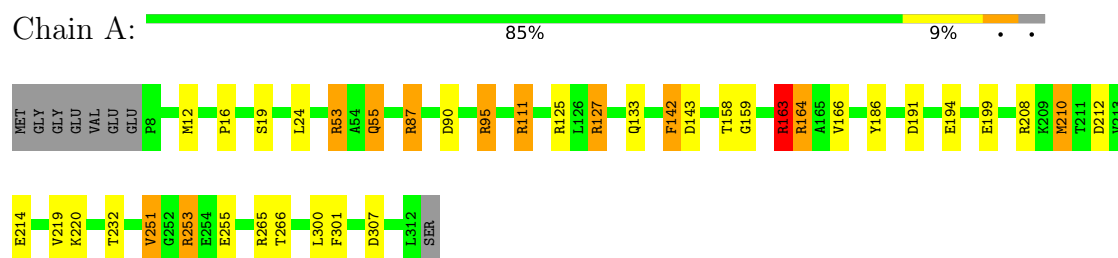
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total 27	O 27	0	0
5	B	6	Total 6	O 6	0	0
5	C	10	Total 10	O 10	0	0
5	D	16	Total 16	O 16	0	0
5	E	7	Total 7	O 7	0	0
5	F	7	Total 7	O 7	0	0

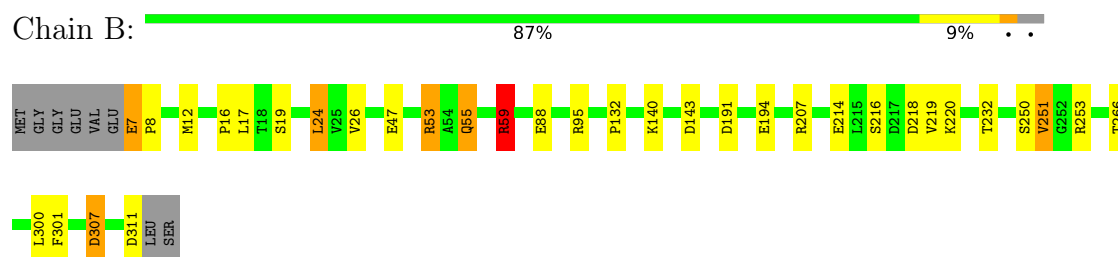
### 3 Residue-property plots [i](#)

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.

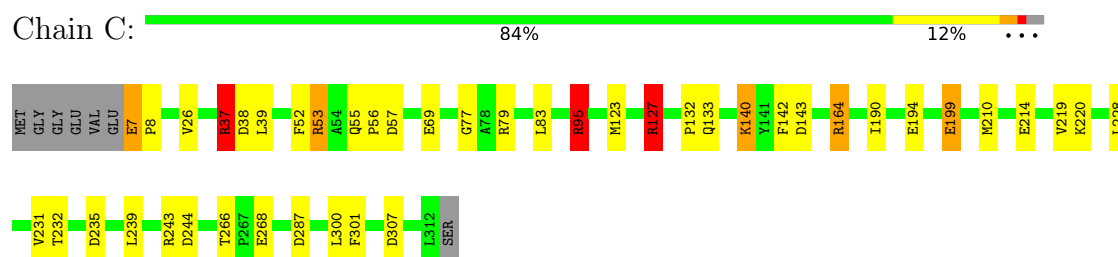
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



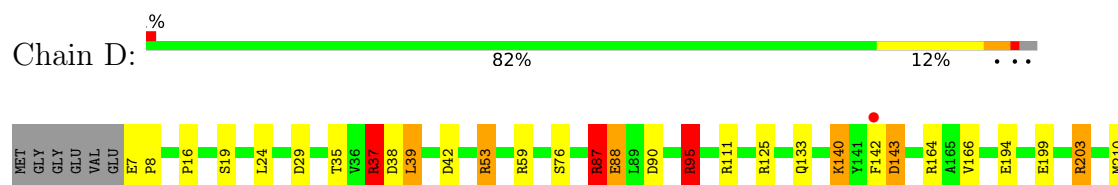
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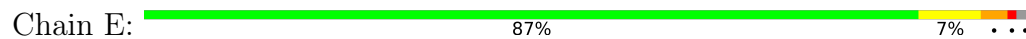


- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup

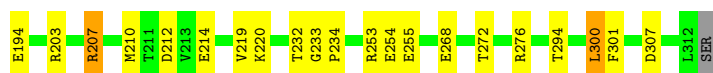
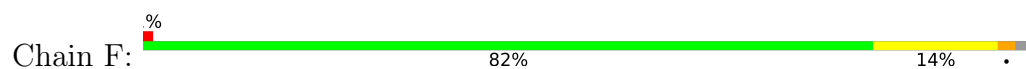




- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.89Å 121.92Å 199.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.12 – 2.02 40.12 – 2.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.12-2.02) 100.0 (40.12-2.02)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.229 , 0.258 0.232 , 0.257	Depositor DCC
$R_{free}$ test set	6931 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 24.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HEM, PG4

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	0.80	0/2363	1.29	12/3210 (0.4%)
1	B	0.75	0/2334	1.25	11/3174 (0.3%)
1	C	0.84	0/2350	1.38	15/3195 (0.5%)
1	D	0.82	1/2351 (0.0%)	1.32	19/3196 (0.6%)
1	E	0.76	0/2355	1.28	13/3202 (0.4%)
1	F	0.81	0/2359	1.42	26/3206 (0.8%)
All	All	0.80	1/14112 (0.0%)	1.32	96/19183 (0.5%)

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	8
1	B	0	3
1	C	0	5
1	D	0	8
1	E	0	7
1	F	0	6
All	All	0	37

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	111	ARG	NE-CZ	5.06	1.38	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	ASP	CB-CA-C	11.16	130.38	111.41
1	F	158	THR	CA-CB-OG1	-10.50	93.85	109.60
1	F	232	THR	CA-CB-OG1	-8.61	96.69	109.60
1	F	111	ARG	CD-NE-CZ	8.42	136.19	124.40
1	E	232	THR	CA-CB-OG1	-8.32	97.12	109.60
1	C	235	ASP	CA-CB-CG	8.27	120.86	112.60
1	C	232	THR	CA-CB-OG1	-8.24	97.24	109.60
1	A	232	THR	CA-CB-OG1	-8.20	97.30	109.60
1	D	199	GLU	CB-CG-CD	7.81	125.87	112.60
1	D	232	THR	CA-CB-OG1	-7.81	97.89	109.60
1	C	7	GLU	CB-CA-C	7.55	124.45	110.10
1	E	87	ARG	CG-CD-NE	-7.41	95.70	112.00
1	E	95	ARG	N-CA-CB	-7.36	98.31	110.68
1	C	199	GLU	CB-CG-CD	7.33	125.06	112.60
1	B	232	THR	CA-CB-OG1	-7.31	98.64	109.60
1	E	164	ARG	CA-CB-CG	7.25	128.59	114.10
1	D	95	ARG	N-CA-CB	-7.24	98.28	110.80
1	E	125	ARG	CG-CD-NE	-7.15	96.28	112.00
1	F	12	MET	CG-SD-CE	7.13	116.59	100.90
1	D	164	ARG	CA-CB-CG	7.13	128.36	114.10
1	A	142	PHE	N-CA-CB	7.03	122.36	110.49
1	A	87	ARG	CG-CD-NE	-7.02	96.55	112.00
1	F	52	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	24	LEU	N-CA-CB	-6.94	99.82	110.65
1	F	38	ASP	CB-CA-C	-6.91	100.03	110.88
1	D	87	ARG	CG-CD-NE	-6.86	96.91	112.00
1	B	7	GLU	CB-CA-C	6.76	122.95	110.10
1	C	127	ARG	CB-CG-CD	-6.62	96.07	111.30
1	C	69	GLU	CB-CG-CD	-6.48	101.58	112.60
1	E	24	LEU	N-CA-CB	-6.35	100.74	110.65
1	A	199	GLU	CB-CG-CD	6.35	123.39	112.60
1	B	218	ASP	CA-CB-CG	6.25	118.85	112.60
1	C	95	ARG	N-CA-CB	-6.18	101.01	110.65
1	F	142	PHE	N-CA-C	-6.13	105.29	112.89
1	D	95	ARG	CG-CD-NE	-6.13	98.52	112.00
1	E	57	ASP	CA-CB-CG	6.11	118.71	112.60
1	D	111	ARG	CD-NE-CZ	6.08	132.92	124.40
1	B	95	ARG	N-CA-CB	-6.06	100.49	110.68
1	C	38	ASP	CB-CA-C	-6.04	101.39	110.88
1	A	210	MET	N-CA-CB	6.04	119.19	110.20
1	D	24	LEU	N-CA-CB	-5.98	101.32	110.65
1	D	38	ASP	CB-CA-C	-5.96	101.53	110.88
1	E	158	THR	CA-CB-OG1	-5.92	100.72	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	24	LEU	N-CA-CB	-5.89	101.52	110.77
1	F	35	THR	CA-CB-OG1	-5.79	100.92	109.60
1	F	163	ARG	N-CA-CB	5.78	118.73	110.06
1	F	207	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	B	47	GLU	CB-CA-C	5.74	119.90	110.88
1	D	35	THR	CA-CB-OG1	-5.69	101.06	109.60
1	C	52	PHE	CA-CB-CG	-5.62	108.18	113.80
1	C	8	PRO	N-CA-C	5.61	120.92	111.32
1	B	207	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	D	311	ASP	CA-CB-CG	5.59	118.19	112.60
1	F	87	ARG	CG-CD-NE	-5.58	99.71	112.00
1	C	37	ARG	CG-CD-NE	-5.57	99.75	112.00
1	F	143	ASP	CA-CB-CG	5.56	118.16	112.60
1	E	42	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	133	GLN	CB-CA-C	-5.54	100.76	109.34
1	A	158	THR	CA-CB-OG1	-5.52	101.32	109.60
1	D	218	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	133	GLN	CB-CA-C	-5.43	100.93	109.34
1	D	307	ASP	CB-CA-C	-5.40	101.83	110.79
1	F	163	ARG	CA-CB-CG	5.39	124.89	114.10
1	C	268	GLU	N-CA-CB	5.39	118.15	110.06
1	F	255	GLU	CB-CA-C	-5.36	101.51	110.19
1	D	140	LYS	CB-CA-C	5.33	118.53	109.53
1	A	210	MET	CB-CG-SD	5.32	128.65	112.70
1	B	307	ASP	CB-CA-C	-5.30	101.99	110.79
1	F	272	THR	CA-CB-OG1	-5.30	101.65	109.60
1	F	38	ASP	N-CA-CB	5.30	117.69	110.01
1	F	210	MET	N-CA-CB	5.27	117.71	110.07
1	B	8	PRO	N-CA-C	5.27	122.07	111.69
1	A	212	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	127	ARG	CA-CB-CG	5.24	124.57	114.10
1	D	133	GLN	CB-CA-C	-5.22	101.25	109.34
1	F	234	PRO	CA-C-N	5.18	127.94	120.38
1	F	234	PRO	C-N-CA	5.18	127.94	120.38
1	F	294	THR	CA-CB-OG1	-5.17	101.84	109.60
1	F	276	ARG	CA-CB-CG	-5.16	103.79	114.10
1	F	254	GLU	N-CA-CB	-5.16	104.30	112.08
1	C	77	GLY	N-CA-C	-5.15	105.46	112.52
1	E	35	THR	CA-CB-OG1	-5.15	101.88	109.60
1	D	287	ASP	CA-CB-CG	5.11	117.70	112.60
1	B	207	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	E	125	ARG	NH1-CZ-NH2	5.08	125.90	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	THR	OG1-CB-CG2	-5.07	99.16	109.30
1	C	244	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	55	GLN	N-CA-CB	5.05	117.49	110.11
1	F	133	GLN	CB-CA-C	-5.05	101.51	109.34
1	B	24	LEU	N-CA-CB	-5.04	102.79	110.65
1	F	268	GLU	CB-CG-CD	-5.04	104.04	112.60
1	B	88	GLU	N-CA-CB	5.03	117.97	109.92
1	F	212	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	29	ASP	CA-CB-CG	5.01	117.61	112.60
1	E	152	ASP	CA-CB-CG	5.01	117.61	112.60
1	E	7	GLU	CB-CA-C	5.01	119.62	110.10

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	125	ARG	Sidechain
1	A	163	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	87	ARG	Sidechain
1	A	95	ARG	Sidechain
1	B	253	ARG	Sidechain
1	B	59	ARG	Sidechain
1	B	7	GLU	Peptide
1	C	127	ARG	Sidechain
1	C	164	ARG	Sidechain
1	C	37	ARG	Sidechain
1	C	7	GLU	Peptide
1	C	95	ARG	Sidechain
1	D	203	ARG	Sidechain
1	D	253	ARG	Sidechain
1	D	276	ARG	Sidechain
1	D	37	ARG	Sidechain
1	D	59	ARG	Sidechain
1	D	7	GLU	Peptide
1	D	87	ARG	Sidechain
1	D	95	ARG	Sidechain
1	E	125	ARG	Sidechain
1	E	253	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	37	ARG	Sidechain
1	E	59	ARG	Sidechain
1	E	7	GLU	Peptide
1	E	87	ARG	Sidechain
1	E	95	ARG	Sidechain
1	F	125[A]	ARG	Sidechain
1	F	164	ARG	Sidechain
1	F	203	ARG	Sidechain
1	F	207	ARG	Sidechain
1	F	233	GLY	Peptide
1	F	253	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	2313	0	2235	21	0
1	B	2284	0	2185	15	0
1	C	2300	0	2216	25	0
1	D	2301	0	2216	18	0
1	E	2305	0	2224	20	0
1	F	2309	0	2225	16	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
2	E	43	0	30	2	0
2	F	43	0	30	1	0
3	A	1	0	0	0	0
4	D	13	0	18	1	0
5	A	27	0	0	0	0
5	B	6	0	0	0	0
5	C	10	0	0	1	0
5	D	16	0	0	1	0
5	E	7	0	0	0	0
5	F	7	0	0	0	0
All	All	14157	0	13499	105	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 (105) 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:210:MET:HE1	1:E:210:MET:HB2	1.38	1.04
1:A:95:ARG:CZ	1:A:95:ARG:HB3	2.09	0.81
1:B:251:VAL:CG1	1:E:123:MET:HG3	2.11	0.80
1:F:125[B]:ARG:HG2	1:F:125[B]:ARG:HH11	1.49	0.78
1:A:210:MET:HE1	1:D:210:MET:HB2	1.65	0.77
1:B:55:GLN:HA	1:B:55:GLN:OE1	1.91	0.70
1:E:53:ARG:NH1	1:E:53:ARG:HG2	2.06	0.70
1:A:55:GLN:HA	1:A:55:GLN:OE1	1.94	0.68
1:E:55:GLN:HA	1:E:55:GLN:OE1	1.92	0.68
1:D:53:ARG:HG2	1:D:53:ARG:NH1	2.10	0.67
1:E:53:ARG:HG2	1:E:53:ARG:HH11	1.60	0.67
1:D:243:ARG:HD2	5:D:501:HOH:O	1.95	0.65
1:A:53:ARG:HG2	1:A:53:ARG:NH1	2.11	0.64
1:C:53:ARG:HG2	1:C:53:ARG:NH1	2.13	0.62
1:F:53:ARG:NH1	1:F:53:ARG:HG2	2.15	0.61
1:F:125[B]:ARG:HG2	1:F:125[B]:ARG:NH1	2.13	0.61
1:B:53:ARG:HG2	1:B:53:ARG:NH1	2.14	0.61
1:A:95:ARG:CZ	1:A:95:ARG:CB	2.77	0.61
1:E:53:ARG:HH11	1:E:53:ARG:CG	2.15	0.60
1:A:53:ARG:HG2	1:A:53:ARG:HH11	1.65	0.60
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.15	0.59
1:D:8:PRO:HB3	1:D:307:ASP:OD2	2.02	0.59
1:F:55:GLN:HA	1:F:55:GLN:OE1	2.04	0.58
1:D:42:ASP:OD2	1:D:125:ARG:NH2	2.38	0.57
1:C:55:GLN:HA	1:C:55:GLN:OE1	2.03	0.57
1:D:39:LEU:O	1:D:39:LEU:HG	2.02	0.57
1:B:17:LEU:O	1:B:59:ARG:NH1	2.38	0.57
1:D:53:ARG:CG	1:D:53:ARG:HH11	2.18	0.56
1:C:243:ARG:HD2	5:C:501:HOH:O	2.03	0.56
1:A:191:ASP:OD1	1:C:127:ARG:NH2	2.39	0.55
1:D:53:ARG:HG2	1:D:53:ARG:HH11	1.69	0.55
1:C:53:ARG:CG	1:C:53:ARG:HH11	2.20	0.55
1:B:251:VAL:HG13	1:E:123:MET:HG3	1.89	0.54
1:E:123:MET:HE2	1:E:127:ARG:HH12	1.72	0.54
1:F:214:GLU:OE2	1:F:220:LYS:NZ	2.40	0.54
1:F:53:ARG:HH11	1:F:53:ARG:CG	2.20	0.54
1:D:143:ASP:OD1	1:D:143:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:N	1:B:143:ASP:OD1	2.42	0.52
1:F:79:ARG:NH2	1:F:83:LEU:O	2.42	0.52
1:C:39:LEU:O	1:C:39:LEU:HG	2.06	0.52
1:F:47:GLU:OE2	1:F:61:SER:HA	2.10	0.51
1:D:76:SER:H	4:D:402:PG4:H51	1.76	0.51
1:C:214:GLU:OE2	1:C:220:LYS:NZ	2.44	0.50
1:A:159:GLY:O	1:A:163:ARG:HG3	2.11	0.50
1:C:300:LEU:HD23	1:C:301:PHE:N	2.27	0.49
1:E:143:ASP:N	1:E:143:ASP:OD1	2.43	0.49
1:C:53:ARG:HG2	1:C:53:ARG:HH11	1.77	0.49
1:A:143:ASP:OD1	1:A:143:ASP:N	2.46	0.49
1:A:111:ARG:HH21	1:C:140:LYS:HE3	1.77	0.48
1:B:53:ARG:NH1	1:B:53:ARG:CG	2.75	0.48
1:D:37:ARG:HG2	1:D:37:ARG:NH1	2.28	0.48
1:A:191:ASP:CG	1:C:127:ARG:HH22	2.21	0.48
1:B:53:ARG:CG	1:B:53:ARG:HH11	2.26	0.47
2:F:401:HEM:HBC2	2:F:401:HEM:HMC2	1.96	0.47
1:F:300:LEU:HD23	1:F:301:PHE:N	2.29	0.47
1:E:253:ARG:HH21	1:E:255:GLU:CD	2.22	0.47
1:A:164:ARG:CZ	1:A:164:ARG:CB	2.94	0.46
1:E:121:GLU:O	1:E:125:ARG:HG2	2.15	0.46
1:C:231:VAL:HG23	1:C:239:LEU:HB2	1.98	0.46
2:E:401:HEM:CMC	2:E:401:HEM:HBC2	2.46	0.45
1:D:214:GLU:OE2	1:D:220:LYS:NZ	2.50	0.45
1:F:123:MET:HE3	1:F:123:MET:HB3	1.82	0.45
1:A:214:GLU:OE2	1:A:220:LYS:NZ	2.49	0.45
1:F:53:ARG:HG2	1:F:53:ARG:HH11	1.80	0.45
1:F:121:GLU:O	1:F:125[B]:ARG:HD3	2.17	0.45
1:A:251:VAL:HG22	1:C:123:MET:HG3	1.97	0.45
1:E:123:MET:CE	1:E:127:ARG:NH1	2.80	0.45
1:C:140:LYS:O	1:C:140:LYS:HD3	2.17	0.45
1:B:214:GLU:OE2	1:B:220:LYS:NZ	2.51	0.44
1:C:79:ARG:NH2	1:C:83:LEU:O	2.48	0.44
1:B:300:LEU:HD23	1:B:301:PHE:N	2.33	0.44
1:D:251:VAL:CG1	1:F:123:MET:HG3	2.48	0.44
1:D:300:LEU:HD23	1:D:301:PHE:N	2.33	0.44
1:C:55:GLN:OE1	1:C:56:PRO:HA	2.18	0.43
2:E:401:HEM:HBC2	2:E:401:HEM:HMC2	2.00	0.43
1:D:88:GLU:OE1	1:D:95:ARG:NH2	2.52	0.43
1:F:26:VAL:HG12	1:F:132:PRO:HA	1.99	0.43
1:C:26:VAL:HG12	1:C:132:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:VAL:CG2	1:D:239:LEU:HB2	2.48	0.42
1:E:300:LEU:HD23	1:E:301:PHE:N	2.33	0.42
1:F:55:GLN:OE1	1:F:56:PRO:HA	2.19	0.42
1:B:216:SER:OG	1:B:219:VAL:HG12	2.19	0.42
1:A:163:ARG:NH1	1:A:163:ARG:HG2	2.35	0.42
1:D:142:PHE:HB3	1:F:113:ASP:OD2	2.19	0.42
1:E:214:GLU:OE2	1:E:220:LYS:NZ	2.52	0.42
1:C:228:LEU:CD1	1:C:287:ASP:HA	2.50	0.42
1:A:111:ARG:HH22	1:C:142:PHE:HA	1.85	0.41
1:C:123:MET:HE3	1:C:123:MET:HB3	1.87	0.41
1:C:143:ASP:OD1	1:C:143:ASP:N	2.52	0.41
1:A:186:TYR:CG	2:A:401:HEM:HBB1	2.56	0.41
1:A:12:MET:HB2	1:A:12:MET:HE2	1.88	0.41
1:B:26:VAL:HG12	1:B:132:PRO:HA	2.02	0.41
1:C:210:MET:CE	1:E:210:MET:HB2	2.28	0.41
1:C:231:VAL:CG2	1:C:239:LEU:HB2	2.50	0.41
1:E:123:MET:CE	1:E:127:ARG:HH12	2.33	0.41
1:E:307:ASP:OD1	1:E:307:ASP:N	2.43	0.41
1:E:300:LEU:HD23	1:E:300:LEU:C	2.46	0.41
1:B:140:LYS:HD2	1:B:140:LYS:HA	1.96	0.40
1:C:190:ILE:O	1:C:194:GLU:HG3	2.20	0.40
1:A:253:ARG:NH1	1:A:255:GLU:OE1	2.32	0.40
1:B:12:MET:HA	1:B:12:MET:HE2	2.03	0.40
1:B:251:VAL:HG12	1:E:123:MET:HG3	1.97	0.40
1:D:300:LEU:HD23	1:D:300:LEU:C	2.46	0.40
1:E:70:ALA:HB2	1:E:102:ASP:HB3	2.03	0.40
1:A:300:LEU:HD23	1:A:301:PHE:N	2.36	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	303/313 (97%)	296 (98%)	5 (2%)	2 (1%)	19	14
1	B	303/313 (97%)	296 (98%)	6 (2%)	1 (0%)	37	34
1	C	304/313 (97%)	294 (97%)	10 (3%)	0	100	100
1	D	304/313 (97%)	297 (98%)	6 (2%)	1 (0%)	37	34
1	E	304/313 (97%)	296 (97%)	8 (3%)	0	100	100
1	F	304/313 (97%)	295 (97%)	9 (3%)	0	100	100
All	All	1822/1878 (97%)	1774 (97%)	44 (2%)	4 (0%)	44	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	PHE
1	D	16	PRO
1	B	16	PRO
1	A	16	PRO

### 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	240/250 (96%)	228 (95%)	12 (5%)	20	17
1	B	233/250 (93%)	221 (95%)	12 (5%)	19	16
1	C	235/250 (94%)	225 (96%)	10 (4%)	25	22
1	D	236/250 (94%)	219 (93%)	17 (7%)	12	8
1	E	237/250 (95%)	226 (95%)	11 (5%)	23	20
1	F	238/250 (95%)	230 (97%)	8 (3%)	32	31
All	All	1419/1500 (95%)	1349 (95%)	70 (5%)	21	18

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER

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Mol	Chain	Res	Type
1	A	53	ARG
1	A	90	ASP
1	A	127	ARG
1	A	163	ARG
1	A	164	ARG
1	A	166	VAL
1	A	194	GLU
1	A	219	VAL
1	A	251	VAL
1	A	266	THR
1	A	307	ASP
1	B	19	SER
1	B	24	LEU
1	B	53	ARG
1	B	55	GLN
1	B	59	ARG
1	B	191	ASP
1	B	194	GLU
1	B	250	SER
1	B	251	VAL
1	B	266	THR
1	B	307	ASP
1	B	311	ASP
1	C	37	ARG
1	C	53	ARG
1	C	57	ASP
1	C	95	ARG
1	C	140	LYS
1	C	164	ARG
1	C	199	GLU
1	C	219	VAL
1	C	266	THR
1	C	307	ASP
1	D	19	SER
1	D	37	ARG
1	D	39	LEU
1	D	53	ARG
1	D	87	ARG
1	D	88	GLU
1	D	90	ASP
1	D	140	LYS
1	D	143	ASP

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Mol	Chain	Res	Type
1	D	166	VAL
1	D	194	GLU
1	D	203	ARG
1	D	219	VAL
1	D	231	VAL
1	D	235	ASP
1	D	251	VAL
1	D	307	ASP
1	E	19	SER
1	E	53	ARG
1	E	55	GLN
1	E	57	ASP
1	E	87	ARG
1	E	143	ASP
1	E	194	GLU
1	E	210	MET
1	E	219	VAL
1	E	266	THR
1	E	307	ASP
1	F	12	MET
1	F	53	ARG
1	F	90	ASP
1	F	166	VAL
1	F	194	GLU
1	F	219	VAL
1	F	300	LEU
1	F	307	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	PG4	D	402	-	12,12,12	0.56	0	11,11,11	0.43	0
2	HEM	B	401	1	41,50,50	1.76	11 (26%)	45,82,82	2.32	18 (40%)
2	HEM	F	401	5,1	41,50,50	1.45	6 (14%)	45,82,82	1.95	11 (24%)
2	HEM	C	401	5,1	41,50,50	1.52	9 (21%)	45,82,82	2.16	14 (31%)
2	HEM	E	401	1	41,50,50	1.56	7 (17%)	45,82,82	2.38	20 (44%)
2	HEM	A	401	5,1	41,50,50	1.55	12 (29%)	45,82,82	1.90	9 (20%)
2	HEM	D	401	5,1	41,50,50	1.40	6 (14%)	45,82,82	2.50	14 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	D	402	-	-	5/10/10/10	-
2	HEM	B	401	1	-	6/12/54/54	-
2	HEM	F	401	5,1	-	5/12/54/54	-
2	HEM	C	401	5,1	-	4/12/54/54	-
2	HEM	E	401	1	-	4/12/54/54	-
2	HEM	A	401	5,1	-	4/12/54/54	-
2	HEM	D	401	5,1	-	4/12/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	HEM	C1B-NB	-4.53	1.32	1.40
2	B	401	HEM	CAD-C3D	4.08	1.61	1.51
2	D	401	HEM	C1B-NB	-3.79	1.33	1.40
2	B	401	HEM	CBD-CAD	3.59	1.63	1.52
2	B	401	HEM	C4D-C3D	3.59	1.51	1.45
2	F	401	HEM	C4D-C3D	3.54	1.51	1.45
2	E	401	HEM	C3B-C4B	3.50	1.51	1.44
2	F	401	HEM	C1B-NB	-3.43	1.34	1.40
2	F	401	HEM	C3C-C2C	-3.39	1.35	1.40
2	A	401	HEM	C1B-NB	-3.39	1.34	1.40
2	C	401	HEM	C4D-C3D	3.14	1.50	1.45
2	E	401	HEM	C4B-NB	-3.14	1.32	1.38
2	B	401	HEM	C1B-NB	-3.08	1.35	1.40
2	D	401	HEM	C4B-NB	-3.08	1.32	1.38
2	A	401	HEM	FE-NB	2.97	2.11	1.96
2	C	401	HEM	C4D-ND	-2.96	1.35	1.40
2	E	401	HEM	O1D-CGD	2.79	1.31	1.22
2	B	401	HEM	C3B-C4B	2.76	1.50	1.44
2	A	401	HEM	C1D-ND	-2.74	1.33	1.38
2	D	401	HEM	C3C-C2C	-2.72	1.36	1.40
2	A	401	HEM	C1A-NA	2.70	1.41	1.36
2	D	401	HEM	C1A-NA	2.67	1.41	1.36
2	B	401	HEM	CBA-CGA	2.67	1.56	1.50
2	E	401	HEM	C4D-ND	-2.66	1.35	1.40
2	C	401	HEM	C3C-C2C	2.61	1.44	1.40
2	C	401	HEM	C1B-NB	-2.59	1.35	1.40
2	C	401	HEM	C4B-NB	-2.59	1.33	1.38
2	E	401	HEM	C1D-ND	-2.57	1.33	1.38
2	A	401	HEM	C4D-C3D	2.52	1.49	1.45
2	C	401	HEM	CBD-CGD	2.52	1.56	1.50
2	A	401	HEM	CBD-CGD	2.49	1.56	1.50
2	C	401	HEM	CHB-C1B	2.45	1.41	1.35
2	B	401	HEM	C1D-ND	-2.38	1.33	1.38
2	C	401	HEM	CHA-C4D	2.38	1.41	1.35
2	F	401	HEM	CHA-C4D	2.37	1.41	1.35
2	B	401	HEM	CHA-C4D	2.34	1.41	1.35
2	B	401	HEM	C1D-C2D	2.33	1.49	1.44
2	A	401	HEM	C4D-ND	-2.32	1.36	1.40
2	A	401	HEM	CHA-C4D	2.27	1.40	1.35
2	E	401	HEM	O1A-CGA	2.26	1.29	1.22
2	B	401	HEM	FE-NB	2.21	2.07	1.96
2	B	401	HEM	O1A-CGA	2.14	1.29	1.22
2	F	401	HEM	CHB-C1B	2.13	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	CBD-CAD	2.12	1.58	1.52
2	D	401	HEM	C1D-ND	-2.10	1.34	1.38
2	D	401	HEM	CBD-CGD	2.09	1.55	1.50
2	A	401	HEM	C1B-C2B	-2.09	1.40	1.44
2	C	401	HEM	FE-NB	2.08	2.07	1.96
2	A	401	HEM	CHB-C1B	2.08	1.40	1.35
2	A	401	HEM	C3B-C4B	2.04	1.48	1.44
2	F	401	HEM	O1D-CGD	2.00	1.28	1.22

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	O2D-CGD-CBD	7.12	136.91	114.03
2	F	401	HEM	CHC-C4B-NB	6.75	131.77	124.43
2	C	401	HEM	CHC-C4B-NB	6.70	131.72	124.43
2	D	401	HEM	O1D-CGD-CBD	-6.40	102.53	123.08
2	D	401	HEM	CHC-C4B-NB	6.34	131.31	124.43
2	A	401	HEM	C1B-NB-C4B	5.80	111.06	105.07
2	D	401	HEM	C1B-NB-C4B	5.51	110.77	105.07
2	B	401	HEM	CBD-CAD-C3D	5.20	127.06	112.63
2	F	401	HEM	C1B-NB-C4B	4.94	110.17	105.07
2	E	401	HEM	C1B-NB-C4B	4.89	110.13	105.07
2	E	401	HEM	CMB-C2B-C1B	4.48	131.87	125.04
2	A	401	HEM	CHC-C4B-NB	4.44	129.26	124.43
2	B	401	HEM	O2D-CGD-CBD	4.44	128.30	114.03
2	E	401	HEM	CHA-C4D-C3D	-4.34	117.18	125.33
2	C	401	HEM	C1B-NB-C4B	4.23	109.44	105.07
2	B	401	HEM	C3D-C4D-ND	4.22	114.86	110.17
2	B	401	HEM	CAD-C3D-C4D	4.19	131.97	124.66
2	E	401	HEM	CHD-C1D-C2D	-4.17	118.46	124.98
2	C	401	HEM	O2D-CGD-CBD	4.10	127.22	114.03
2	E	401	HEM	CHD-C1D-ND	4.10	128.88	124.43
2	C	401	HEM	CMC-C2C-C3C	4.04	132.24	124.68
2	B	401	HEM	O1D-CGD-CBD	-4.04	110.11	123.08
2	B	401	HEM	C4D-C3D-C2D	-3.99	101.09	106.90
2	A	401	HEM	CHB-C1B-NB	3.91	129.22	124.38
2	E	401	HEM	C4A-C3A-C2A	3.90	109.71	107.00
2	C	401	HEM	C2D-C1D-ND	3.72	114.34	109.88
2	D	401	HEM	CMC-C2C-C3C	3.72	131.63	124.68
2	B	401	HEM	CHB-C1B-NB	3.71	128.97	124.38
2	F	401	HEM	O1D-CGD-CBD	-3.66	111.31	123.08
2	E	401	HEM	CMA-C3A-C4A	-3.59	122.95	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	C3D-C4D-ND	3.49	114.06	110.17
2	E	401	HEM	CHA-C4D-ND	3.47	128.67	124.38
2	B	401	HEM	C2C-C3C-C4C	-3.45	104.49	106.90
2	C	401	HEM	CHC-C4B-C3B	-3.36	119.43	124.57
2	B	401	HEM	O2A-CGA-O1A	-3.35	114.95	123.30
2	E	401	HEM	CMC-C2C-C3C	3.24	130.75	124.68
2	E	401	HEM	CAB-C3B-C2B	-3.09	118.42	128.60
2	D	401	HEM	C3B-C2B-C1B	-3.09	104.19	106.49
2	C	401	HEM	CHB-C1B-NB	3.08	128.19	124.38
2	B	401	HEM	C1B-NB-C4B	3.05	108.23	105.07
2	E	401	HEM	C4D-C3D-C2D	-3.02	102.50	106.90
2	A	401	HEM	C2D-C1D-ND	2.98	113.45	109.88
2	D	401	HEM	CHB-C1B-NB	2.92	127.99	124.38
2	D	401	HEM	C3D-C4D-ND	2.89	113.39	110.17
2	A	401	HEM	O2D-CGD-O1D	-2.88	116.12	123.30
2	A	401	HEM	O1A-CGA-CBA	-2.88	113.83	123.08
2	C	401	HEM	O1D-CGD-CBD	-2.81	114.06	123.08
2	C	401	HEM	CBB-CAB-C3B	-2.79	113.73	127.62
2	B	401	HEM	CHB-C1B-C2B	-2.78	119.02	126.72
2	A	401	HEM	C4C-CHD-C1D	2.70	126.13	122.56
2	D	401	HEM	CAD-C3D-C4D	2.69	129.36	124.66
2	D	401	HEM	C2D-C1D-ND	2.66	113.07	109.88
2	E	401	HEM	CMB-C2B-C3B	-2.65	121.82	128.30
2	B	401	HEM	CAB-C3B-C2B	-2.62	119.99	128.60
2	A	401	HEM	CAB-C3B-C2B	-2.58	120.11	128.60
2	B	401	HEM	CHC-C4B-NB	2.58	127.23	124.43
2	F	401	HEM	O2A-CGA-CBA	2.53	122.15	114.03
2	F	401	HEM	C2D-C1D-ND	2.50	112.88	109.88
2	F	401	HEM	C4A-C3A-C2A	2.49	108.73	107.00
2	D	401	HEM	C4C-CHD-C1D	2.45	125.79	122.56
2	C	401	HEM	C3B-C2B-C1B	-2.41	104.70	106.49
2	F	401	HEM	O1A-CGA-CBA	-2.39	115.41	123.08
2	B	401	HEM	C4C-CHD-C1D	2.37	125.68	122.56
2	D	401	HEM	C4D-C3D-C2D	-2.36	103.45	106.90
2	F	401	HEM	CMA-C3A-C4A	-2.34	124.87	128.46
2	E	401	HEM	C2D-C1D-ND	2.31	112.65	109.88
2	E	401	HEM	CHC-C4B-NB	2.30	126.93	124.43
2	E	401	HEM	CAB-C3B-C4B	2.30	135.17	124.47
2	A	401	HEM	C4D-C3D-C2D	-2.29	103.56	106.90
2	D	401	HEM	CMA-C3A-C4A	-2.26	124.98	128.46
2	F	401	HEM	O2D-CGD-CBD	2.26	121.28	114.03
2	C	401	HEM	C4D-ND-C1D	-2.25	102.75	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CHD-C1D-C2D	-2.25	121.46	124.98
2	B	401	HEM	CBB-CAB-C3B	-2.22	116.57	127.62
2	B	401	HEM	C2D-C1D-ND	2.21	112.52	109.88
2	C	401	HEM	CMD-C2D-C1D	2.20	128.38	125.04
2	B	401	HEM	CMB-C2B-C1B	2.19	128.37	125.04
2	E	401	HEM	C4D-ND-C1D	-2.16	102.84	105.07
2	E	401	HEM	C4C-CHD-C1D	-2.15	119.72	122.56
2	B	401	HEM	C4D-ND-C1D	-2.12	102.88	105.07
2	C	401	HEM	C4A-C3A-C2A	2.11	108.46	107.00
2	E	401	HEM	O1D-CGD-CBD	2.10	129.83	123.08
2	E	401	HEM	C4B-C3B-C2B	-2.08	105.47	107.11
2	F	401	HEM	CHD-C1D-C2D	-2.07	121.75	124.98
2	F	401	HEM	CMB-C2B-C1B	2.04	128.15	125.04
2	C	401	HEM	C3D-C4D-ND	2.04	112.44	110.17

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	HEM	C2D-C3D-CAD-CBD
2	B	401	HEM	C4D-C3D-CAD-CBD
4	D	402	PG4	O3-C5-C6-O4
4	D	402	PG4	O4-C7-C8-O5
4	D	402	PG4	O2-C3-C4-O3
2	B	401	HEM	C2B-C3B-CAB-CBB
4	D	402	PG4	C1-C2-O2-C3
2	A	401	HEM	CAA-CBA-CGA-O2A
4	D	402	PG4	C5-C6-O4-C7
2	E	401	HEM	CAD-CBD-CGD-O2D
2	E	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAA-CBA-CGA-O1A
2	F	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	E	401	HEM	CAA-CBA-CGA-O2A

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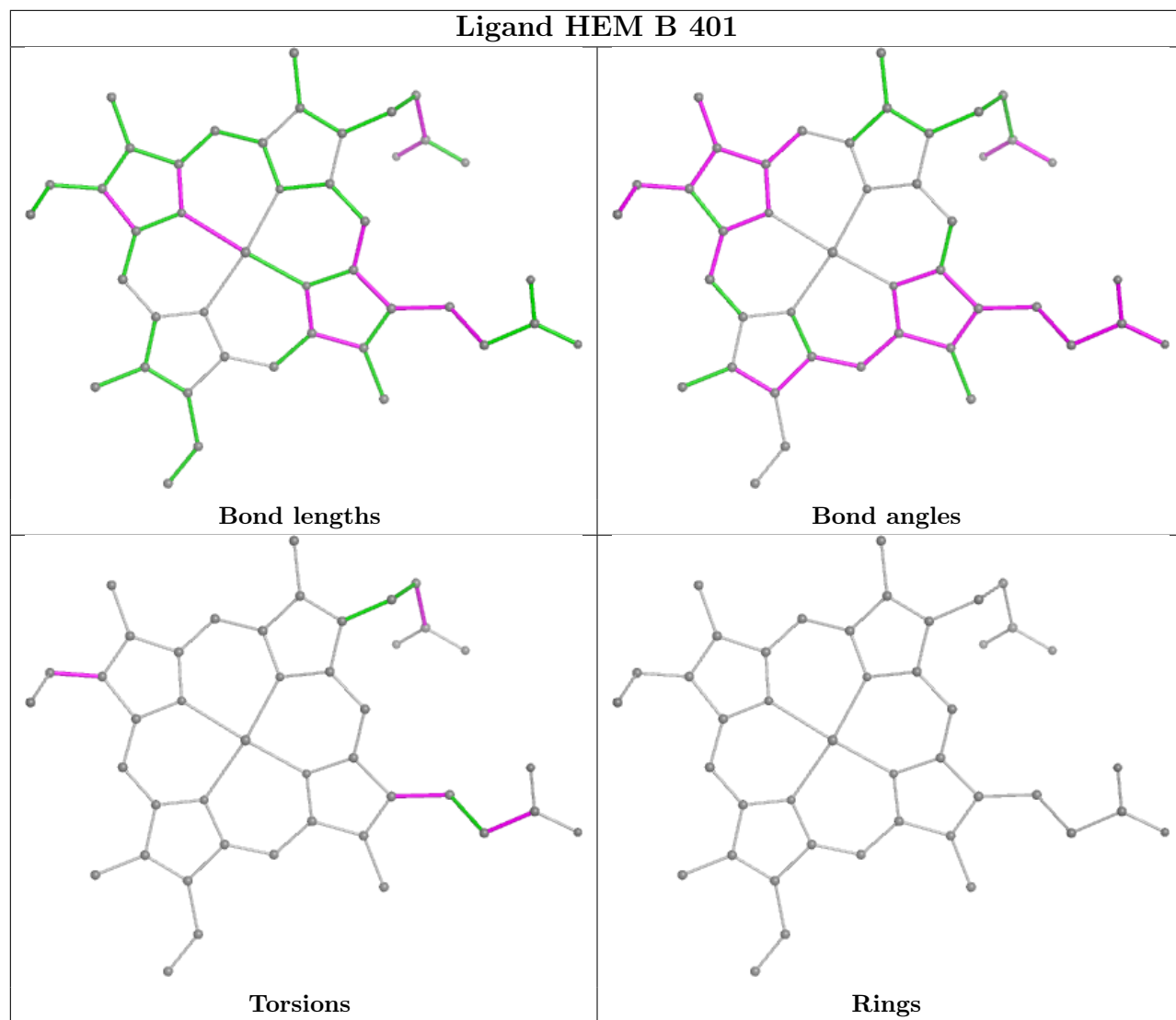
Mol	Chain	Res	Type	Atoms
2	F	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	F	401	HEM	C2D-C3D-CAD-CBD
2	B	401	HEM	CAD-CBD-CGD-O2D

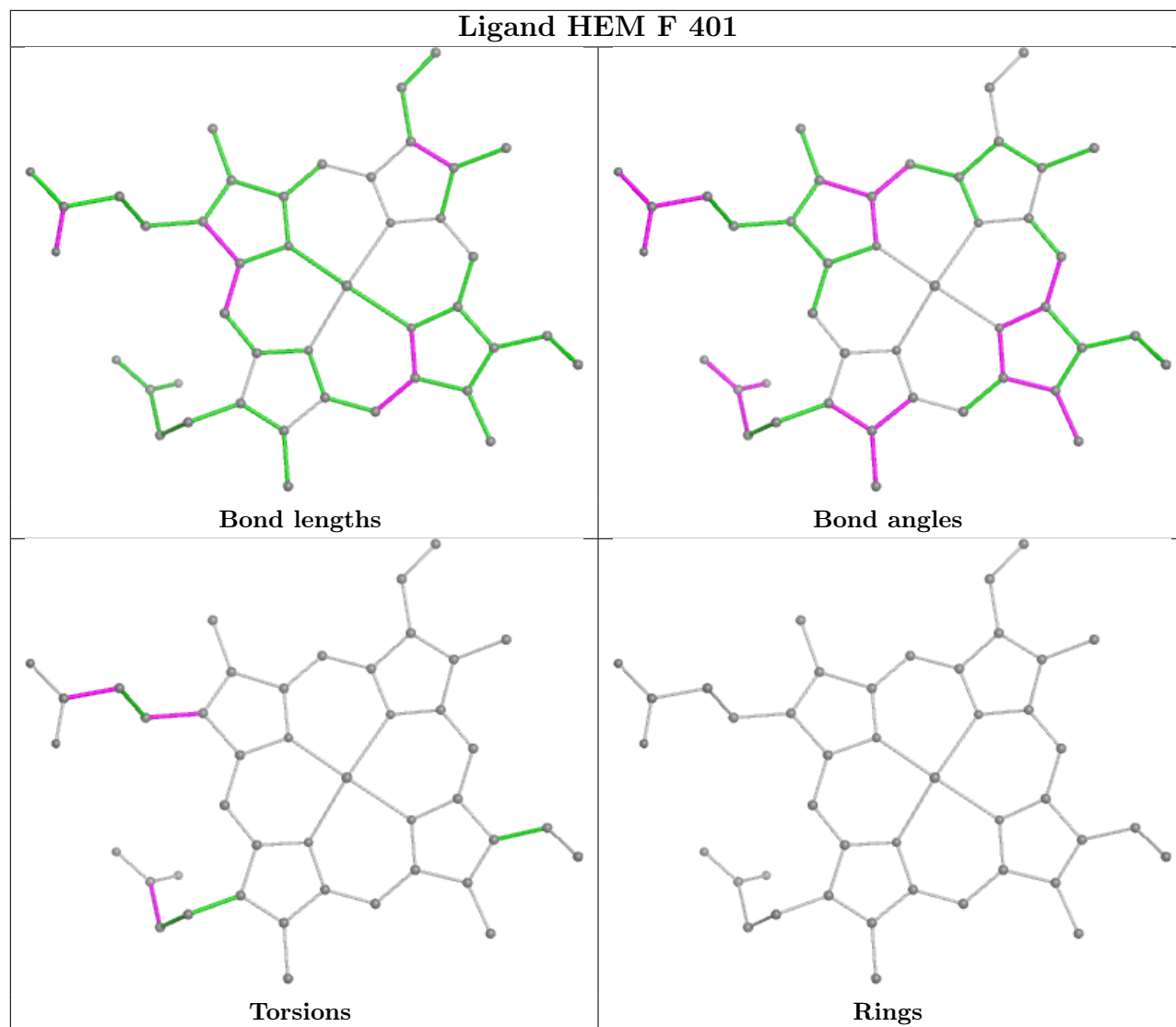
There are no ring outliers.

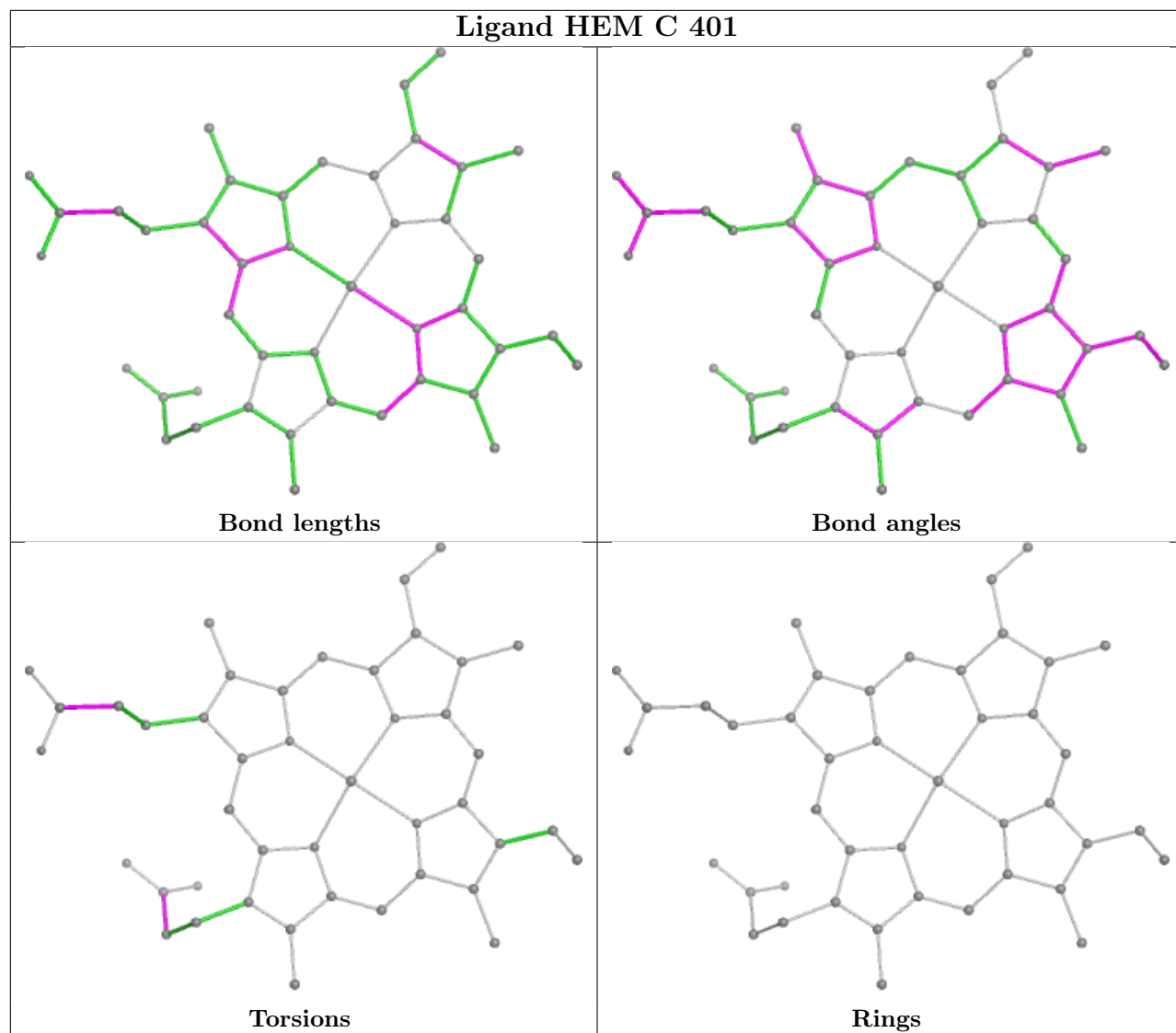
4 monomers are involved in 5 short contacts:

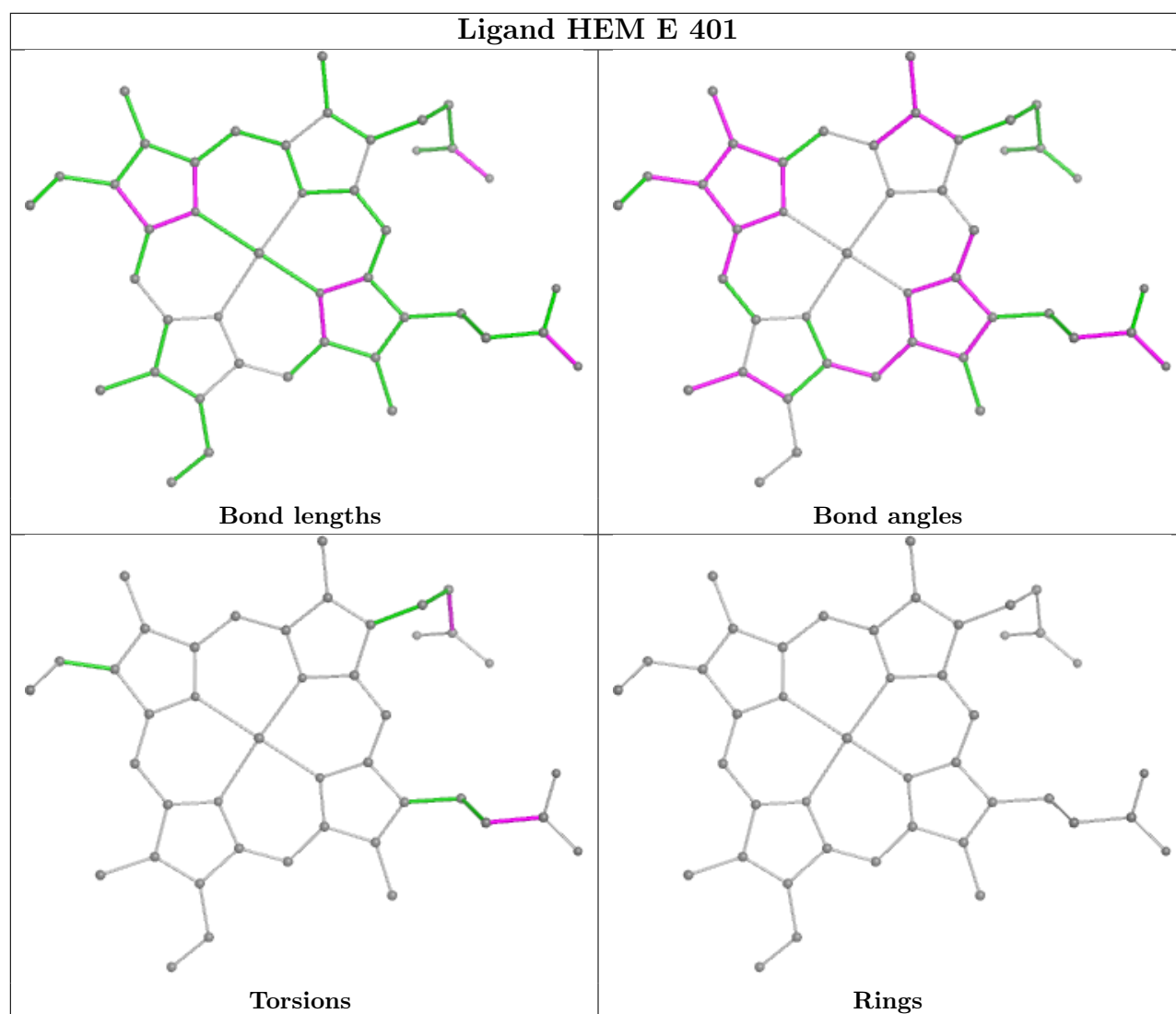
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	402	PG4	1	0
2	F	401	HEM	1	0
2	E	401	HEM	2	0
2	A	401	HEM	1	0

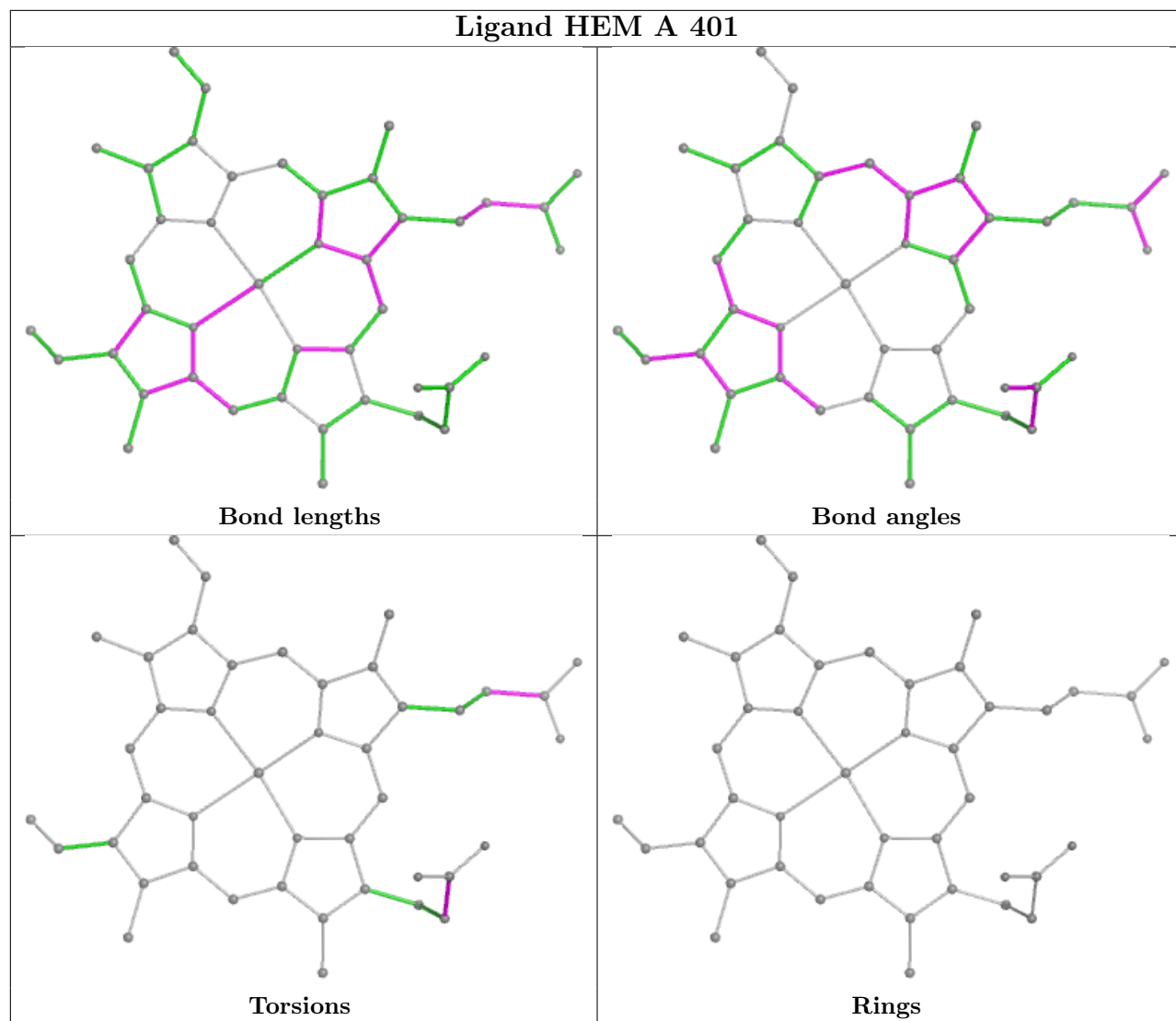
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

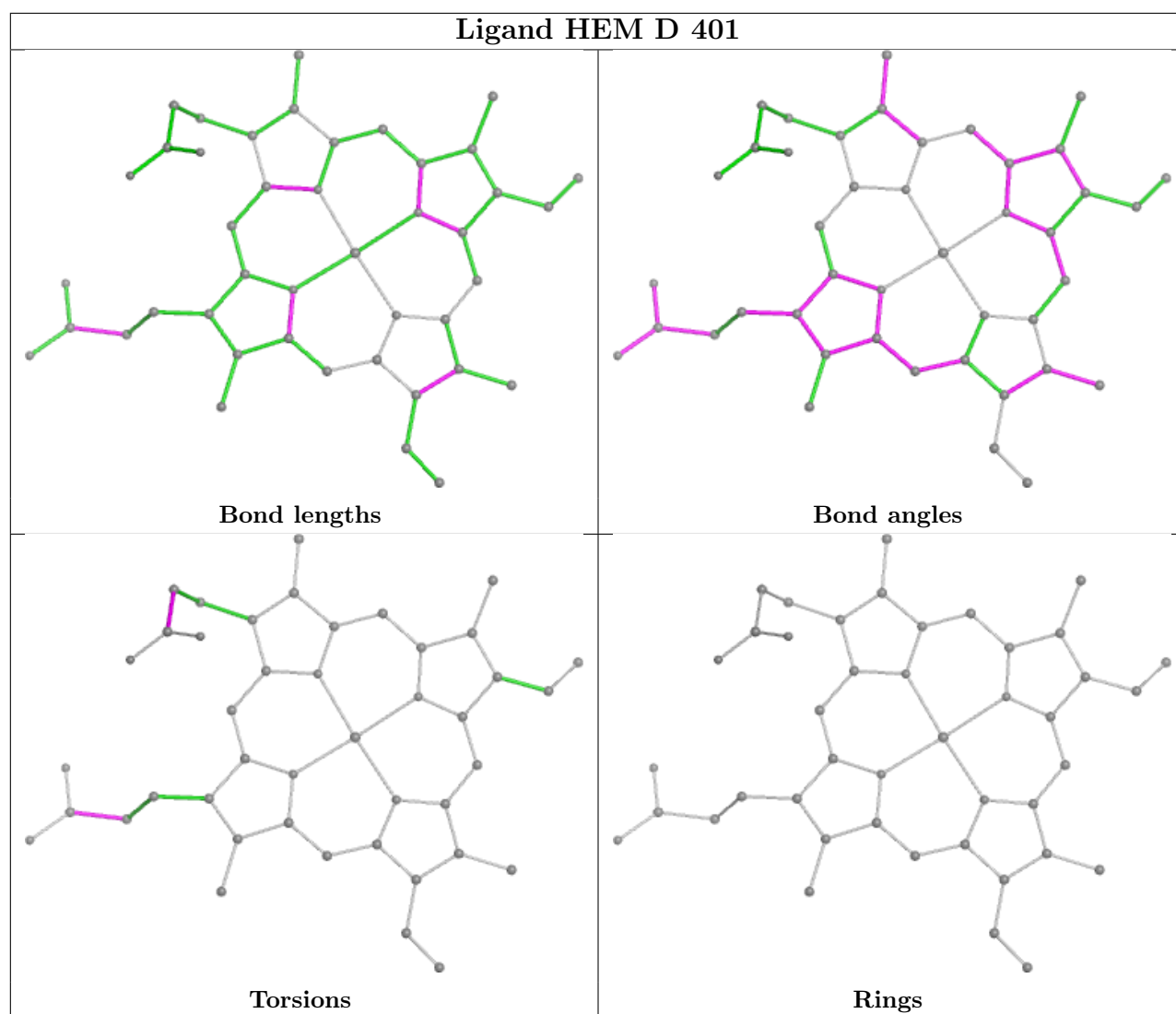












## 5.7 Other polymers [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	305/313 (97%)	-0.93	0	100 100	18, 29, 58, 81	0
1	B	305/313 (97%)	-0.76	0	100 100	22, 36, 61, 89	0
1	C	306/313 (97%)	-0.89	0	100 100	19, 31, 63, 97	0
1	D	306/313 (97%)	-0.88	2 (0%)	84 84	18, 29, 61, 97	0
1	E	306/313 (97%)	-0.81	0	100 100	20, 33, 64, 107	0
1	F	305/313 (97%)	-0.86	2 (0%)	84 84	13, 31, 62, 100	1 (0%)
All	All	1833/1878 (97%)	-0.86	4 (0%)	92 91	13, 32, 62, 107	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	142	PHE	3.6
1	F	8	PRO	2.5
1	D	312	LEU	2.3
1	D	142	PHE	2.1

### 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.

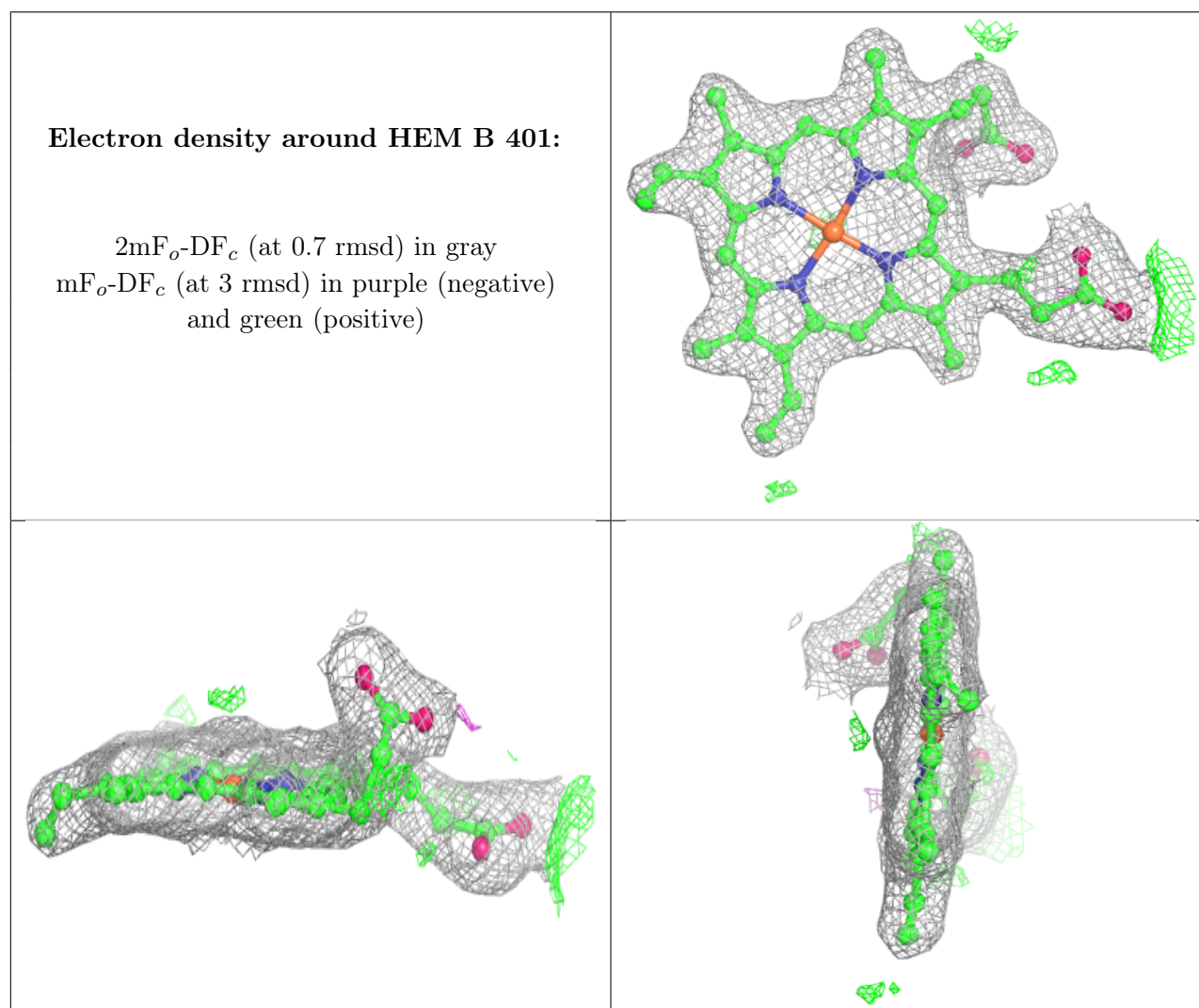
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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.

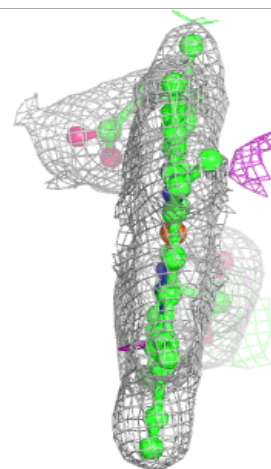
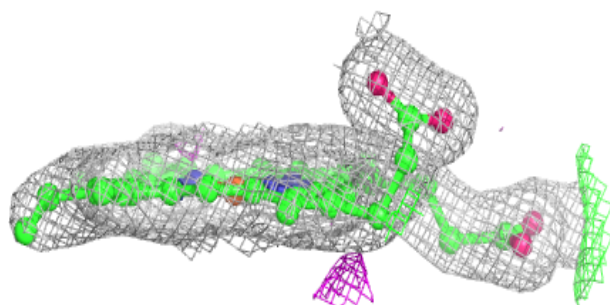
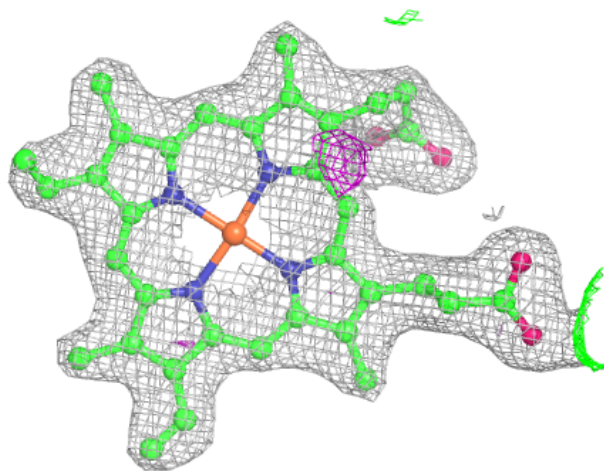
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PG4	D	402	13/13	0.84	0.12	45,72,81,87	0
2	HEM	B	401	43/43	0.99	0.04	19,24,35,48	0
2	HEM	C	401	43/43	0.99	0.05	22,29,35,38	0
2	HEM	D	401	43/43	0.99	0.04	19,22,27,34	0
2	HEM	E	401	43/43	0.99	0.04	22,26,31,34	0
2	HEM	F	401	43/43	0.99	0.05	22,26,33,42	0
2	HEM	A	401	43/43	0.99	0.04	24,28,32,35	0
3	MG	A	402	1/1	1.00	0.04	26,26,26,26	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.



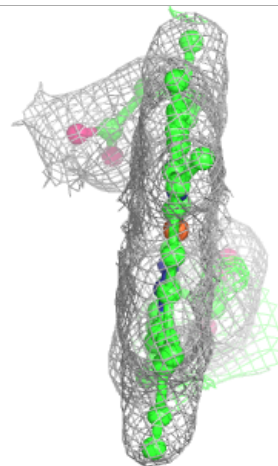
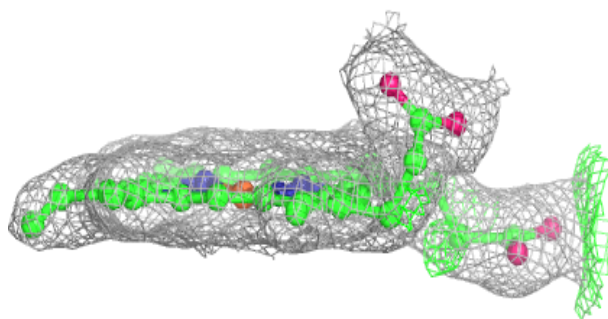
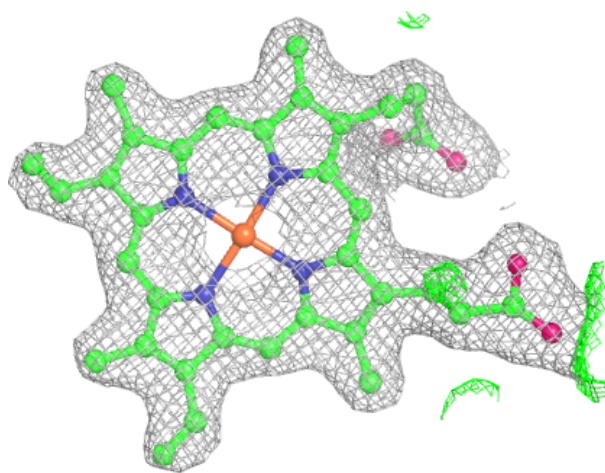
**Electron density around HEM C 401:**

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



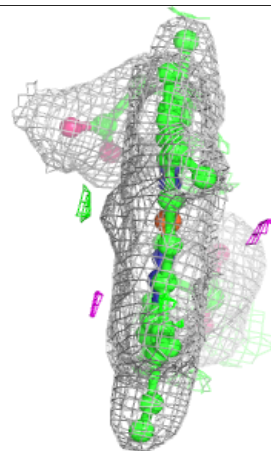
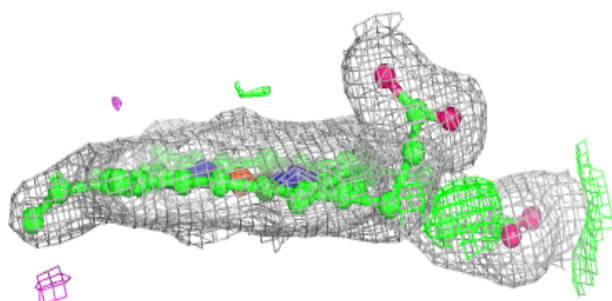
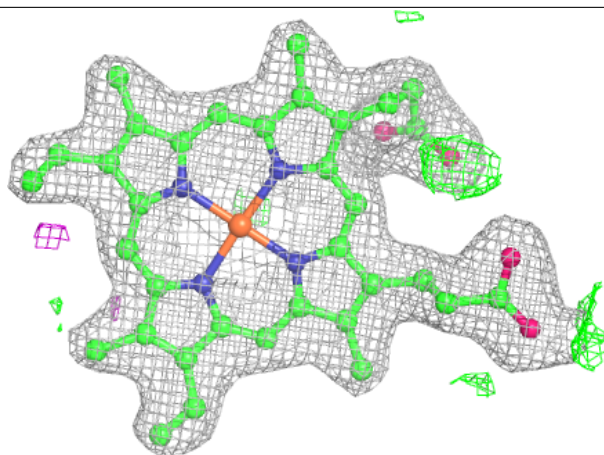
**Electron density around HEM D 401:**

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



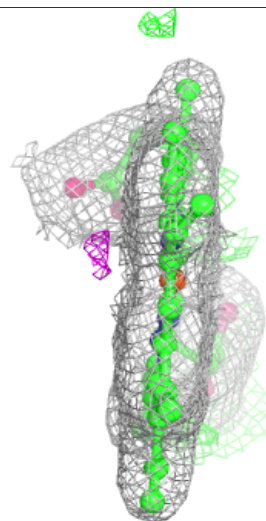
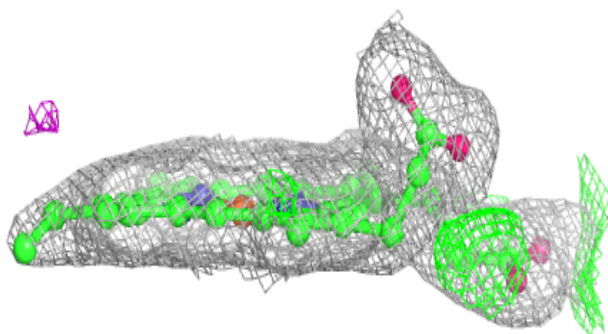
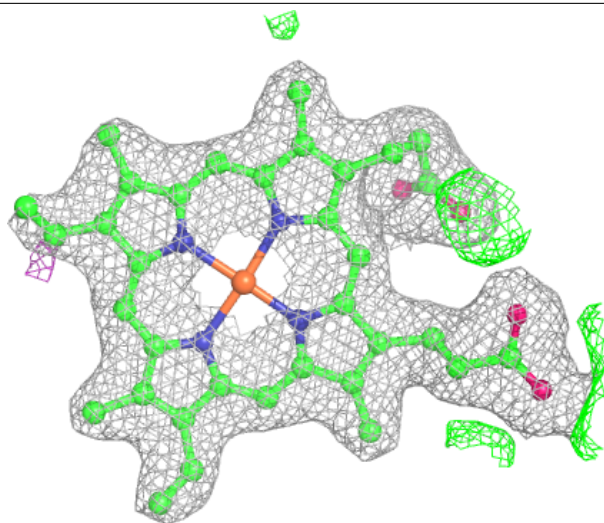
**Electron density around HEM E 401:**

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

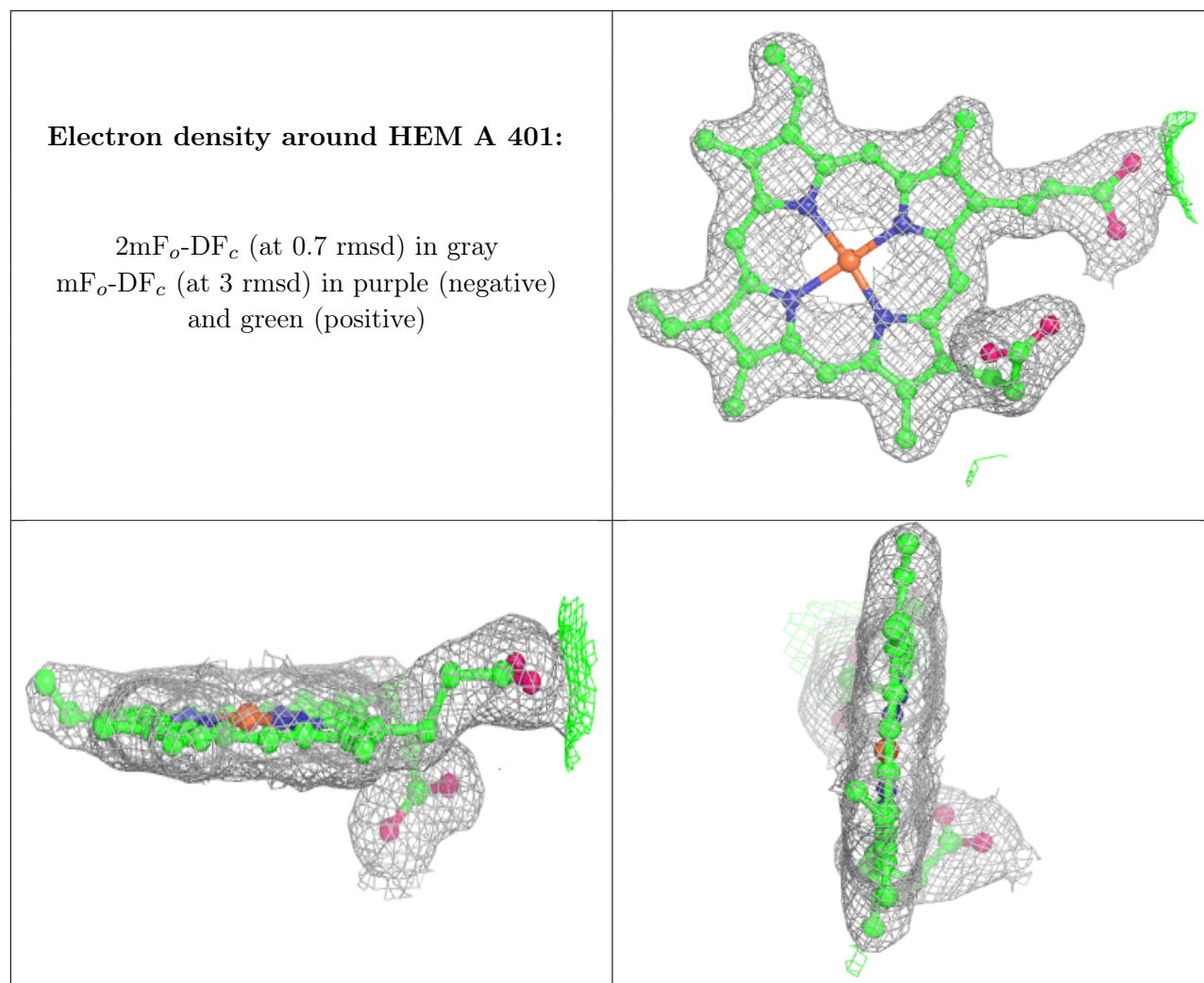


**Electron density around HEM F 401:**

$2mF_o-DF_c$  (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.