



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 10:19 am BST

PDB ID : 9EWJ / pdb_00009ewj
Title : Dye-decolourising peroxidase DtpB (224 kGy)
Authors : Lucic, M.; Worrall, J.A.R.; Hough, M.A.; Owen, R.L.; Strange, R.W.
Deposited on : 2024-04-03
Resolution : 1.92 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) : 2.42

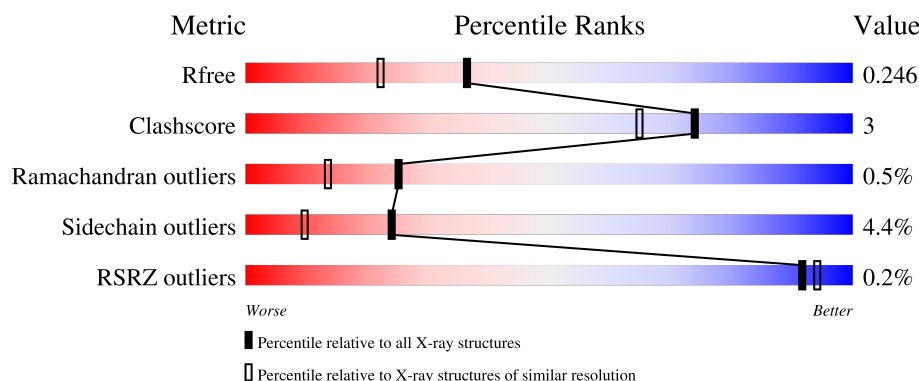
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 1.92 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	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	312	 87% 8% . . .
1	B	312	 86% 8% . . .
1	C	312	 83% 12% . . .
1	D	312	 82% 11% . . .
1	E	312	 84% 11% . . .

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Mol	Chain	Length	Quality of chain
1	F	312	<div><div></div><div>82%</div><div>12%</div><div></div><div></div></div>

2 Entry composition [i](#)

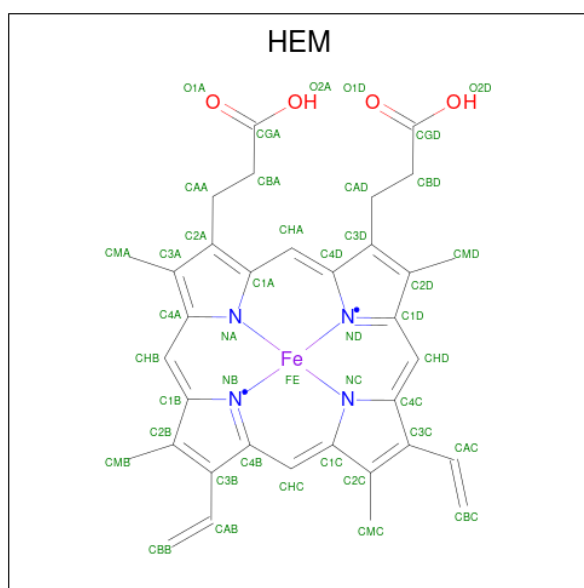
There are 6 unique types of molecules in this entry. The entry contains 14342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			2291	1447	389	446	9			
1	C	306	Total	C	N	O	S	0	0	0
			2311	1459	397	446	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	306	Total	C	N	O	S	0	0	0
			2303	1454	392	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		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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


- Molecule 6 is water.

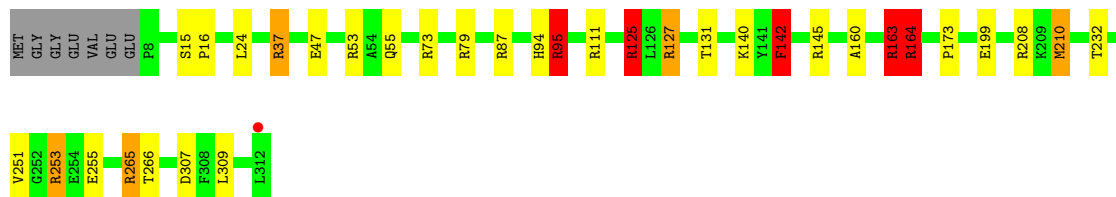
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total	O	0	0
			58	58		
6	B	29	Total	O	0	0
			29	29		
6	C	41	Total	O	0	0
			41	41		
6	D	49	Total	O	0	0
			49	49		
6	E	30	Total	O	0	0
			30	30		
6	F	36	Total	O	0	0
			36	36		

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

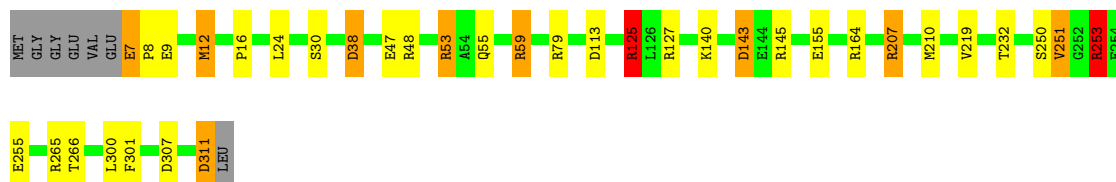
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup

Chain A: 




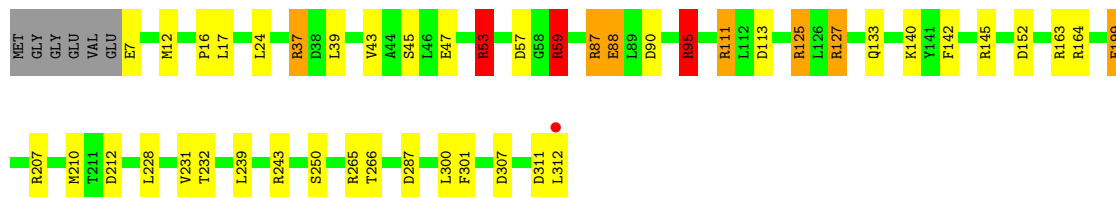
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup

Chain B: 




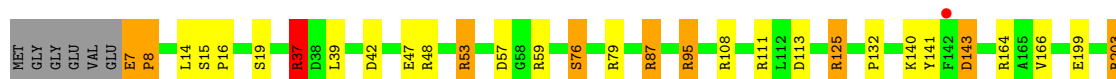
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup

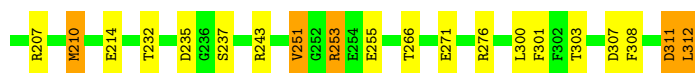
Chain C: 



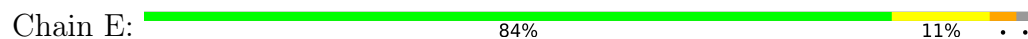
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup

Chain D: 

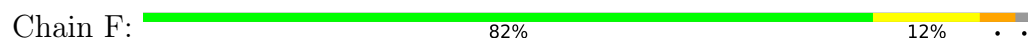




- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



- 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, α , β , γ	86.85Å 121.90Å 199.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.11 – 1.92 40.11 – 1.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.11-1.92) 100.0 (40.11-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.208 , 0.245 0.213 , 0.246	Depositor DCC
R_{free} test set	8044 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14342	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.86	3/2363 (0.1%)	1.35	31/3210 (1.0%)
1	B	0.75	1/2341 (0.0%)	1.27	21/3183 (0.7%)
1	C	0.87	4/2361 (0.2%)	1.33	28/3209 (0.9%)
1	D	0.86	4/2351 (0.2%)	1.37	32/3196 (1.0%)
1	E	0.79	2/2355 (0.1%)	1.29	24/3202 (0.7%)
1	F	0.78	3/2353 (0.1%)	1.35	31/3200 (1.0%)
All	All	0.82	17/14124 (0.1%)	1.33	167/19200 (0.9%)

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	7
1	B	0	5
1	C	0	8
1	D	0	7
1	E	0	8
1	F	0	7
All	All	0	42

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	GLU	CD-OE1	9.30	1.35	1.25
1	C	199	GLU	CD-OE2	9.12	1.35	1.25
1	D	199	GLU	CD-OE2	8.60	1.35	1.25
1	E	199	GLU	CD-OE1	7.49	1.33	1.25
1	A	47	GLU	CD-OE1	-6.28	1.18	1.25
1	A	47	GLU	CD-OE2	-6.26	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	GLU	CD-OE1	6.26	1.32	1.25
1	F	243	ARG	NE-CZ	6.19	1.41	1.33
1	D	214	GLU	CD-OE1	6.17	1.32	1.25
1	F	47	GLU	CD-OE1	-5.63	1.19	1.25
1	D	47	GLU	CD-OE2	-5.53	1.19	1.25
1	F	111	ARG	NE-CZ	5.32	1.40	1.33
1	D	199	GLU	CG-CD	5.29	1.59	1.51
1	C	47	GLU	CD-OE1	-5.25	1.19	1.25
1	C	111	ARG	NE-CZ	5.16	1.39	1.33
1	B	155	GLU	CD-OE1	-5.15	1.20	1.25
1	E	199	GLU	CD-OE2	5.08	1.31	1.25

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	E	87	ARG	CG-CD-NE	-11.22	88.23	111.80
1	D	276	ARG	NE-CZ-NH1	-10.55	115.02	120.30
1	A	125	ARG	NE-CZ-NH2	9.92	125.26	120.30
1	A	232	THR	CA-CB-OG1	-9.91	88.18	109.00
1	A	253	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	D	111	ARG	CD-NE-CZ	9.06	136.28	123.60
1	A	145	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	D	207	ARG	NE-CZ-NH2	8.89	124.74	120.30
1	D	125	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	C	127	ARG	CB-CG-CD	-8.82	88.67	111.60
1	B	232	THR	CA-CB-OG1	-8.65	90.83	109.00
1	D	87	ARG	CG-CD-NE	-8.29	94.39	111.80
1	E	57	ASP	CB-CA-C	-8.22	93.97	110.40
1	C	12	MET	CG-SD-CE	-8.20	87.08	100.20
1	E	164	ARG	CA-CB-CG	8.19	131.42	113.40
1	B	7	GLU	CB-CA-C	8.18	126.75	110.40
1	B	48	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	F	163	ARG	CA-CB-CG	8.11	131.23	113.40
1	C	7	GLU	CB-CA-C	8.09	126.58	110.40
1	F	210	MET	CG-SD-CE	-8.08	87.27	100.20
1	A	210	MET	CB-CG-SD	8.05	136.54	112.40
1	A	37	ARG	NE-CZ-NH2	8.03	124.32	120.30
1	D	95	ARG	N-CA-CB	-8.01	96.18	110.60
1	B	12	MET	CG-SD-CE	7.90	112.84	100.20
1	F	208	ARG	NE-CZ-NH2	7.83	124.21	120.30
1	C	163	ARG	CA-CB-CG	7.78	130.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	ASP	CB-CG-OD1	-7.68	111.39	118.30
1	F	87	ARG	CG-CD-NE	-7.67	95.69	111.80
1	D	164	ARG	CA-CB-CG	7.59	130.11	113.40
1	F	87	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	E	232	THR	CA-CB-OG1	-7.48	93.29	109.00
1	E	113	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	B	207	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	D	232	THR	CA-CB-OG1	-7.35	93.56	109.00
1	D	111	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	B	113	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	E	276	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	127	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	E	111	ARG	CD-NE-CZ	7.03	133.44	123.60
1	E	163	ARG	CA-CB-CG	6.96	128.72	113.40
1	C	127	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	E	125	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	E	207	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	F	158	THR	CA-CB-OG1	-6.90	94.51	109.00
1	F	268	GLU	CB-CG-CD	-6.89	95.60	114.20
1	F	113	ASP	CB-CG-OD1	-6.85	112.13	118.30
1	F	111	ARG	CD-NE-CZ	6.85	133.19	123.60
1	C	53	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	D	95	ARG	CG-CD-NE	-6.70	97.74	111.80
1	D	57	ASP	CB-CA-C	6.68	123.75	110.40
1	A	265	ARG	CB-CG-CD	6.67	128.93	111.60
1	A	127	ARG	CA-CB-CG	6.63	127.99	113.40
1	D	7	GLU	CB-CA-C	6.61	123.63	110.40
1	C	43	VAL	CG1-CB-CG2	-6.60	100.34	110.90
1	F	57	ASP	CB-CA-C	-6.59	97.23	110.40
1	F	108	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	142	PHE	N-CA-CB	6.51	122.32	110.60
1	F	24	LEU	CB-CG-CD2	-6.50	99.95	111.00
1	C	265	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	212	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	79	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	E	95	ARG	N-CA-CB	-6.43	99.03	110.60
1	B	8	PRO	N-CA-CB	-6.42	95.54	102.60
1	B	210	MET	CA-CB-CG	-6.41	102.40	113.30
1	F	111	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	A	73	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	C	232	THR	CA-CB-OG1	-6.31	95.74	109.00
1	C	95	ARG	N-CA-CB	-6.29	99.28	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	108	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	309	LEU	CB-CG-CD1	-6.27	100.34	111.00
1	C	207	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	C	57	ASP	CB-CA-C	-6.26	97.87	110.40
1	F	240	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	D	79	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	265	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	D	53	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	24	LEU	CB-CG-CD2	-6.17	100.51	111.00
1	A	87	ARG	CG-CD-NE	-6.16	98.87	111.80
1	F	265	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	210	MET	N-CA-CB	6.10	121.57	110.60
1	A	47	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	F	152	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	D	53	ARG	CD-NE-CZ	-6.08	115.09	123.60
1	C	145	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	E	273	MET	CG-SD-CE	6.00	109.81	100.20
1	B	307	ASP	CB-CA-C	-5.98	98.44	110.40
1	B	253	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	F	53	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	D	311	ASP	CB-CG-OD1	5.90	123.61	118.30
1	F	111	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	127	ARG	CA-CB-CG	5.87	126.32	113.40
1	F	127	ARG	CB-CA-C	5.83	122.06	110.40
1	B	79	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	24	LEU	N-CA-CB	-5.81	98.79	110.40
1	B	145	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	E	265	ARG	CD-NE-CZ	5.78	131.70	123.60
1	B	47	GLU	CG-CD-OE2	-5.76	106.78	118.30
1	B	251	VAL	N-CA-CB	-5.76	98.83	111.50
1	C	87	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	E	88	GLU	CB-CA-C	-5.75	98.90	110.40
1	A	95	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	D	14	LEU	CB-CG-CD1	5.74	120.77	111.00
1	C	87	ARG	CG-CD-NE	-5.74	99.75	111.80
1	F	12	MET	CG-SD-CE	5.70	109.31	100.20
1	C	111	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	D	253	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	59	ARG	CG-CD-NE	-5.66	99.92	111.80
1	D	48	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	95	ARG	CG-CD-NE	-5.63	99.97	111.80
1	A	127	ARG	CD-NE-CZ	5.61	131.46	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	111	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
1	F	203	ARG	CG-CD-NE	-5.60	100.04	111.80
1	B	207	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	E	127	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	D	111	ARG	CA-CB-CG	5.55	125.62	113.40
1	E	312	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	125	ARG	CB-CG-CD	5.55	126.02	111.60
1	E	108	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	D	199	GLU	CB-CG-CD	5.53	129.14	114.20
1	A	251	VAL	N-CA-CB	-5.52	99.36	111.50
1	C	212	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	F	240	GLU	CG-CD-OE1	-5.44	107.42	118.30
1	B	9	GLU	N-CA-CB	5.42	120.36	110.60
1	D	271	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	F	37	ARG	CG-CD-NE	-5.39	100.49	111.80
1	C	125	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	F	95	ARG	N-CA-CB	-5.34	100.99	110.60
1	A	37	ARG	CD-NE-CZ	5.33	131.07	123.60
1	A	127	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	255	GLU	N-CA-CB	-5.33	101.00	110.60
1	D	255	GLU	CG-CD-OE2	-5.33	107.64	118.30
1	B	125	ARG	CB-CG-CD	5.30	125.38	111.60
1	F	7	GLU	CB-CA-C	5.29	120.98	110.40
1	E	29	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	C	57	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	E	7	GLU	CB-CA-C	5.28	120.95	110.40
1	F	207	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	C	45	SER	CB-CA-C	-5.26	100.10	110.10
1	F	232	THR	CA-CB-OG1	-5.25	97.96	109.00
1	D	132	PRO	N-CD-CG	-5.24	95.33	103.20
1	A	37	ARG	CG-CD-NE	-5.24	100.80	111.80
1	A	140	LYS	CA-CB-CG	5.23	124.90	113.40
1	F	14	LEU	CB-CG-CD1	5.22	119.87	111.00
1	D	37	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	133	GLN	CB-CA-C	-5.16	100.08	110.40
1	A	131	THR	CA-CB-OG1	-5.16	98.17	109.00
1	A	164	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	53	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	E	127	ARG	CB-CA-C	-5.13	100.14	110.40
1	A	79	ARG	CB-CA-C	-5.12	100.16	110.40
1	D	79	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	59	ARG	CB-CG-CD	5.11	124.88	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	218	ASP	CB-CA-C	5.10	120.59	110.40
1	D	111	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	F	79	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	E	88	GLU	CG-CD-OE2	-5.08	108.13	118.30
1	C	59	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	152	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	111	ARG	CG-CD-NE	5.08	122.46	111.80
1	B	38	ASP	CB-CA-C	-5.07	100.27	110.40
1	D	53	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	303	THR	OG1-CB-CG2	-5.05	98.38	110.00
1	E	95	ARG	CG-CD-NE	-5.04	101.21	111.80
1	A	163	ARG	N-CA-CB	5.03	119.66	110.60
1	C	111	ARG	CA-CB-CG	5.03	124.47	113.40
1	C	88	GLU	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	A	127	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	95	ARG	Sidechain
1	B	125	ARG	Sidechain
1	B	207	ARG	Sidechain
1	B	253	ARG	Sidechain
1	B	59	ARG	Sidechain
1	B	7	GLU	Peptide
1	C	111	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	127	ARG	Sidechain
1	C	164	ARG	Sidechain
1	C	37	ARG	Sidechain
1	C	59	ARG	Sidechain
1	C	87	ARG	Sidechain
1	C	95	ARG	Sidechain
1	D	141	TYR	Peptide
1	D	203	ARG	Sidechain
1	D	253	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	37	ARG	Sidechain
1	D	7	GLU	Peptide
1	D	87	ARG	Sidechain
1	D	95	ARG	Sidechain
1	E	125	ARG	Sidechain
1	E	203	ARG	Sidechain
1	E	253	ARG	Sidechain
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	ARG	Sidechain
1	F	145	ARG	Sidechain
1	F	203	ARG	Sidechain
1	F	207	ARG	Sidechain
1	F	233	GLY	Peptide
1	F	37	ARG	Sidechain
1	F	7	GLU	Peptide

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	2313	0	2235	17	0
1	B	2291	0	2201	14	0
1	C	2311	0	2232	17	0
1	D	2301	0	2216	19	0
1	E	2305	0	2224	15	0
1	F	2303	0	2214	9	0
2	A	43	0	30	1	0
2	B	43	0	30	1	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	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	D	1	0	0	1	0
5	D	13	0	18	1	0
6	A	58	0	0	1	0
6	B	29	0	0	0	0
6	C	41	0	0	1	0
6	D	49	0	0	0	0
6	E	30	0	0	1	0
6	F	36	0	0	2	0
All	All	14342	0	13520	82	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 (82) 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:F:125:ARG:HD3	6:F:522:HOH:O	1.72	0.90
1:D:53:ARG:HG2	1:D:53:ARG:HH11	1.45	0.81
1:A:210:MET:HE1	1:D:210:MET:HB2	1.66	0.77
1:B:53:ARG:HG2	1:B:53:ARG:NH1	1.99	0.77
1:A:53:ARG:HH11	1:A:53:ARG:HG2	1.49	0.76
1:D:53:ARG:HG2	1:D:53:ARG:NH1	2.00	0.76
1:A:53:ARG:HG2	1:A:53:ARG:NH1	2.03	0.73
1:D:42:ASP:OD2	1:D:125:ARG:NH2	2.22	0.72
1:A:210:MET:HE1	1:D:210:MET:CB	2.20	0.71
1:B:251:VAL:CG1	1:E:123:MET:HG3	2.21	0.70
1:C:243:ARG:HD2	6:C:505:HOH:O	1.92	0.68
1:D:143:ASP:OD1	1:D:143:ASP:N	2.28	0.67
1:B:53:ARG:HG2	1:B:53:ARG:HH11	1.60	0.66
1:C:210:MET:CE	1:E:210:MET:HB2	2.26	0.65
1:E:53:ARG:NH1	1:E:53:ARG:HG2	2.12	0.64
1:C:53:ARG:HG2	1:C:53:ARG:NH1	2.12	0.64
1:B:143:ASP:OD1	1:B:143:ASP:N	2.32	0.61
1:E:53:ARG:HG2	1:E:53:ARG:HH11	1.66	0.61
1:D:53:ARG:HH11	1:D:53:ARG:CG	2.11	0.61
1:E:253:ARG:HH21	1:E:255:GLU:CD	2.04	0.59
1:C:231:VAL:HG23	1:C:239:LEU:HD12	1.85	0.58
1:C:210:MET:HE1	1:E:210:MET:HB2	1.86	0.57
1:C:231:VAL:CG2	1:C:239:LEU:HD12	2.36	0.56
1:A:210:MET:CE	1:D:210:MET:HB2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:HG12	1:E:123:MET:HG3	1.89	0.55
1:D:37:ARG:HG2	1:D:37:ARG:NH1	2.21	0.55
1:A:53:ARG:NH1	1:A:53:ARG:CG	2.70	0.54
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.13	0.54
1:A:160:ALA:HA	1:A:163:ARG:HG3	1.88	0.54
1:A:164:ARG:CZ	1:A:164:ARG:CB	2.86	0.54
2:E:401:HEM:CMC	2:E:401:HEM:HBC2	2.39	0.53
1:B:53:ARG:HH11	1:B:53:ARG:CG	2.20	0.53
1:C:228:LEU:HD12	1:C:287:ASP:HA	1.89	0.53
1:D:251:VAL:CG1	1:F:123:MET:HG3	2.39	0.53
1:C:39:LEU:O	1:C:39:LEU:HG	2.09	0.52
1:D:76:SER:H	5:D:403:PG4:H51	1.74	0.52
1:C:95:ARG:HG2	1:C:95:ARG:NH1	2.24	0.52
2:E:401:HEM:HBC2	2:E:401:HEM:HMC2	1.90	0.52
1:D:39:LEU:O	1:D:39:LEU:HG	2.08	0.52
1:D:8:PRO:CB	1:D:307:ASP:OD2	2.59	0.51
1:F:53:ARG:NH1	1:F:53:ARG:HG2	2.24	0.51
1:A:210:MET:HE1	1:D:210:MET:SD	2.51	0.50
1:C:53:ARG:HG2	1:C:53:ARG:HH11	1.74	0.50
1:B:55:GLN:HA	1:B:55:GLN:OE1	2.12	0.49
1:F:300:LEU:HD23	1:F:301:PHE:N	2.28	0.48
1:A:173:PRO:HD2	6:A:535:HOH:O	2.13	0.48
1:E:143:ASP:OD1	1:E:143:ASP:N	2.46	0.48
1:C:53:ARG:HH11	1:C:53:ARG:CG	2.27	0.47
1:B:12:MET:HA	1:B:12:MET:HE2	1.94	0.47
1:E:228:LEU:HD12	1:E:287:ASP:HA	1.95	0.47
1:F:243:ARG:HD2	6:F:515:HOH:O	2.13	0.47
1:C:300:LEU:HD23	1:C:301:PHE:N	2.31	0.46
1:A:94:HIS:C	1:A:95:ARG:HG3	2.36	0.46
1:D:8:PRO:HB2	1:D:307:ASP:OD2	2.16	0.46
1:C:228:LEU:CD1	1:C:287:ASP:HA	2.46	0.45
1:C:88:GLU:OE2	1:C:95:ARG:NH2	2.48	0.45
1:B:55:GLN:HB3	1:C:17:LEU:HD12	1.98	0.45
1:E:300:LEU:HD23	1:E:301:PHE:N	2.31	0.45
1:F:99:THR:HB	1:F:100:PRO:HD2	1.99	0.45
1:A:142:PHE:N	1:C:113:ASP:OD2	2.50	0.45
1:A:210:MET:CE	1:D:210:MET:HA	2.47	0.44
1:F:253:ARG:NH1	1:F:253:ARG:HG3	2.32	0.44
1:E:243:ARG:HD2	6:E:505:HOH:O	2.16	0.44
2:A:401:HEM:HMC2	2:A:401:HEM:HBC2	2.00	0.44
1:E:53:ARG:HH11	1:E:53:ARG:CG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ASP:O	1:C:312:LEU:HD23	2.17	0.44
1:A:55:GLN:HA	1:A:55:GLN:OE1	2.18	0.43
1:E:219:VAL:O	1:E:219:VAL:HG23	2.17	0.43
1:D:243:ARG:HD2	4:D:404:O:O	2.19	0.42
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	2.00	0.42
1:A:95:ARG:CB	1:A:95:ARG:CZ	2.97	0.42
1:B:251:VAL:HG23	1:E:116:PHE:CE1	2.55	0.42
1:D:308:PHE:O	1:D:312:LEU:HD23	2.20	0.42
1:F:228:LEU:HD12	1:F:287:ASP:HA	2.01	0.42
1:D:300:LEU:HD23	1:D:301:PHE:N	2.35	0.41
1:E:253:ARG:NH2	1:E:255:GLU:OE2	2.52	0.41
1:B:253:ARG:HH21	1:B:255:GLU:CD	2.24	0.41
1:A:164:ARG:CZ	1:A:164:ARG:HB2	2.49	0.41
1:B:300:LEU:HD23	1:B:301:PHE:N	2.36	0.41
1:F:79:ARG:NH2	1:F:83:LEU:O	2.52	0.41
1:B:311:ASP:OD1	1:B:311:ASP:N	2.55	0.40
1:B:164:ARG:O	1:B:265:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/312 (97%)	296 (98%)	5 (2%)	2 (1%)	19	9
1	B	303/312 (97%)	294 (97%)	8 (3%)	1 (0%)	37	26
1	C	304/312 (97%)	293 (96%)	9 (3%)	2 (1%)	19	9
1	D	304/312 (97%)	297 (98%)	6 (2%)	1 (0%)	37	26
1	E	304/312 (97%)	298 (98%)	5 (2%)	1 (0%)	37	26
1	F	304/312 (97%)	295 (97%)	6 (2%)	3 (1%)	13	4
All	All	1822/1872 (97%)	1773 (97%)	39 (2%)	10 (0%)	25	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	PHE
1	C	142	PHE
1	F	235	ASP
1	D	16	PRO
1	B	16	PRO
1	F	16	PRO
1	A	16	PRO
1	C	16	PRO
1	E	16	PRO
1	F	234	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	240/249 (96%)	233 (97%)	7 (3%)	37	20
1	B	235/249 (94%)	225 (96%)	10 (4%)	25	10
1	C	238/249 (96%)	229 (96%)	9 (4%)	28	13
1	D	236/249 (95%)	220 (93%)	16 (7%)	13	3
1	E	237/249 (95%)	228 (96%)	9 (4%)	28	13
1	F	237/249 (95%)	226 (95%)	11 (5%)	23	9
All	All	1423/1494 (95%)	1361 (96%)	62 (4%)	24	10

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	95	ARG
1	A	125	ARG
1	A	163	ARG
1	A	164	ARG
1	A	266	THR
1	A	307	ASP

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Mol	Chain	Res	Type
1	B	24	LEU
1	B	30	SER
1	B	38	ASP
1	B	125	ARG
1	B	140	LYS
1	B	143	ASP
1	B	219	VAL
1	B	250	SER
1	B	266	THR
1	B	311	ASP
1	C	37	ARG
1	C	53	ARG
1	C	59	ARG
1	C	90	ASP
1	C	140	LYS
1	C	199	GLU
1	C	250	SER
1	C	266	THR
1	C	307	ASP
1	D	8	PRO
1	D	15	SER
1	D	19	SER
1	D	37	ARG
1	D	76	SER
1	D	140	LYS
1	D	143	ASP
1	D	166	VAL
1	D	203	ARG
1	D	210	MET
1	D	235	ASP
1	D	237	SER
1	D	251	VAL
1	D	266	THR
1	D	311	ASP
1	D	312	LEU
1	E	19	SER
1	E	90	ASP
1	E	111	ARG
1	E	140	LYS
1	E	143	ASP
1	E	210	MET
1	E	219	VAL

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Mol	Chain	Res	Type
1	E	266	THR
1	E	307	ASP
1	F	14	LEU
1	F	30	SER
1	F	90	ASP
1	F	92	PRO
1	F	111	ARG
1	F	140	LYS
1	F	158	THR
1	F	219	VAL
1	F	234	PRO
1	F	251	VAL
1	F	266	THR

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

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](#)

Of 11 ligands modelled in this entry, 4 are 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
2	HEM	D	401	4,1	41,50,50	1.85	13 (31%)	45,82,82	3.42	22 (48%)
2	HEM	A	401	4,1	41,50,50	1.80	13 (31%)	45,82,82	2.24	16 (35%)
5	PG4	D	403	-	12,12,12	0.89	0	11,11,11	0.76	0
2	HEM	C	401	6,1	41,50,50	1.63	7 (17%)	45,82,82	2.90	20 (44%)
2	HEM	E	401	6,1	41,50,50	1.65	10 (24%)	45,82,82	2.61	23 (51%)
2	HEM	F	401	6,1	41,50,50	1.77	8 (19%)	45,82,82	2.48	19 (42%)
2	HEM	B	501	1	41,50,50	1.59	7 (17%)	45,82,82	2.26	21 (46%)

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	D	401	4,1	-	4/12/54/54	-
2	HEM	A	401	4,1	-	5/12/54/54	-
5	PG4	D	403	-	-	7/10/10/10	-
2	HEM	C	401	6,1	-	5/12/54/54	-
2	HEM	E	401	6,1	-	6/12/54/54	-
2	HEM	F	401	6,1	-	4/12/54/54	-
2	HEM	B	501	1	-	7/12/54/54	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1B-NB	-4.94	1.31	1.40
2	C	401	HEM	CHA-C4D	4.76	1.47	1.35
2	A	401	HEM	C4D-ND	-4.63	1.32	1.40
2	F	401	HEM	C4D-C3D	4.52	1.52	1.45
2	F	401	HEM	C3C-C2C	-4.36	1.34	1.40
2	D	401	HEM	C4D-C3D	4.31	1.52	1.45
2	D	401	HEM	O2D-CGD	4.28	1.45	1.30
2	E	401	HEM	O1D-CGD	3.89	1.35	1.22
2	C	401	HEM	C1B-NB	-3.73	1.33	1.40
2	B	501	HEM	CAD-C3D	3.67	1.60	1.51
2	D	401	HEM	CBD-CGD	3.63	1.59	1.50
2	D	401	HEM	C3C-C2C	-3.57	1.35	1.40
2	E	401	HEM	C3B-C4B	3.54	1.52	1.44
2	A	401	HEM	FE-NB	3.50	2.14	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C4D-C3D	3.41	1.50	1.45
2	C	401	HEM	C4D-C3D	3.37	1.50	1.45
2	A	401	HEM	C1B-NB	-3.35	1.34	1.40
2	C	401	HEM	CBD-CGD	3.32	1.58	1.50
2	E	401	HEM	C1A-CHA	-3.32	1.31	1.41
2	F	401	HEM	CHD-C1D	-3.27	1.31	1.41
2	F	401	HEM	C1B-NB	-3.07	1.35	1.40
2	D	401	HEM	C1D-C2D	3.05	1.50	1.44
2	B	501	HEM	CBD-CAD	3.05	1.61	1.52
2	A	401	HEM	CBD-CAD	2.79	1.60	1.52
2	D	401	HEM	C1A-NA	2.79	1.41	1.36
2	D	401	HEM	O1A-CGA	2.77	1.31	1.22
2	E	401	HEM	C1D-ND	-2.76	1.33	1.38
2	F	401	HEM	C4D-ND	-2.76	1.35	1.40
2	A	401	HEM	C1D-ND	-2.67	1.33	1.38
2	A	401	HEM	CBD-CGD	2.66	1.56	1.50
2	E	401	HEM	C4D-ND	-2.63	1.35	1.40
2	A	401	HEM	CHA-C4D	2.61	1.41	1.35
2	A	401	HEM	C4A-CHB	-2.57	1.33	1.41
2	E	401	HEM	C3C-C2C	2.57	1.43	1.40
2	F	401	HEM	CBD-CGD	2.56	1.56	1.50
2	F	401	HEM	C3B-C4B	2.54	1.49	1.44
2	B	501	HEM	O1D-CGD	2.47	1.30	1.22
2	E	401	HEM	CBD-CAD	2.45	1.59	1.52
2	F	401	HEM	C1A-NA	2.34	1.41	1.36
2	B	501	HEM	CBA-CGA	2.34	1.56	1.50
2	E	401	HEM	C4B-NB	-2.33	1.34	1.38
2	D	401	HEM	O1D-CGD	2.31	1.29	1.22
2	A	401	HEM	C1A-NA	2.30	1.40	1.36
2	D	401	HEM	C4D-ND	-2.30	1.36	1.40
2	A	401	HEM	CMB-C2B	2.28	1.55	1.50
2	D	401	HEM	C1D-ND	-2.26	1.34	1.38
2	A	401	HEM	CHB-C1B	2.23	1.40	1.35
2	D	401	HEM	C1B-NB	-2.21	1.36	1.40
2	A	401	HEM	O2D-CGD	-2.19	1.23	1.30
2	E	401	HEM	O1A-CGA	2.16	1.29	1.22
2	B	501	HEM	CHA-C4D	2.14	1.40	1.35
2	C	401	HEM	C4B-NB	-2.14	1.34	1.38
2	D	401	HEM	CMB-C2B	2.13	1.55	1.50
2	D	401	HEM	C4B-NB	-2.12	1.34	1.38
2	C	401	HEM	C4A-CHB	-2.11	1.35	1.41
2	B	501	HEM	C4A-CHB	-2.07	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	HEM	C1B-NB	-2.03	1.36	1.40
2	C	401	HEM	C3D-C2D	-2.01	1.32	1.36

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	O2D-CGD-CBD	11.07	149.59	114.03
2	D	401	HEM	O1D-CGD-CBD	-10.65	88.87	123.08
2	C	401	HEM	CHC-C4B-NB	9.33	134.57	124.43
2	A	401	HEM	C1B-NB-C4B	7.09	112.40	105.07
2	B	501	HEM	O2D-CGD-CBD	6.07	133.55	114.03
2	D	401	HEM	CHC-C4B-NB	6.00	130.95	124.43
2	E	401	HEM	CMB-C2B-C1B	5.85	133.95	125.04
2	F	401	HEM	CMA-C3A-C4A	-5.79	119.57	128.46
2	C	401	HEM	C1B-NB-C4B	5.52	110.78	105.07
2	B	501	HEM	O1D-CGD-CBD	-5.52	105.36	123.08
2	F	401	HEM	CHC-C4B-NB	5.41	130.31	124.43
2	F	401	HEM	O1D-CGD-CBD	-5.29	106.09	123.08
2	F	401	HEM	O2D-CGD-CBD	5.13	130.51	114.03
2	D	401	HEM	CMC-C2C-C3C	5.09	134.21	124.68
2	C	401	HEM	O2D-CGD-CBD	5.01	130.12	114.03
2	D	401	HEM	C3D-C4D-ND	4.86	115.57	110.17
2	C	401	HEM	CHD-C1D-ND	-4.83	119.18	124.43
2	C	401	HEM	C2D-C1D-ND	4.80	115.64	109.88
2	D	401	HEM	C4C-CHD-C1D	4.74	128.82	122.56
2	A	401	HEM	CHC-C4B-NB	4.73	129.56	124.43
2	D	401	HEM	C2D-C1D-ND	4.62	115.41	109.88
2	D	401	HEM	C1B-NB-C4B	4.51	109.73	105.07
2	E	401	HEM	CHC-C4B-NB	4.44	129.25	124.43
2	B	501	HEM	CBD-CAD-C3D	4.43	124.94	112.63
2	E	401	HEM	CMC-C2C-C3C	4.15	132.43	124.68
2	E	401	HEM	C4D-C3D-C2D	-4.11	100.91	106.90
2	E	401	HEM	O1D-CGD-CBD	4.11	136.28	123.08
2	E	401	HEM	CHA-C4D-C3D	-4.05	117.72	125.33
2	C	401	HEM	C3B-C2B-C1B	-4.05	103.48	106.49
2	F	401	HEM	CMD-C2D-C1D	4.01	131.15	125.04
2	D	401	HEM	C3B-C2B-C1B	-3.96	103.55	106.49
2	E	401	HEM	C1B-NB-C4B	3.96	109.16	105.07
2	C	401	HEM	O1D-CGD-CBD	-3.95	110.40	123.08
2	A	401	HEM	C2D-C1D-ND	3.94	114.60	109.88
2	E	401	HEM	C3D-C4D-ND	3.94	114.55	110.17
2	A	401	HEM	C4C-CHD-C1D	3.92	127.73	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	C4A-C3A-C2A	3.87	109.69	107.00
2	A	401	HEM	O2D-CGD-O1D	-3.86	113.69	123.30
2	F	401	HEM	C1B-NB-C4B	3.84	109.04	105.07
2	F	401	HEM	CHA-C4D-ND	3.81	129.09	124.38
2	C	401	HEM	CHC-C4B-C3B	-3.70	118.90	124.57
2	C	401	HEM	CHB-C1B-NB	3.68	128.93	124.38
2	B	501	HEM	C2C-C3C-C4C	-3.67	104.34	106.90
2	F	401	HEM	CMA-C3A-C2A	3.67	131.85	124.94
2	D	401	HEM	CAD-CBD-CGD	3.51	121.15	113.60
2	C	401	HEM	C4D-ND-C1D	-3.47	101.49	105.07
2	F	401	HEM	C4C-CHD-C1D	3.39	127.03	122.56
2	C	401	HEM	CMC-C2C-C3C	3.37	130.98	124.68
2	D	401	HEM	C4D-ND-C1D	-3.36	101.60	105.07
2	D	401	HEM	C4D-C3D-C2D	-3.27	102.14	106.90
2	E	401	HEM	CAB-C3B-C2B	-3.26	117.85	128.60
2	F	401	HEM	C2D-C1D-ND	3.25	113.77	109.88
2	D	401	HEM	CBD-CAD-C3D	3.20	121.52	112.63
2	D	401	HEM	C4B-C3B-C2B	3.19	109.65	107.11
2	E	401	HEM	C3B-C2B-C1B	-3.19	104.12	106.49
2	E	401	HEM	O2D-CGD-CBD	-3.12	103.99	114.03
2	A	401	HEM	CHB-C1B-NB	3.12	128.24	124.38
2	E	401	HEM	CMA-C3A-C4A	-3.12	123.67	128.46
2	C	401	HEM	C4B-C3B-C2B	3.09	109.57	107.11
2	F	401	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
2	C	401	HEM	CBB-CAB-C3B	-3.01	112.66	127.62
2	B	501	HEM	CAD-C3D-C4D	3.00	129.90	124.66
2	A	401	HEM	O1A-CGA-CBA	-2.97	113.53	123.08
2	C	401	HEM	O2A-CGA-CBA	2.95	123.50	114.03
2	D	401	HEM	CMA-C3A-C4A	-2.92	123.98	128.46
2	C	401	HEM	CMB-C2B-C1B	2.85	129.37	125.04
2	E	401	HEM	CAD-C3D-C4D	2.81	129.57	124.66
2	B	501	HEM	O2A-CGA-O1A	-2.80	116.31	123.30
2	F	401	HEM	C2C-C3C-C4C	-2.77	104.96	106.90
2	B	501	HEM	C1B-NB-C4B	2.77	107.93	105.07
2	B	501	HEM	CAB-C3B-C2B	-2.76	119.50	128.60
2	C	401	HEM	CMA-C3A-C4A	-2.76	124.23	128.46
2	C	401	HEM	C3C-C4C-NC	-2.75	105.75	110.94
2	D	401	HEM	CAB-C3B-C2B	2.75	137.66	128.60
2	B	501	HEM	C4D-C3D-C2D	-2.75	102.89	106.90
2	B	501	HEM	C3D-C4D-ND	2.75	113.22	110.17
2	D	401	HEM	CAB-C3B-C4B	-2.72	111.78	124.47
2	F	401	HEM	O2A-CGA-CBA	2.71	122.73	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	CHA-C4D-ND	2.70	127.72	124.38
2	C	401	HEM	C2C-C3C-C4C	2.68	108.77	106.90
2	E	401	HEM	C1D-C2D-C3D	2.67	109.77	106.96
2	C	401	HEM	CAA-CBA-CGA	2.65	121.19	113.76
2	E	401	HEM	CHD-C1D-ND	2.61	127.27	124.43
2	A	401	HEM	CHD-C1D-C2D	-2.60	120.92	124.98
2	E	401	HEM	CMB-C2B-C3B	-2.60	121.93	128.30
2	A	401	HEM	C4A-C3A-C2A	2.58	108.79	107.00
2	B	501	HEM	CMC-C2C-C3C	2.53	129.40	124.68
2	E	401	HEM	C2C-C3C-C4C	2.52	108.66	106.90
2	A	401	HEM	CHA-C4D-ND	2.51	127.48	124.38
2	A	401	HEM	C4B-CHC-C1C	2.50	125.86	122.56
2	A	401	HEM	CAB-C3B-C2B	-2.48	120.44	128.60
2	E	401	HEM	CHD-C1D-C2D	-2.45	121.14	124.98
2	F	401	HEM	C1D-C2D-C3D	-2.44	104.39	106.96
2	E	401	HEM	O2A-CGA-O1A	2.43	129.36	123.30
2	B	501	HEM	O2A-CGA-CBA	2.41	121.79	114.03
2	F	401	HEM	CAB-C3B-C2B	2.41	136.53	128.60
2	F	401	HEM	CHA-C4D-C3D	-2.40	120.82	125.33
2	C	401	HEM	O1A-CGA-CBA	-2.40	115.37	123.08
2	B	501	HEM	CBB-CAB-C3B	-2.39	115.73	127.62
2	B	501	HEM	C4C-CHD-C1D	2.36	125.67	122.56
2	D	401	HEM	CHD-C1D-C2D	-2.31	121.37	124.98
2	D	401	HEM	CMB-C2B-C1B	2.29	128.52	125.04
2	F	401	HEM	C4A-C3A-C2A	2.27	108.58	107.00
2	B	501	HEM	CHC-C4B-NB	2.26	126.89	124.43
2	B	501	HEM	CBA-CAA-C2A	2.26	116.47	112.62
2	E	401	HEM	C3C-C4C-NC	-2.21	106.76	110.94
2	B	501	HEM	CHB-C1B-NB	2.21	127.11	124.38
2	A	401	HEM	CBB-CAB-C3B	-2.13	117.01	127.62
2	A	401	HEM	C1D-C2D-C3D	-2.12	104.73	106.96
2	E	401	HEM	CBD-CAD-C3D	2.11	118.49	112.63
2	B	501	HEM	C2D-C1D-ND	2.10	112.40	109.88
2	D	401	HEM	CHA-C4D-ND	-2.08	121.81	124.38
2	B	501	HEM	CMB-C2B-C1B	2.08	128.20	125.04
2	A	401	HEM	CMD-C2D-C1D	2.07	128.19	125.04
2	F	401	HEM	O1A-CGA-CBA	-2.07	116.44	123.08
2	A	401	HEM	CHA-C4D-C3D	-2.05	121.48	125.33
2	B	501	HEM	CHD-C1D-C2D	-2.05	121.78	124.98
2	D	401	HEM	CAD-C3D-C4D	2.04	128.22	124.66
2	F	401	HEM	CBA-CAA-C2A	-2.01	109.18	112.62
2	D	401	HEM	CBB-CAB-C3B	-2.01	117.64	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CAB-C3B-C4B	2.01	133.81	124.47

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	HEM	C2A-CAA-CBA-CGA
5	D	403	PG4	O3-C5-C6-O4
2	A	401	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C2B-C3B-CAB-CBB
2	E	401	HEM	C2B-C3B-CAB-CBB
5	D	403	PG4	O2-C3-C4-O3
2	B	501	HEM	C2D-C3D-CAD-CBD
5	D	403	PG4	O1-C1-C2-O2
5	D	403	PG4	O4-C7-C8-O5
5	D	403	PG4	C4-C3-O2-C2
2	B	501	HEM	C4D-C3D-CAD-CBD
5	D	403	PG4	C3-C4-O3-C5
2	A	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	E	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAA-CBA-CGA-O2A
5	D	403	PG4	C6-C5-O3-C4
2	E	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAD-CBD-CGD-O1D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	E	401	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	E	401	HEM	CAA-CBA-CGA-O1A
2	F	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAD-CBD-CGD-O1D

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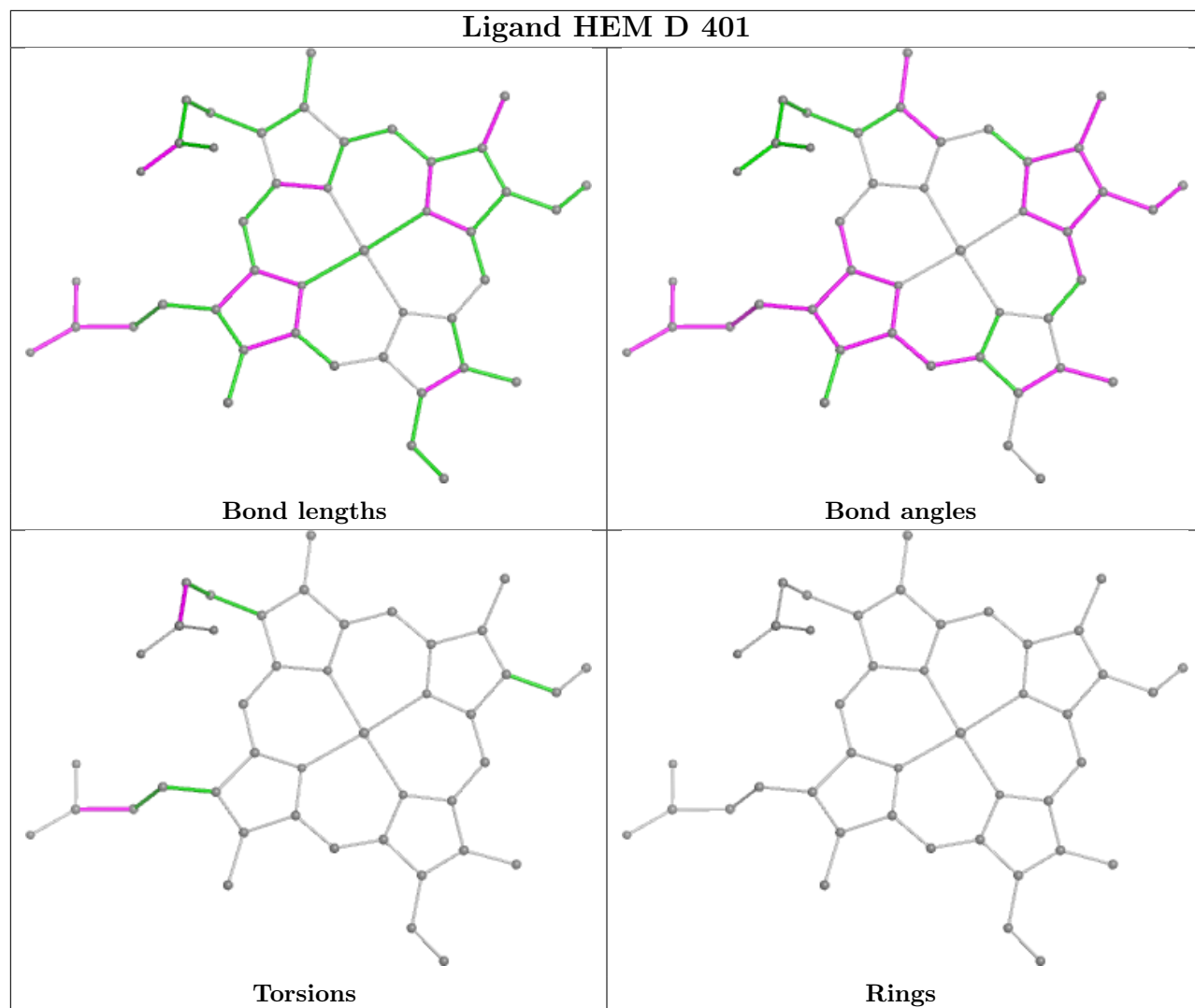
Mol	Chain	Res	Type	Atoms
2	E	401	HEM	C2D-C3D-CAD-CBD
2	B	501	HEM	CAD-CBD-CGD-O1D

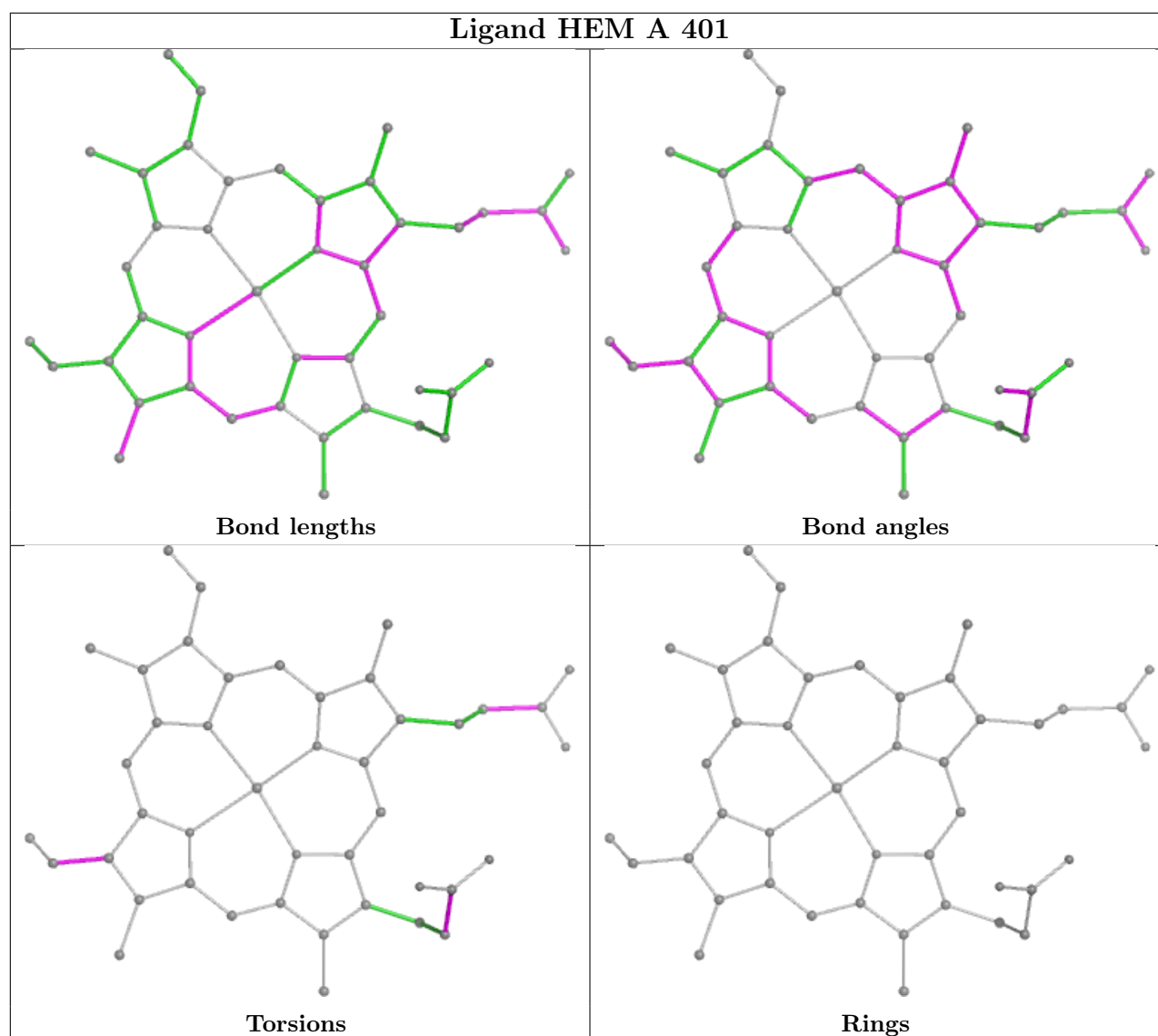
There are no ring outliers.

4 monomers are involved in 5 short contacts:

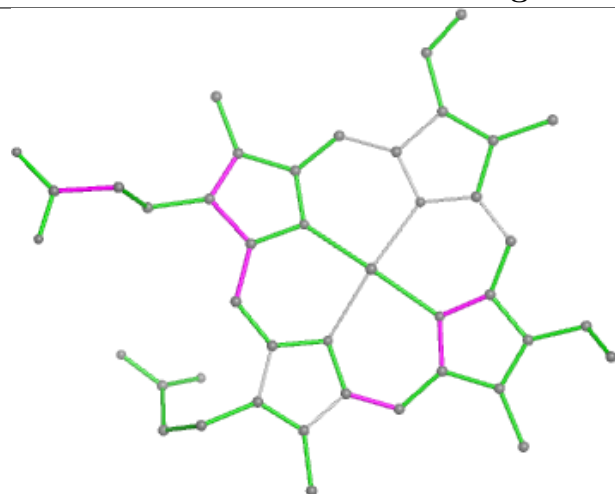
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	1	0
5	D	403	PG4	1	0
2	E	401	HEM	2	0
2	B	501	HEM	1	0

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.

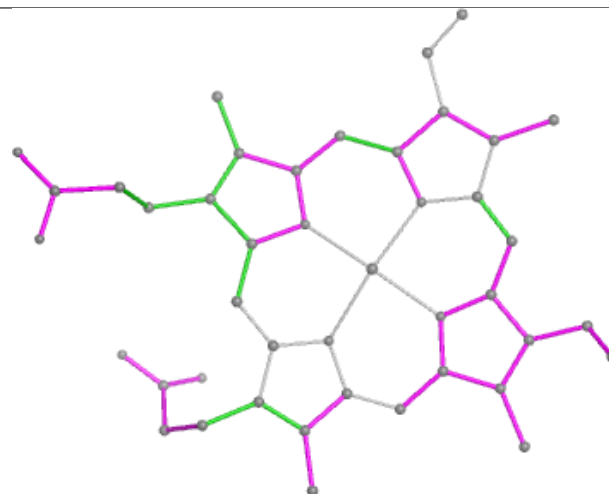




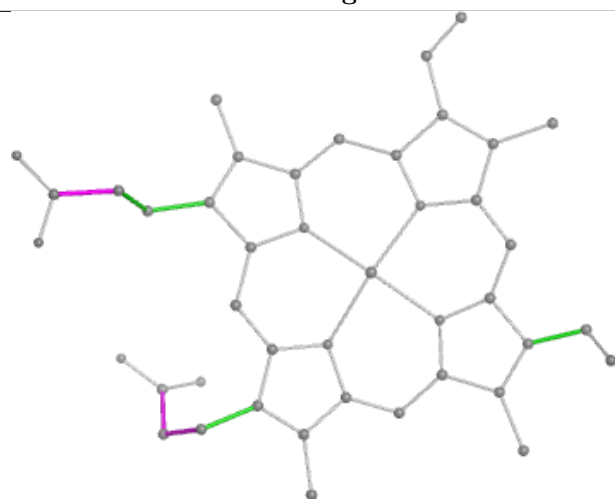
Ligand HEM C 401



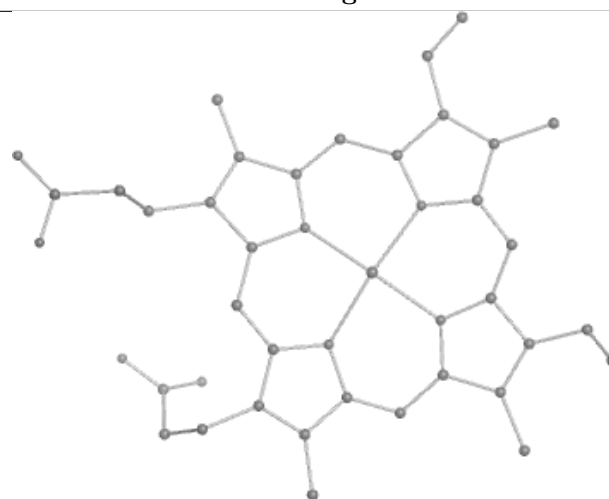
Bond lengths



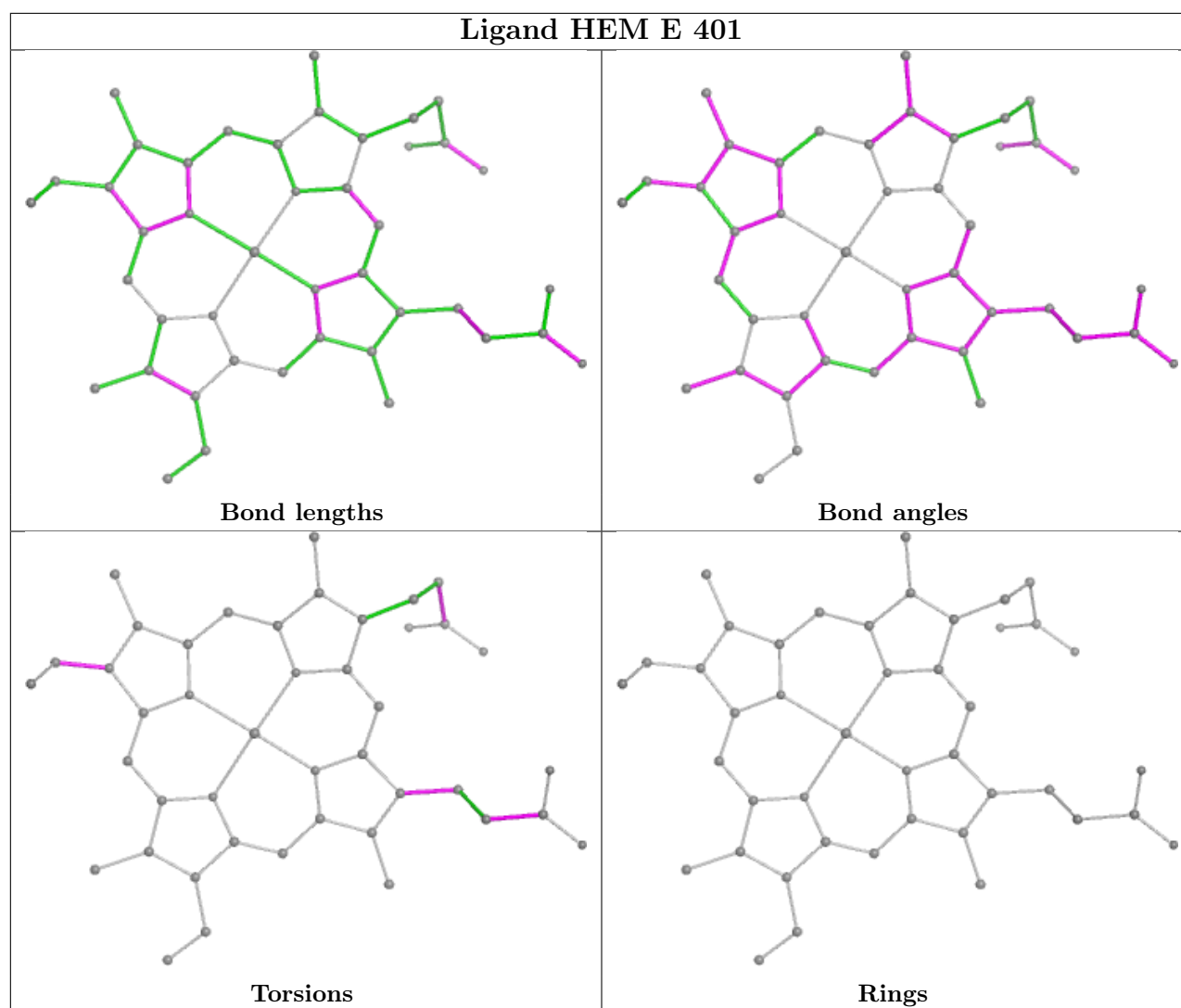
Bond angles

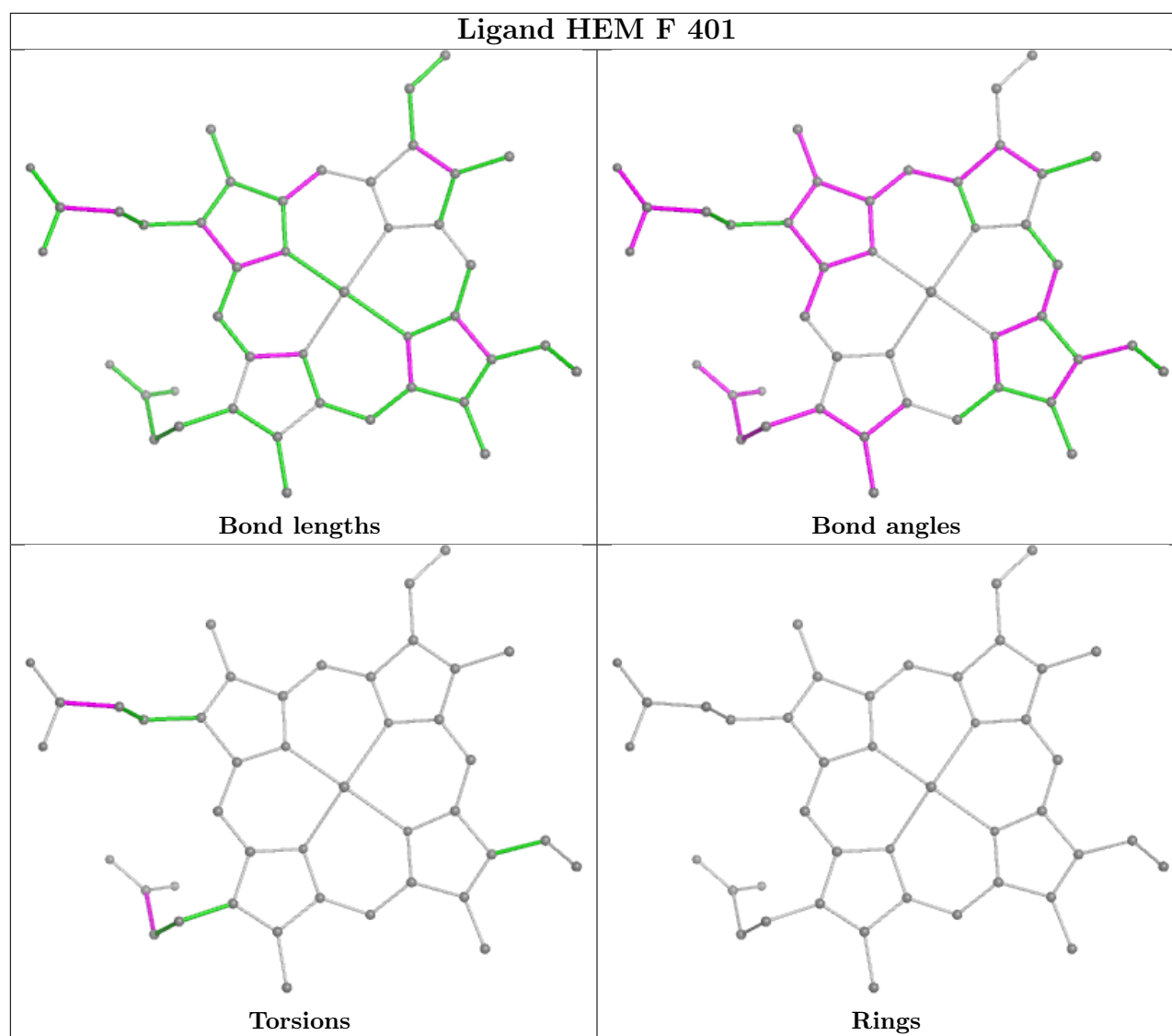


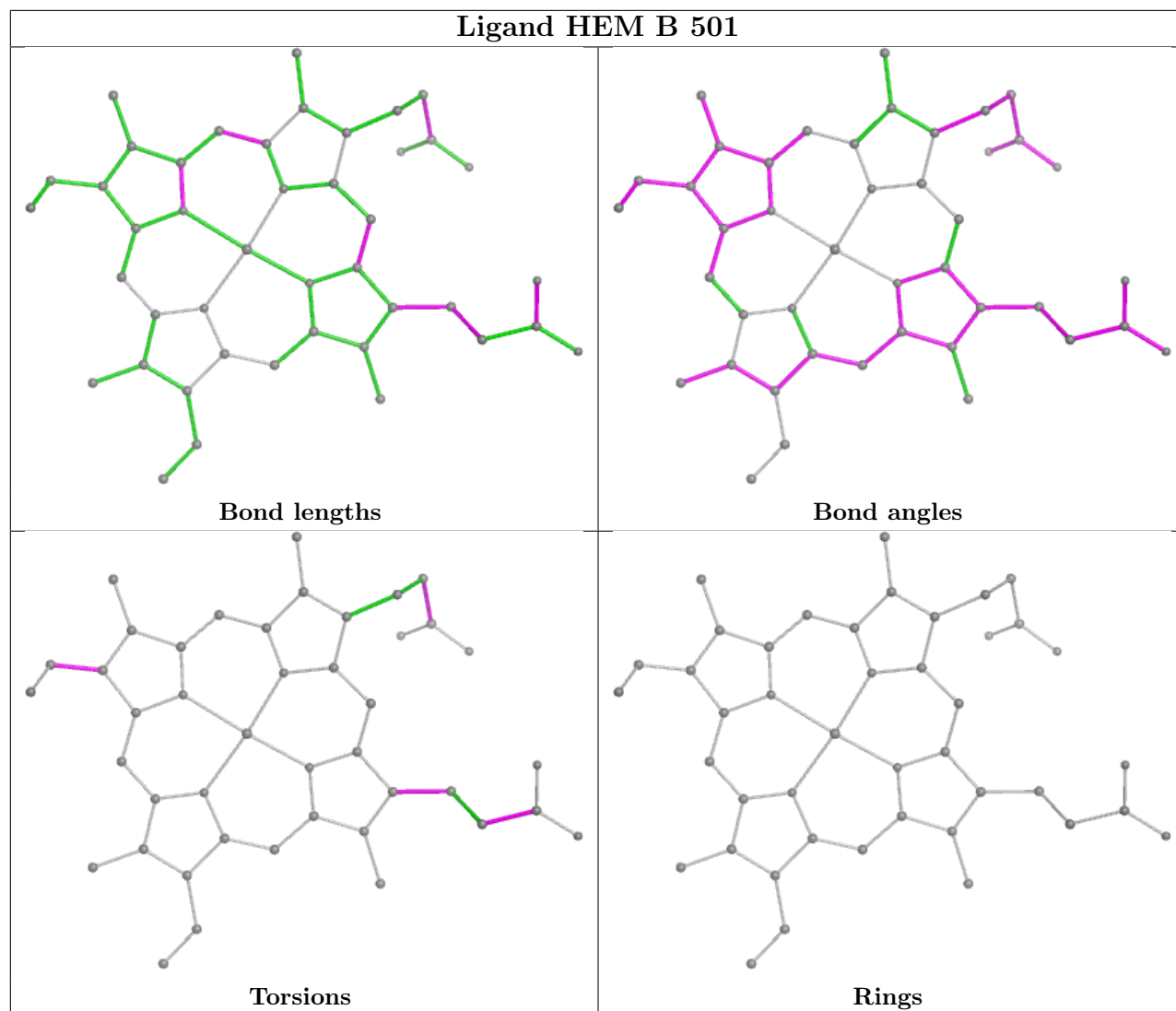
Torsions



Rings







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	305/312 (97%)	-0.83	1 (0%) 90 93	19, 27, 54, 76	0
1	B	305/312 (97%)	-0.67	0 100 100	23, 33, 60, 91	0
1	C	306/312 (98%)	-0.75	1 (0%) 90 93	18, 30, 62, 97	0
1	D	306/312 (98%)	-0.78	1 (0%) 90 93	18, 28, 58, 98	0
1	E	306/312 (98%)	-0.71	0 100 100	20, 30, 62, 111	0
1	F	306/312 (98%)	-0.74	1 (0%) 90 93	19, 30, 60, 104	0
All	All	1834/1872 (97%)	-0.75	4 (0%) 92 94	18, 30, 61, 111	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	142	PHE	5.0
1	D	142	PHE	2.5
1	A	312	LEU	2.2
1	C	312	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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,

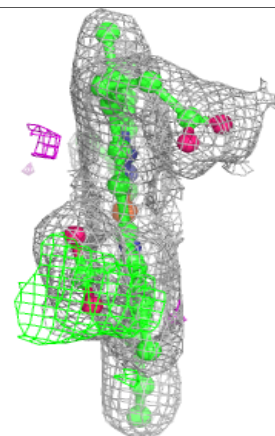
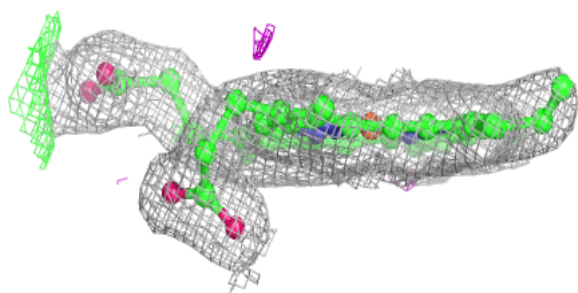
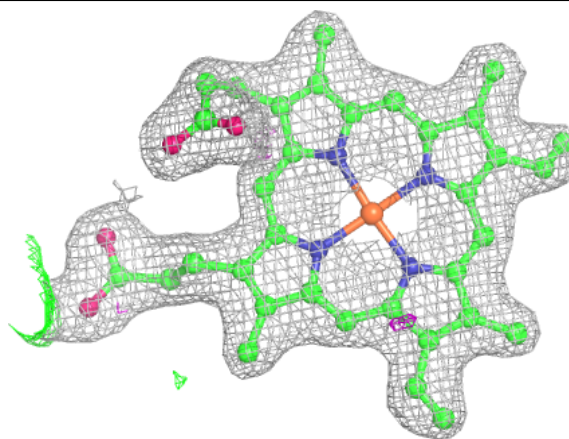
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PG4	D	403	13/13	0.83	0.14	46,62,84,85	0
3	MG	D	402	1/1	0.96	0.05	47,47,47,47	0
2	HEM	C	401	43/43	0.99	0.05	22,28,32,40	0
2	HEM	D	401	43/43	0.99	0.04	15,20,25,37	0
2	HEM	E	401	43/43	0.99	0.04	20,25,30,39	0
2	HEM	F	401	43/43	0.99	0.04	20,24,30,41	0
2	HEM	A	401	43/43	0.99	0.04	21,26,31,33	0
4	O	A	403	1/1	0.99	0.04	21,21,21,21	1
4	O	D	404	1/1	0.99	0.08	22,22,22,22	1
2	HEM	B	501	43/43	0.99	0.04	19,23,30,50	0
3	MG	A	402	1/1	1.00	0.03	24,24,24,24	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.

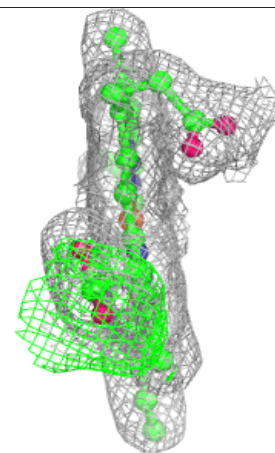
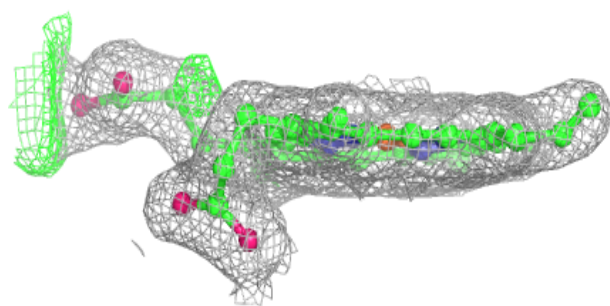
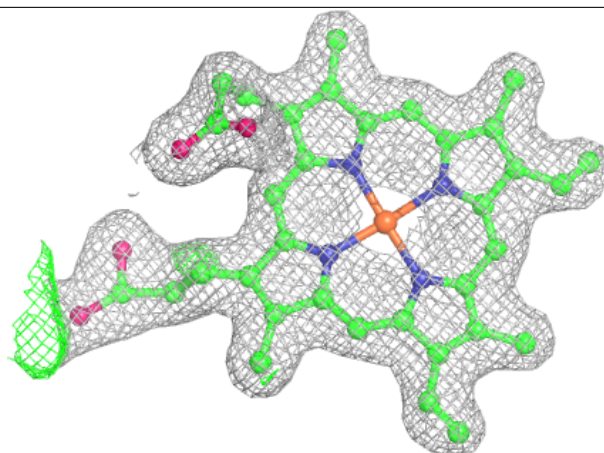
Electron density around HEM C 401:

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



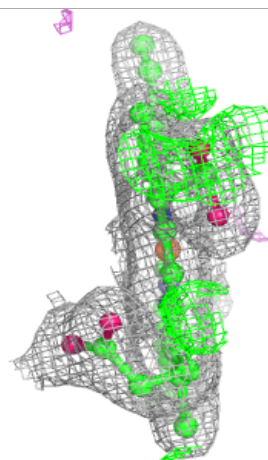
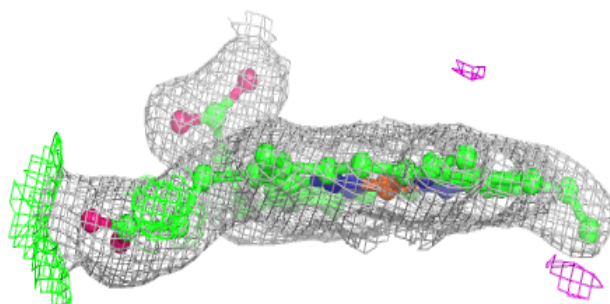
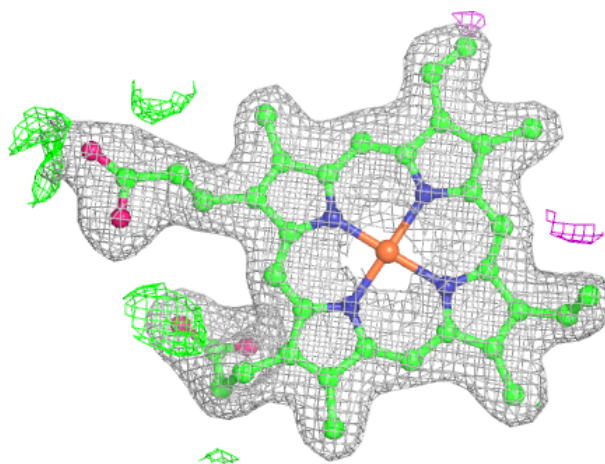
Electron density around HEM D 401:

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



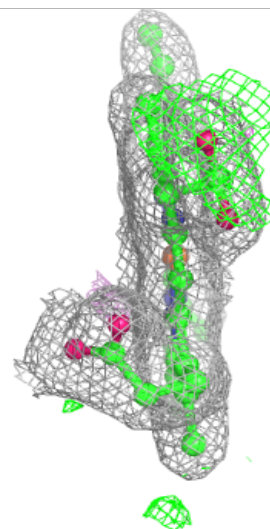
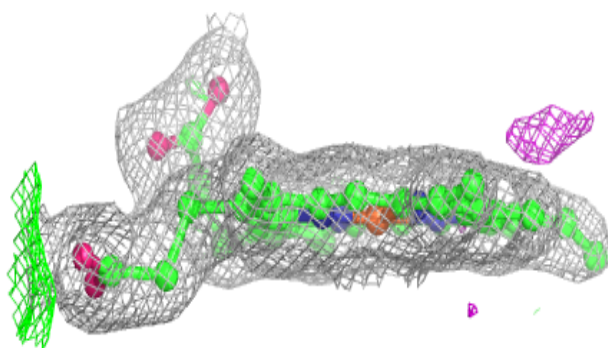
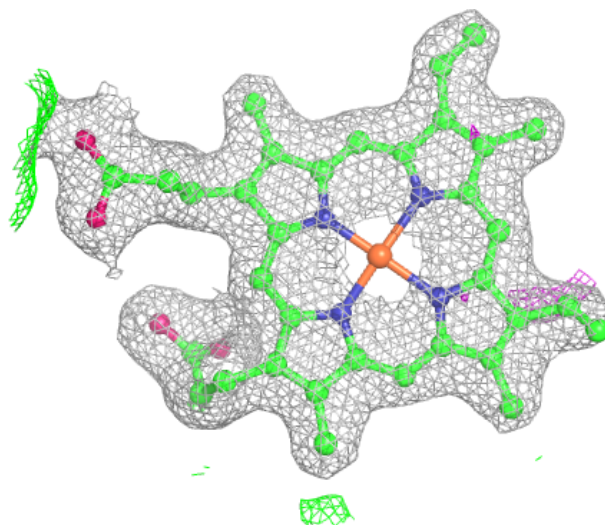
Electron density around HEM E 401:

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



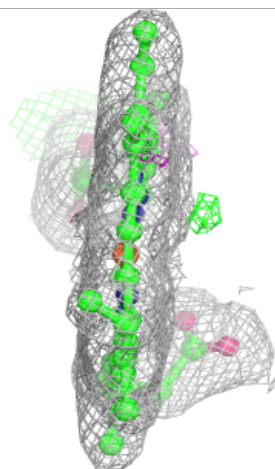
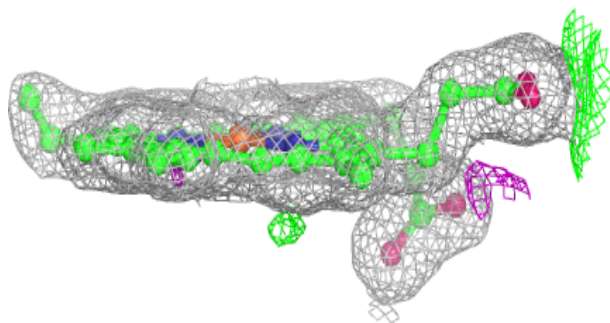
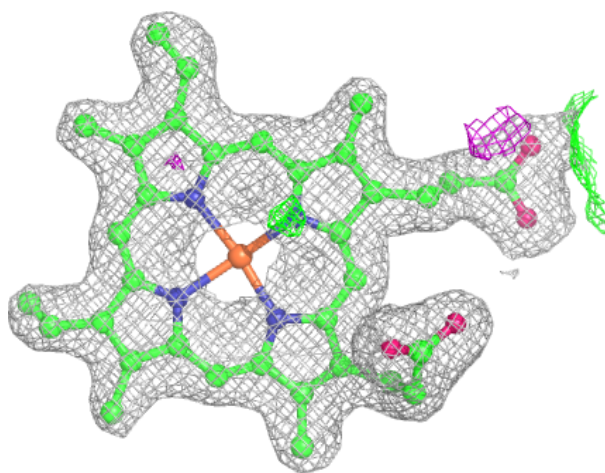
Electron density around HEM F 401:

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



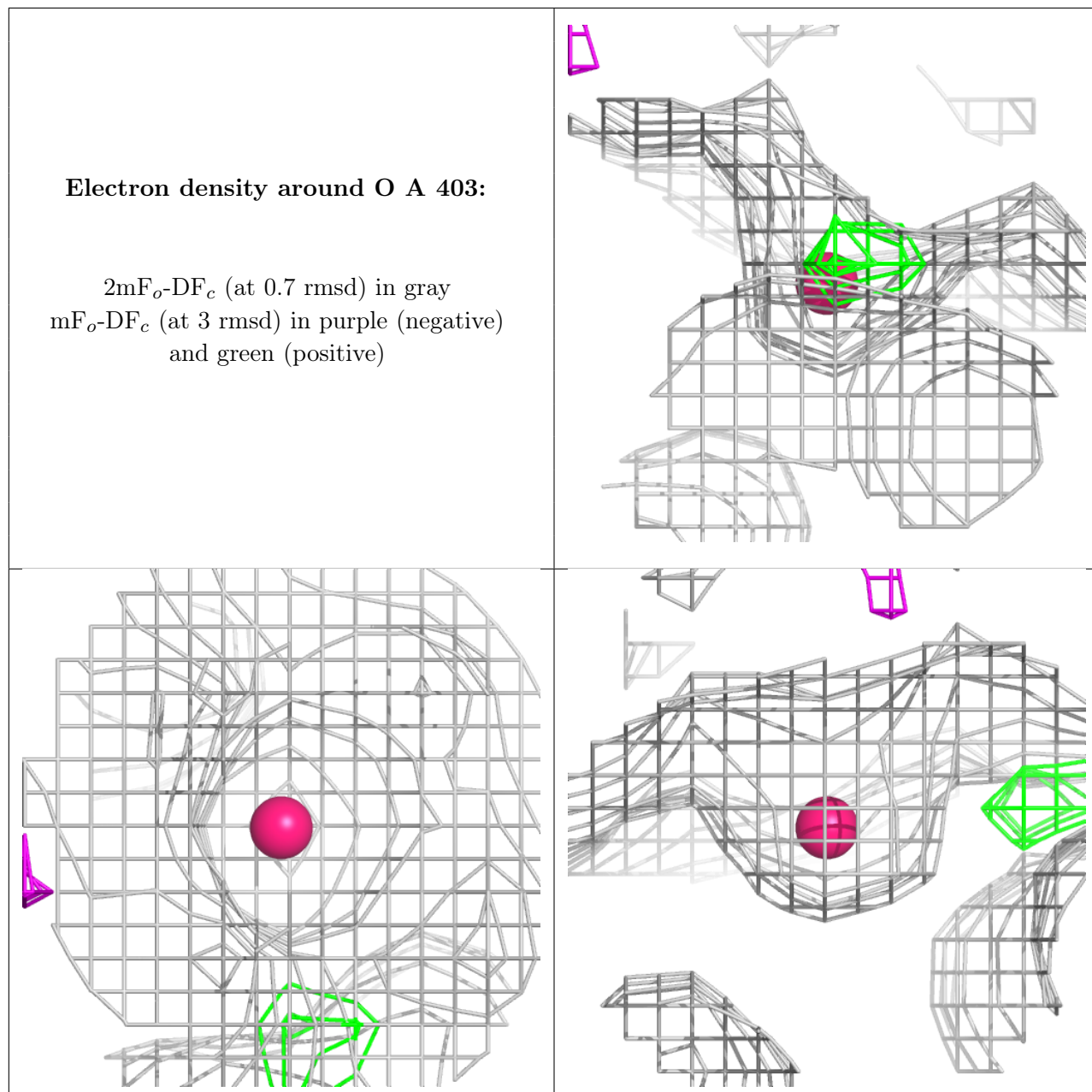
Electron density around HEM A 401:

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



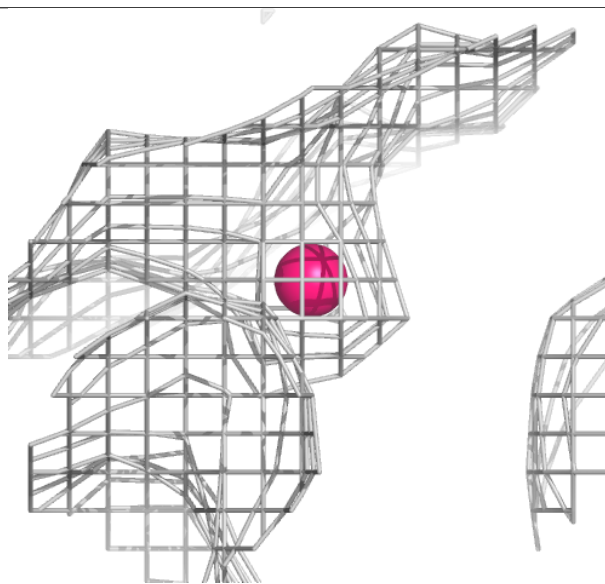
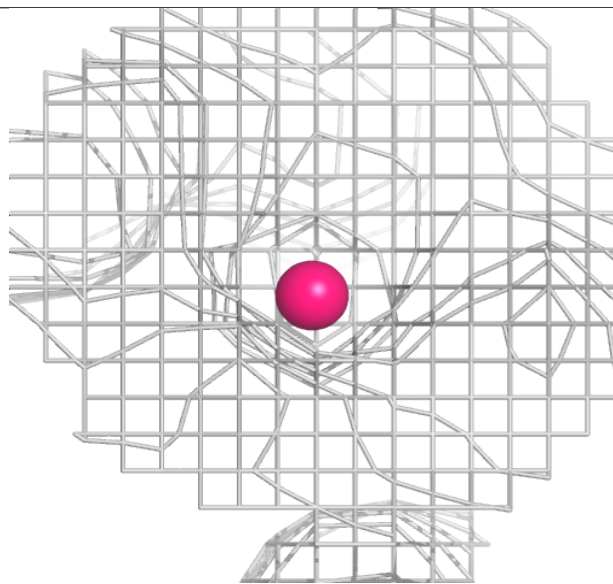
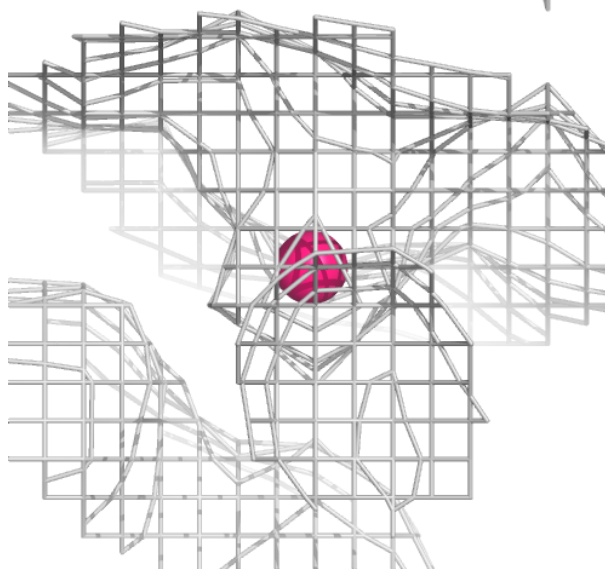
Electron density around O A 403:

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



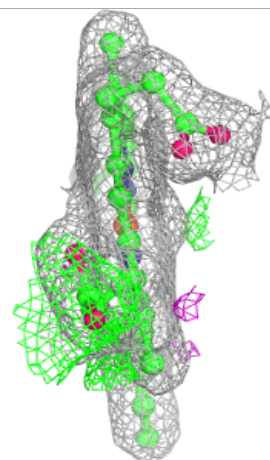
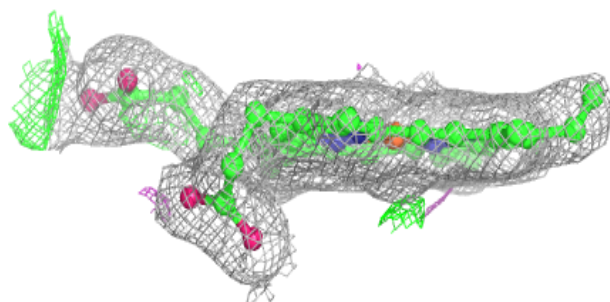
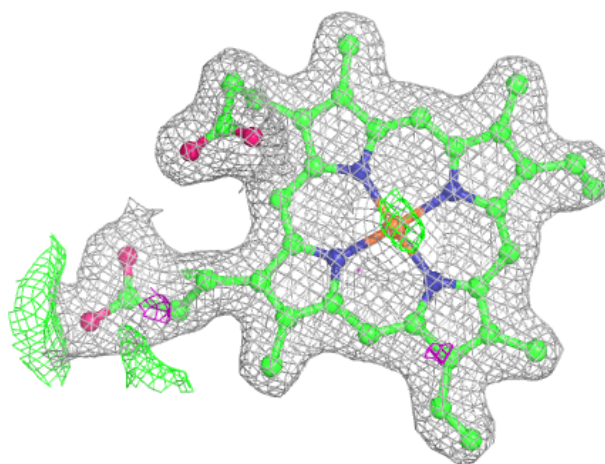
Electron density around O D 404:

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



Electron density around HEM B 501:

$2mF_o-DF_c$ (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.