Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2025 – 04:41 pm BST

PDB ID	:	9FBC / pdb_00009fbc
Title	:	Dye-decolourising peroxidase DtpB (448 kGy)
Authors	:	Lucic, M.; Worrall, J.A.R.; Hough, M.A.; Strange, R.W.; Owen, R.L.
Deposited on	:	2024-05-13
Resolution	:	2.72 Å(reported)

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

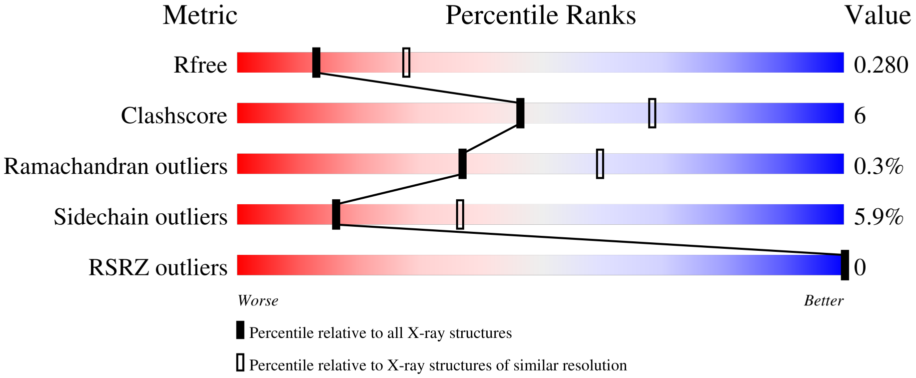
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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 <=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	
1	B	313	
1	C	313	
1	D	313	
1	E	313	

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Mol	Chain	Length	Quality of chain
1	F	313	

2 Entry composition (i)

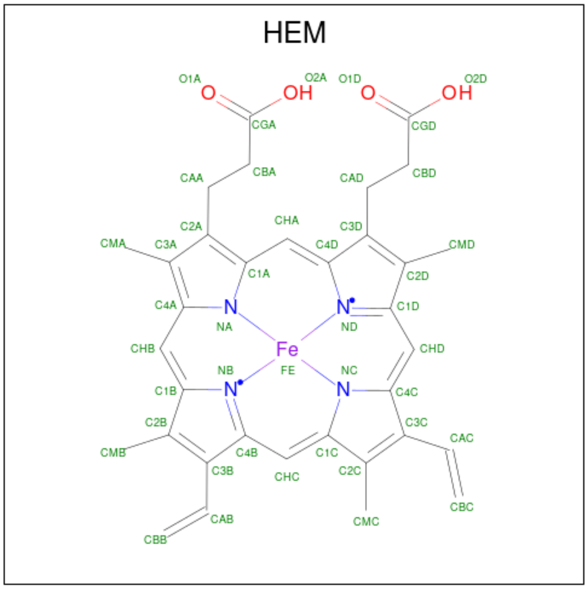
There are 3 unique types of molecules in this entry. The entry contains 14026 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2303	C 1453	N 391	O 450	S 9	0	0	0
1	B	305	Total 2277	C 1439	N 385	O 444	S 9	0	0	0
1	C	306	Total 2293	C 1452	N 388	O 444	S 9	0	0	0
1	D	306	Total 2299	C 1452	N 394	O 444	S 9	0	0	0
1	E	306	Total 2305	C 1456	N 396	O 444	S 9	0	0	0
1	F	305	Total 2289	C 1445	N 388	O 447	S 9	0	0	0

- 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 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	E	1	Total C Fe N O 43 34 1 4 4	0	0
2	F	1	Total C Fe N O 43 34 1 4 4	0	0

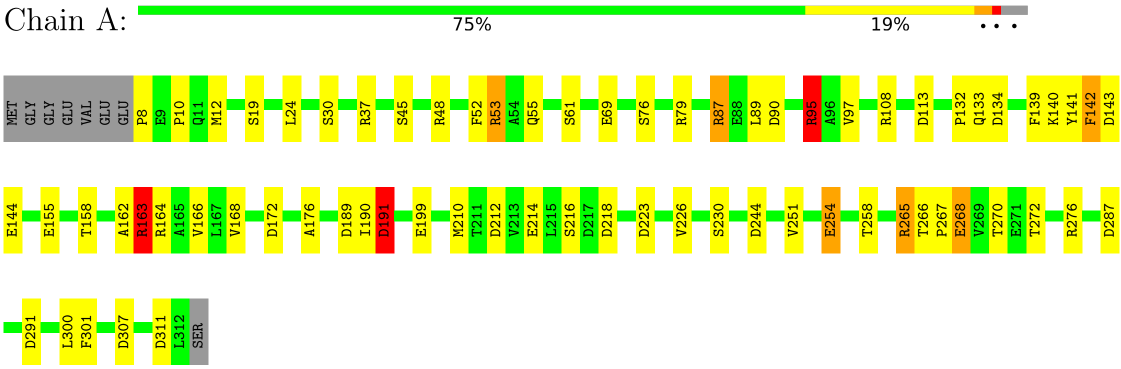
- Molecule 3 is water.

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

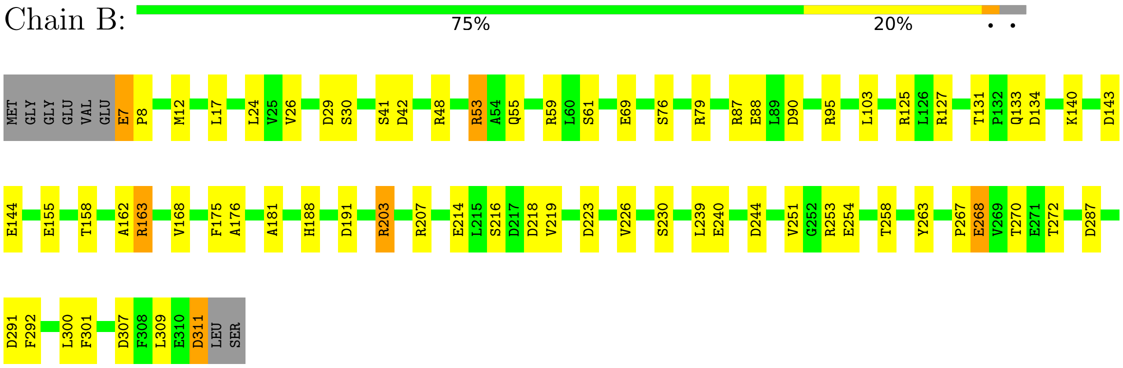
3 Residue-property plots ⓘ

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.

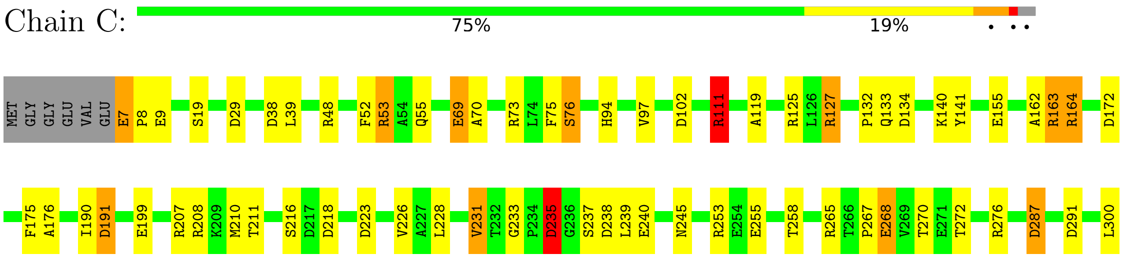
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



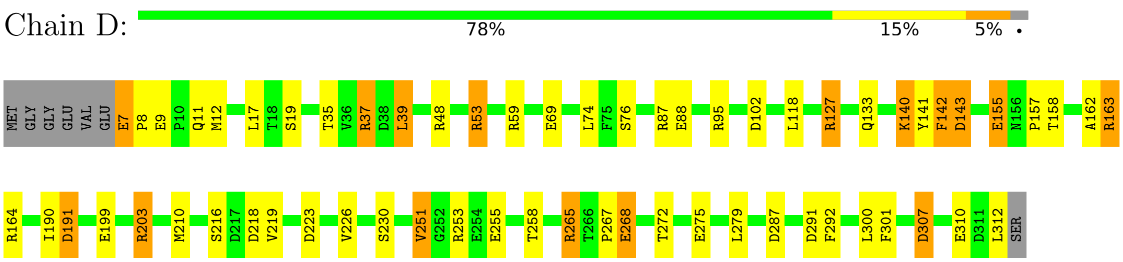
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



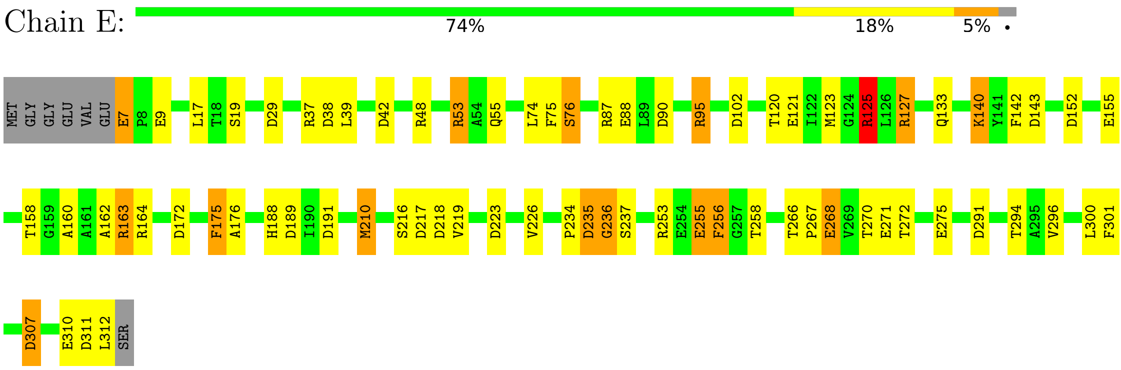
- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



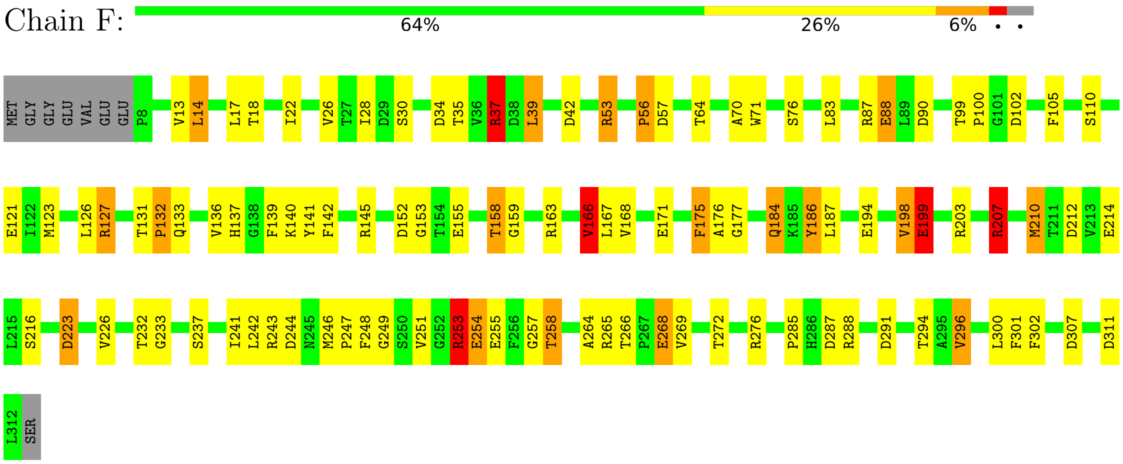
• Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



• 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	86.98Å 121.96Å 199.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.16 – 2.72 40.16 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.16-2.72) 99.9 (40.16-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.235 , 0.286 0.234 , 0.280	Depositor DCC
R_{free} test set	2931 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 0.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14026	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.94	4/2353 (0.2%)	1.71	57/3198 (1.8%)
1	B	0.83	0/2327	1.66	36/3165 (1.1%)
1	C	0.92	2/2343 (0.1%)	1.65	38/3187 (1.2%)
1	D	0.88	0/2349	1.65	37/3193 (1.2%)
1	E	0.86	1/2355 (0.0%)	1.63	47/3202 (1.5%)
1	F	0.98	1/2339 (0.0%)	1.90	64/3181 (2.0%)
All	All	0.90	8/14066 (0.1%)	1.70	279/19126 (1.5%)

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	4
1	B	0	4
1	C	0	9
1	D	0	8
1	E	0	6
1	F	0	6
All	All	0	37

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	ARG	NE-CZ	6.81	1.40	1.33
1	A	144	GLU	CD-OE1	6.77	1.38	1.25
1	A	163	ARG	NE-CZ	5.96	1.39	1.33
1	A	191	ASP	CA-C	5.74	1.60	1.52
1	F	285	PRO	CA-CB	5.70	1.61	1.53
1	E	188	HIS	CG-CD2	-5.27	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ASP	CG-OD2	5.21	1.35	1.25
1	C	94	HIS	CE1-NE2	5.20	1.37	1.32

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	ASP	CA-CB-CG	15.43	128.03	112.60
1	F	158	THR	CA-CB-OG1	-13.70	89.06	109.60
1	C	8	PRO	N-CA-C	11.98	130.08	110.55
1	C	69	GLU	CB-CG-CD	-11.04	93.83	112.60
1	C	7	GLU	CB-CA-C	10.78	130.59	110.10
1	B	268	GLU	CB-CA-C	10.76	133.01	110.32
1	F	152	ASP	CA-CB-CG	10.65	123.25	112.60
1	E	164	ARG	CA-CB-CG	10.25	134.60	114.10
1	A	144	GLU	CG-CD-OE2	-10.12	95.13	118.40
1	B	311	ASP	CA-CB-CG	10.12	122.72	112.60
1	B	8	PRO	N-CA-C	9.88	126.66	110.55
1	A	270	THR	CA-CB-OG1	9.79	124.29	109.60
1	F	88	GLU	CB-CA-C	9.64	124.84	109.61
1	A	191	ASP	CB-CA-C	9.42	129.16	110.42
1	E	218	ASP	CB-CA-C	9.39	125.84	110.81
1	F	232	THR	CA-CB-OG1	-9.21	95.79	109.60
1	C	127	ARG	CA-CB-CG	9.20	132.51	114.10
1	C	270	THR	CA-CB-OG1	9.18	123.37	109.60
1	A	158	THR	CA-CB-OG1	-9.08	95.98	109.60
1	D	307	ASP	CB-CA-C	-8.89	95.56	110.68
1	F	88	GLU	CB-CG-CD	8.66	127.32	112.60
1	F	163	ARG	CA-CB-CG	8.63	131.37	114.10
1	A	95	ARG	CB-CG-CD	8.52	130.90	111.30
1	D	140	LYS	CB-CA-C	8.49	123.67	109.84
1	B	307	ASP	CB-CA-C	-8.44	96.34	110.68
1	D	158	THR	CA-CB-OG1	-8.38	97.03	109.60
1	A	142	PHE	CA-CB-CG	8.33	122.13	113.80
1	E	125	ARG	CG-CD-NE	-8.31	93.71	112.00
1	B	163	ARG	CB-CA-C	8.29	124.59	110.84
1	F	254	GLU	CB-CG-CD	8.28	126.68	112.60
1	E	270	THR	CA-CB-OG1	8.26	121.99	109.60
1	E	191	ASP	CA-CB-CG	8.25	120.85	112.60
1	D	87	ARG	CG-CD-NE	-8.21	93.95	112.00
1	D	265	ARG	CA-CB-CG	8.20	130.51	114.10
1	E	158	THR	CA-CB-OG1	-8.17	97.35	109.60
1	F	223	ASP	CA-CB-CG	8.16	120.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	THR	CA-CB-OG1	-8.12	97.41	109.60
1	D	164	ARG	CA-CB-CG	8.09	130.28	114.10
1	B	90	ASP	CA-CB-CG	8.06	120.66	112.60
1	F	175	PHE	CB-CA-C	-8.05	97.98	111.02
1	B	223	ASP	CA-CB-CG	8.02	120.62	112.60
1	F	184	GLN	CB-CA-C	-7.96	96.44	109.89
1	D	7	GLU	CB-CA-C	7.92	125.14	110.10
1	A	311	ASP	CA-CB-CG	7.88	120.48	112.60
1	D	191	ASP	CA-CB-CG	7.82	120.42	112.60
1	A	268	GLU	CB-CA-C	7.82	125.62	110.46
1	C	211	THR	OG1-CB-CG2	-7.82	93.67	109.30
1	F	244	ASP	CA-CB-CG	7.79	120.39	112.60
1	E	311	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	163	ARG	CD-NE-CZ	7.62	135.07	124.40
1	B	268	GLU	N-CA-C	-7.62	103.09	112.38
1	B	144	GLU	CB-CA-C	7.57	123.47	111.51
1	D	163	ARG	CB-CA-C	7.56	123.39	110.84
1	D	223	ASP	CA-CB-CG	7.51	120.11	112.60
1	D	310	GLU	N-CA-CB	7.51	121.78	110.22
1	F	105	PHE	CA-CB-CG	-7.42	106.38	113.80
1	B	291	ASP	CA-CB-CG	7.41	120.01	112.60
1	B	270	THR	CA-CB-OG1	7.36	120.64	109.60
1	E	296	VAL	N-CA-CB	7.26	120.97	112.33
1	D	127	ARG	N-CA-CB	7.25	120.36	109.19
1	E	163	ARG	CB-CA-C	7.24	122.86	110.84
1	A	90	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	8	PRO	CA-N-CD	7.17	122.04	112.00
1	A	163	ARG	CB-CG-CD	7.14	127.72	111.30
1	A	95	ARG	CB-CA-C	7.13	122.75	109.71
1	B	140	LYS	CB-CA-C	7.11	121.27	109.53
1	D	291	ASP	CA-CB-CG	7.11	119.71	112.60
1	D	127	ARG	CA-CB-CG	7.08	128.25	114.10
1	E	7	GLU	CB-CA-C	7.04	123.48	110.10
1	E	223	ASP	CA-CB-CG	7.01	119.61	112.60
1	F	255	GLU	CB-CA-C	-7.00	99.27	110.81
1	F	127	ARG	CB-CA-C	6.98	118.39	109.80
1	F	56	PRO	N-CA-CB	-6.93	94.98	102.60
1	C	240	GLU	CB-CG-CD	6.82	124.20	112.60
1	A	140	LYS	CA-CB-CG	6.81	127.72	114.10
1	C	141	TYR	N-CA-CB	-6.80	99.16	110.37
1	E	120	THR	CA-CB-OG1	-6.79	99.41	109.60
1	C	268	GLU	N-CA-C	-6.78	103.08	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	87	ARG	CG-CD-NE	-6.77	97.11	112.00
1	E	294	THR	OG1-CB-CG2	-6.75	95.80	109.30
1	E	140	LYS	CB-CA-C	6.74	121.86	109.46
1	E	236	GLY	CA-C-N	6.72	130.38	120.90
1	E	236	GLY	C-N-CA	6.72	130.38	120.90
1	A	163	ARG	CG-CD-NE	6.70	126.75	112.00
1	F	265	ARG	CB-CG-CD	6.70	126.71	111.30
1	F	214	GLU	CB-CA-C	6.68	120.81	109.53
1	C	191	ASP	CA-CB-CG	6.66	119.26	112.60
1	D	140	LYS	CB-CG-CD	6.66	126.62	111.30
1	C	140	LYS	CB-CG-CD	6.65	126.60	111.30
1	C	272	THR	CA-CB-OG1	-6.60	99.70	109.60
1	C	255	GLU	CB-CA-C	-6.59	100.04	110.79
1	D	35	THR	CA-CB-OG1	-6.59	99.72	109.60
1	A	191	ASP	CA-C-O	6.55	129.88	120.51
1	A	87	ARG	CG-CD-NE	-6.54	97.61	112.00
1	E	42	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	240	GLU	CB-CG-CD	6.53	123.70	112.60
1	F	268	GLU	CB-CA-C	6.52	121.77	110.68
1	D	155	GLU	CG-CD-OE2	-6.52	103.40	118.40
1	D	268	GLU	CB-CA-C	6.52	123.11	110.46
1	B	69	GLU	N-CA-CB	6.51	119.45	110.01
1	C	163	ARG	CB-CA-C	6.50	121.64	110.84
1	A	223	ASP	CA-CB-CG	6.50	119.10	112.60
1	D	255	GLU	CB-CA-C	-6.49	100.21	110.79
1	E	127	ARG	N-CA-CB	6.46	119.23	109.34
1	F	171	GLU	CB-CG-CD	6.46	123.58	112.60
1	D	133	GLN	CB-CA-C	-6.45	98.91	109.56
1	C	9	GLU	N-CA-CB	6.45	118.68	110.23
1	C	52	PHE	CA-CB-CG	-6.45	107.35	113.80
1	F	37	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	F	294	THR	CA-CB-OG1	-6.45	99.93	109.60
1	A	69	GLU	CB-CG-CD	-6.44	101.65	112.60
1	F	64	THR	OG1-CB-CG2	-6.42	96.45	109.30
1	B	214	GLU	CB-CG-CD	6.41	123.50	112.60
1	D	158	THR	OG1-CB-CG2	6.41	122.11	109.30
1	F	153	GLY	CA-C-N	6.39	129.17	120.54
1	F	153	GLY	C-N-CA	6.39	129.17	120.54
1	C	163	ARG	CA-CB-CG	6.36	126.82	114.10
1	F	199	GLU	CB-CG-CD	6.35	123.40	112.60
1	C	291	ASP	CA-CB-CG	6.35	118.95	112.60
1	D	268	GLU	N-CA-C	-6.34	103.63	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	ASP	CA-CB-CG	6.34	118.94	112.60
1	E	307	ASP	CA-CB-CG	6.34	118.94	112.60
1	E	127	ARG	CA-CB-CG	6.26	126.62	114.10
1	F	42	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	155	GLU	CG-CD-OE2	-6.24	104.05	118.40
1	B	218	ASP	CA-CB-CG	6.24	118.84	112.60
1	E	163	ARG	CA-C-N	6.23	130.56	120.60
1	E	163	ARG	C-N-CA	6.23	130.56	120.60
1	B	163	ARG	CG-CD-NE	-6.19	98.38	112.00
1	A	141	TYR	CB-CA-C	6.18	120.20	110.19
1	A	133	GLN	CB-CA-C	-6.18	99.37	109.56
1	C	223	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	141	TYR	N-CA-CB	-6.15	100.40	110.42
1	A	172	ASP	CA-CB-CG	6.14	118.75	112.60
1	E	268	GLU	N-CA-C	-6.12	103.91	111.75
1	E	90	ASP	CA-CB-CG	6.12	118.72	112.60
1	F	137	HIS	CA-CB-CG	6.11	119.91	113.80
1	A	190	ILE	O-C-N	6.10	127.79	121.87
1	C	164	ARG	CA-CB-CG	6.10	126.30	114.10
1	F	311	ASP	CA-CB-CG	6.09	118.69	112.60
1	C	38	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	8	PRO	N-CA-C	6.07	127.28	112.10
1	A	139	PHE	CA-C-N	6.07	129.38	120.82
1	A	139	PHE	C-N-CA	6.07	129.38	120.82
1	B	287	ASP	CA-CB-CG	6.05	118.66	112.60
1	F	199	GLU	CB-CA-C	6.05	120.97	110.68
1	C	133	GLN	CB-CA-C	-6.01	99.64	109.56
1	A	24	LEU	N-CA-CB	-6.00	101.35	110.77
1	B	87	ARG	CA-CB-CG	6.00	126.10	114.10
1	B	133	GLN	CB-CA-C	-5.99	99.68	109.56
1	D	279	LEU	CA-C-O	5.97	125.98	119.24
1	E	152	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	29	ASP	CA-CB-CG	5.95	118.55	112.60
1	F	127	ARG	N-CA-CB	5.95	118.35	109.19
1	B	95	ARG	CB-CA-C	5.92	120.54	109.71
1	F	28	ILE	CB-CA-C	5.90	118.10	110.96
1	A	140	LYS	CB-CG-CD	5.87	124.80	111.30
1	F	210	MET	CG-SD-CE	-5.84	88.05	100.90
1	F	307	ASP	CA-CB-CG	5.83	118.43	112.60
1	E	163	ARG	CA-CB-CG	5.81	125.72	114.10
1	F	142	PHE	N-CA-C	-5.81	106.04	113.01
1	B	69	GLU	CB-CA-C	-5.79	101.79	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	218	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	287	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	207	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	C	268	GLU	CB-CA-C	5.76	121.63	110.46
1	E	175	PHE	CA-CB-CG	-5.74	108.06	113.80
1	D	287	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	144	GLU	CG-CD-OE1	5.70	131.52	118.40
1	E	102	ASP	CB-CA-C	5.70	121.00	110.56
1	D	219	VAL	CB-CA-C	-5.69	105.00	111.55
1	F	198	VAL	N-CA-CB	-5.68	103.91	110.55
1	F	186	TYR	N-CA-CB	5.68	120.71	110.83
1	E	255	GLU	N-CA-CB	5.67	119.50	110.65
1	F	242	LEU	O-C-N	5.66	129.84	123.27
1	E	271	GLU	CB-CG-CD	5.65	122.21	112.60
1	A	244	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	7	GLU	CB-CA-C	5.61	120.77	110.10
1	C	97	VAL	O-C-N	5.61	127.33	122.12
1	A	52	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	8	PRO	N-CA-CB	-5.60	96.84	103.00
1	D	275	GLU	CB-CG-CD	5.59	122.10	112.60
1	F	35	THR	CA-CB-OG1	-5.58	101.23	109.60
1	F	272	THR	CA-CB-OG1	-5.58	101.23	109.60
1	F	166	VAL	N-CA-C	5.58	116.42	111.90
1	F	102	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	212	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	218	ASP	CB-CA-C	5.55	121.47	110.42
1	C	311	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	113	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	37	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	A	163	ARG	N-CA-CB	5.54	119.14	109.72
1	E	133	GLN	CB-CA-C	-5.54	100.42	109.56
1	F	132	PRO	CA-C-O	-5.53	114.67	121.31
1	E	189	ASP	CA-CB-CG	5.52	118.12	112.60
1	F	17	LEU	N-CA-CB	5.52	118.14	109.69
1	F	37	ARG	CB-CG-CD	5.52	124.00	111.30
1	F	131	THR	CA-CB-OG1	5.51	117.87	109.60
1	E	268	GLU	CB-CA-C	5.51	121.14	110.46
1	F	133	GLN	CB-CA-C	-5.50	100.82	109.34
1	E	29	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	268	GLU	N-CA-C	-5.48	104.74	111.75
1	F	145	ARG	CB-CA-C	5.48	118.84	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	214	GLU	CG-CD-OE2	-5.47	105.83	118.40
1	D	218	ASP	CA-CB-CG	5.47	118.07	112.60
1	E	160	ALA	N-CA-C	-5.46	106.62	113.28
1	E	9	GLU	N-CA-CB	5.45	118.40	109.90
1	B	203	ARG	CB-CG-CD	5.45	123.83	111.30
1	E	291	ASP	CA-CB-CG	5.43	118.03	112.60
1	E	142	PHE	CB-CA-C	5.43	121.66	110.31
1	E	172	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	254	GLU	CG-CD-OE2	-5.41	105.95	118.40
1	F	37	ARG	N-CA-CB	5.41	118.08	110.12
1	B	69	GLU	CB-CG-CD	5.39	121.76	112.60
1	F	258	THR	CB-CA-C	5.38	118.74	110.14
1	A	272	THR	CA-CB-OG1	-5.37	101.55	109.60
1	C	199	GLU	CB-CG-CD	5.36	121.71	112.60
1	D	272	THR	CA-CB-OG1	-5.34	101.59	109.60
1	F	287	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	97	VAL	O-C-N	5.34	128.76	122.36
1	A	276	ARG	CA-CB-CG	-5.34	103.43	114.10
1	A	108	ARG	NH1-CZ-NH2	5.33	126.23	119.30
1	F	18	THR	N-CA-C	-5.33	100.34	109.24
1	C	238	ASP	CA-CB-CG	5.33	117.92	112.60
1	F	253	ARG	CB-CG-CD	5.32	123.54	111.30
1	F	83	LEU	O-C-N	-5.30	116.84	123.04
1	D	199	GLU	CB-CG-CD	5.30	121.61	112.60
1	F	246	MET	CG-SD-CE	-5.29	89.25	100.90
1	B	191	ASP	CB-CA-C	5.29	119.67	110.68
1	F	203	ARG	CB-CA-C	5.28	119.56	110.79
1	C	127	ARG	N-CA-CB	5.28	117.94	109.28
1	A	37	ARG	CD-NE-CZ	5.28	131.79	124.40
1	E	312	LEU	CB-CG-CD2	5.26	126.48	110.70
1	F	207	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	B	140	LYS	N-CA-C	-5.25	101.14	109.96
1	A	291	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	134	ASP	CA-CB-CG	5.24	117.84	112.60
1	E	38	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	132	PRO	N-CD-CG	-5.23	95.35	103.20
1	D	142	PHE	CB-CA-C	5.22	120.83	110.17
1	C	287	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	172	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	239	LEU	CB-CG-CD2	5.19	126.28	110.70
1	F	121	GLU	CB-CA-C	5.19	120.64	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	PRO	N-CA-CB	-5.19	99.05	103.36
1	A	199	GLU	N-CA-CB	5.18	117.66	109.94
1	F	121	GLU	CA-C-N	5.17	127.02	120.72
1	F	121	GLU	C-N-CA	5.17	127.02	120.72
1	D	87	ARG	CB-CA-C	-5.16	102.15	110.77
1	D	9	GLU	N-CA-CB	5.16	117.94	109.90
1	F	249	GLY	N-CA-C	5.15	117.15	110.45
1	D	11	GLN	N-CA-CB	5.15	117.80	110.44
1	D	17	LEU	CB-CA-C	5.15	117.22	110.06
1	B	134	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	127	ARG	CB-CA-C	5.14	117.20	110.06
1	A	191	ASP	N-CA-C	-5.14	99.86	110.80
1	B	207	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	B	42	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	8	PRO	N-CA-CB	-5.10	99.12	103.36
1	B	175	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	214	GLU	CB-CG-CD	5.10	121.27	112.60
1	F	291	ASP	CB-CA-C	5.10	120.16	110.27
1	F	177	GLY	CA-C-O	5.09	124.83	119.03
1	D	102	ASP	CB-CA-C	5.08	119.71	110.11
1	E	7	GLU	N-CA-CB	-5.07	101.88	110.50
1	D	157	PRO	N-CA-CB	-5.06	98.07	103.38
1	B	272	THR	OG1-CB-CG2	-5.06	99.19	109.30
1	A	134	ASP	CA-CB-CG	5.05	117.66	112.60
1	E	275	GLU	CB-CG-CD	5.05	121.19	112.60
1	E	310	GLU	CB-CG-CD	5.04	121.17	112.60
1	E	125	ARG	CB-CG-CD	5.04	122.89	111.30
1	A	95	ARG	CA-CB-CG	-5.04	104.03	114.10
1	B	244	ASP	CA-CB-CG	5.02	117.62	112.60
1	F	56	PRO	N-CD-CG	-5.02	97.77	103.80
1	C	216	SER	CA-CB-OG	5.02	121.14	111.10
1	C	191	ASP	N-CA-C	-5.00	105.11	111.11
1	C	235	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	A	79	ARG	Sidechain
1	A	87	ARG	Sidechain
1	A	95	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	203	ARG	Sidechain
1	B	253	ARG	Sidechain
1	B	7	GLU	Peptide
1	B	79	ARG	Sidechain
1	C	111	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	208	ARG	Sidechain
1	C	233	GLY	Peptide
1	C	253	ARG	Sidechain
1	C	276	ARG	Sidechain
1	C	7	GLU	Peptide
1	C	75	PHE	Peptide
1	C	76	SER	Peptide
1	D	127	ARG	Sidechain
1	D	141	TYR	Peptide
1	D	203	ARG	Sidechain
1	D	253	ARG	Sidechain
1	D	265	ARG	Sidechain
1	D	37	ARG	Sidechain
1	D	59	ARG	Sidechain
1	D	7	GLU	Peptide
1	E	125	ARG	Sidechain
1	E	253	ARG	Sidechain
1	E	7	GLU	Peptide
1	E	75	PHE	Peptide
1	E	76	SER	Peptide
1	E	95	ARG	Sidechain
1	F	141	TYR	Peptide
1	F	207	ARG	Sidechain
1	F	233	GLY	Peptide
1	F	243	ARG	Sidechain
1	F	253	ARG	Sidechain
1	F	276	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	2303	0	2216	26	0
1	B	2277	0	2169	21	0
1	C	2293	0	2199	29	0
1	D	2299	0	2212	23	0
1	E	2305	0	2224	28	0
1	F	2289	0	2193	38	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	4	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
All	All	14026	0	13393	154	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 6.

All (154) 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:A:210:MET:HE1	1:D:210:MET:HB2	1.10	1.07
2:E:401:HEM:HBC2	2:E:401:HEM:HMC2	1.43	0.97
1:A:210:MET:CE	1:D:210:MET:HB2	1.94	0.96
1:C:210:MET:HE1	1:E:210:MET:HB2	1.49	0.95
1:A:210:MET:HE1	1:D:210:MET:CB	1.98	0.93
1:A:191:ASP:OD1	1:C:127:ARG:NH2	2.03	0.91
1:F:184:GLN:OE1	1:F:186:TYR:OH	1.89	0.88
1:B:48:ARG:NH2	1:C:155:GLU:OE2	2.10	0.84
1:F:187:LEU:HD12	1:F:296:VAL:HG11	1.59	0.83
1:A:254:GLU:OE1	1:C:127:ARG:NH1	2.16	0.79
1:A:189:ASP:OD1	1:A:191:ASP:HB2	1.85	0.76
1:A:142:PHE:O	1:C:111:ARG:NH2	2.20	0.74
2:F:401:HEM:HBC2	2:F:401:HEM:HMC2	1.70	0.73
2:C:401:HEM:HMC2	2:C:401:HEM:HBC2	1.70	0.73
1:E:53:ARG:HH11	1:E:53:ARG:HG2	1.54	0.72
2:E:401:HEM:HBC2	2:E:401:HEM:CMC	2.11	0.72
1:E:48:ARG:NH2	1:F:155:GLU:OE2	2.25	0.69
1:F:39:LEU:C	1:F:39:LEU:HD13	2.20	0.67
1:F:158:THR:HG22	1:F:159:GLY:N	2.10	0.65
1:B:254:GLU:HG2	1:E:127:ARG:CZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:HEM:HMC2	2:D:401:HEM:HBC2	1.80	0.63
1:E:53:ARG:HG2	1:E:53:ARG:NH1	2.13	0.61
1:D:8:PRO:HB3	1:D:307:ASP:OD2	2.01	0.60
1:C:300:LEU:HD23	1:C:301:PHE:N	2.15	0.60
1:B:300:LEU:HD23	1:B:301:PHE:N	2.17	0.59
1:D:53:ARG:HG2	1:D:53:ARG:NH1	2.18	0.59
1:F:300:LEU:HD23	1:F:301:PHE:N	2.18	0.58
1:E:300:LEU:HD23	1:E:301:PHE:N	2.17	0.58
1:A:300:LEU:HD23	1:A:301:PHE:N	2.18	0.58
1:A:53:ARG:HH11	1:A:53:ARG:HG2	1.69	0.57
1:D:53:ARG:HG2	1:D:53:ARG:HH11	1.68	0.57
1:D:300:LEU:HD23	1:D:301:PHE:N	2.19	0.57
1:B:17:LEU:O	1:B:59:ARG:NH1	2.38	0.56
1:A:191:ASP:OD1	1:C:127:ARG:NH1	2.38	0.56
1:A:53:ARG:HG2	1:A:53:ARG:NH1	2.19	0.56
1:F:37:ARG:HB2	1:F:37:ARG:NH1	2.20	0.56
1:E:256:PHE:N	1:E:256:PHE:CD1	2.73	0.55
1:A:164:ARG:O	1:A:265:ARG:NH1	2.40	0.55
1:F:241:ILE:HG22	1:F:264:ALA:HB2	1.88	0.55
2:A:401:HEM:HBB2	2:A:401:HEM:HHC	1.88	0.55
1:D:53:ARG:HH11	1:D:53:ARG:CG	2.20	0.55
1:C:132:PRO:O	1:C:132:PRO:HG2	2.07	0.55
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.19	0.55
1:F:139:PHE:O	1:F:247:PRO:HD2	2.08	0.54
1:F:37:ARG:HB2	1:F:37:ARG:CZ	2.37	0.54
1:C:39:LEU:HG	1:C:39:LEU:O	2.07	0.54
1:C:48:ARG:NH2	1:D:155:GLU:OE2	2.41	0.54
1:F:99:THR:HB	1:F:100:PRO:HD2	1.90	0.54
1:B:53:ARG:HG2	1:B:53:ARG:NH1	2.23	0.54
1:C:210:MET:SD	1:E:210:MET:HE3	2.48	0.53
1:C:231:VAL:HB	1:C:239:LEU:HD12	1.90	0.53
1:B:181:ALA:HB2	1:B:263:TYR:CE1	2.43	0.53
2:A:401:HEM:HMC2	2:A:401:HEM:HBC2	1.90	0.52
1:D:39:LEU:O	1:D:39:LEU:HG	2.07	0.52
2:D:401:HEM:CMB	2:D:401:HEM:HBB2	2.39	0.52
1:C:309:LEU:O	1:C:312:LEU:HD12	2.08	0.52
2:C:401:HEM:HBC2	2:C:401:HEM:CMC	2.35	0.52
1:E:53:ARG:HH11	1:E:53:ARG:CG	2.21	0.52
1:F:126:LEU:O	1:F:127:ARG:C	2.52	0.52
1:A:48:ARG:NH2	1:E:155:GLU:OE2	2.39	0.51
1:E:37:ARG:NH1	1:E:74:LEU:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:PHE:HB3	1:F:302:PHE:HZ	1.75	0.51
1:F:39:LEU:HD13	1:F:39:LEU:O	2.11	0.51
1:E:48:ARG:HH21	1:F:155:GLU:CD	2.19	0.50
2:D:401:HEM:HBB2	2:D:401:HEM:HMB1	1.92	0.50
1:B:251:VAL:HG12	1:E:123:MET:HG3	1.93	0.49
1:E:121:GLU:O	1:E:125:ARG:HG2	2.12	0.49
1:A:55:GLN:HA	1:A:55:GLN:OE1	2.12	0.49
1:A:12:MET:HG2	1:A:61:SER:HB2	1.94	0.49
1:A:143:ASP:CG	1:A:143:ASP:O	2.56	0.49
1:C:53:ARG:HG2	1:C:53:ARG:NH1	2.28	0.48
1:B:12:MET:HG2	1:B:61:SER:HB2	1.95	0.48
1:F:223:ASP:OD2	1:F:288:ARG:HD3	2.13	0.48
1:E:234:PRO:C	1:E:236:GLY:H	2.22	0.48
1:E:55:GLN:HA	1:E:55:GLN:OE1	2.14	0.48
1:F:198:VAL:O	1:F:199:GLU:C	2.54	0.48
1:F:266:THR:HG23	1:F:269:VAL:HG23	1.95	0.48
1:C:55:GLN:HA	1:C:55:GLN:OE1	2.14	0.47
1:A:191:ASP:OD1	1:C:127:ARG:CZ	2.62	0.47
1:A:300:LEU:HD23	1:A:300:LEU:C	2.39	0.47
1:F:248:PHE:CZ	1:F:257:GLY:HA3	2.49	0.47
1:F:158:THR:CG2	1:F:159:GLY:N	2.76	0.47
1:D:37:ARG:NH1	1:D:74:LEU:O	2.47	0.46
1:B:29:ASP:OD1	1:B:131:THR:OG1	2.32	0.46
1:E:39:LEU:HD23	1:E:125:ARG:HB2	1.98	0.46
1:C:53:ARG:CG	1:C:53:ARG:HH11	2.29	0.46
1:F:39:LEU:C	1:F:39:LEU:CD1	2.88	0.46
1:D:300:LEU:HD23	1:D:300:LEU:C	2.40	0.46
1:F:168:VAL:O	1:F:176:ALA:HA	2.16	0.46
1:A:55:GLN:HB3	1:E:17:LEU:CD1	2.45	0.46
1:C:69:GLU:O	1:C:73:ARG:HG3	2.16	0.46
1:B:53:ARG:HH11	1:B:53:ARG:CG	2.29	0.45
1:F:166:VAL:HG12	1:F:167:LEU:HD23	1.97	0.45
1:A:251:VAL:HG11	1:C:119:ALA:HB1	1.99	0.45
1:C:267:PRO:O	1:C:268:GLU:C	2.60	0.45
2:F:401:HEM:HBC2	2:F:401:HEM:CMC	2.43	0.45
1:B:300:LEU:HD23	1:B:300:LEU:C	2.41	0.45
1:E:255:GLU:C	1:E:256:PHE:CD1	2.94	0.45
1:F:26:VAL:HG12	1:F:132:PRO:HA	1.99	0.45
1:C:228:LEU:HD12	1:C:287:ASP:HA	1.99	0.45
1:D:53:ARG:NH1	1:D:53:ARG:CG	2.80	0.45
1:A:89:LEU:O	1:A:95:ARG:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:HD23	1:C:300:LEU:C	2.42	0.45
1:E:235:ASP:C	1:E:237:SER:H	2.24	0.44
1:D:267:PRO:O	1:D:268:GLU:C	2.60	0.44
2:D:401:HEM:HBC2	2:D:401:HEM:CMC	2.46	0.44
1:F:87:ARG:O	1:F:88:GLU:C	2.60	0.44
1:F:166:VAL:HG12	1:F:167:LEU:CD2	2.48	0.44
1:E:267:PRO:O	1:E:268:GLU:C	2.60	0.44
1:D:143:ASP:OD1	1:D:143:ASP:N	2.50	0.44
1:E:300:LEU:HD23	1:E:300:LEU:C	2.43	0.44
1:B:53:ARG:NH1	1:B:53:ARG:CG	2.81	0.43
1:F:22:ILE:HA	1:F:136:VAL:O	2.18	0.43
1:A:267:PRO:O	1:A:268:GLU:C	2.60	0.43
1:D:162:ALA:O	1:D:163:ARG:C	2.60	0.43
1:F:175:PHE:HB3	1:F:302:PHE:CZ	2.52	0.43
1:B:162:ALA:O	1:B:163:ARG:C	2.62	0.43
1:C:53:ARG:NH1	1:C:53:ARG:CG	2.81	0.43
1:C:164:ARG:O	1:C:265:ARG:NH1	2.52	0.43
1:D:12:MET:HE2	1:D:12:MET:HB2	1.99	0.43
1:A:48:ARG:HH21	1:E:155:GLU:CD	2.26	0.43
1:D:142:PHE:CZ	1:F:53:ARG:HG3	2.54	0.43
2:B:401:HEM:HBC2	2:B:401:HEM:HMC2	2.00	0.43
1:D:142:PHE:HZ	1:F:53:ARG:HG3	1.83	0.42
1:B:155:GLU:CD	1:D:48:ARG:HH21	2.27	0.42
1:C:70:ALA:HB2	1:C:102:ASP:HB3	2.01	0.42
1:C:175:PHE:O	1:C:176:ALA:C	2.63	0.42
1:E:88:GLU:OE1	1:E:95:ARG:NH2	2.52	0.42
1:A:168:VAL:HG12	1:A:176:ALA:HA	2.01	0.42
1:B:26:VAL:HG22	1:B:103:LEU:HB2	2.02	0.42
1:E:162:ALA:O	1:E:163:ARG:C	2.62	0.42
1:B:143:ASP:OD1	1:B:143:ASP:N	2.53	0.41
1:F:207:ARG:HD2	2:F:401:HEM:CAA	2.50	0.41
1:E:123:MET:CE	1:E:127:ARG:HH12	2.33	0.41
1:B:267:PRO:O	1:B:268:GLU:C	2.62	0.41
1:E:175:PHE:O	1:E:176:ALA:C	2.63	0.41
1:C:235:ASP:C	1:C:237:SER:H	2.27	0.41
1:B:55:GLN:HA	1:B:55:GLN:OE1	2.20	0.41
1:D:251:VAL:CG1	1:F:123:MET:HG3	2.51	0.41
1:D:118:LEU:HD12	1:D:118:LEU:HA	1.77	0.41
1:E:143:ASP:OD1	1:E:143:ASP:N	2.53	0.41
1:C:190:ILE:O	1:C:191:ASP:C	2.64	0.41
1:A:162:ALA:O	1:A:163:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:HIS:HA	1:B:292:PHE:O	2.21	0.40
1:F:266:THR:CG2	1:F:269:VAL:HG23	2.52	0.40
1:D:190:ILE:O	1:D:191:ASP:C	2.64	0.40
1:F:70:ALA:O	1:F:71:TRP:C	2.64	0.40
1:F:210:MET:HB3	1:F:210:MET:HE3	1.71	0.40
1:B:41:SER:HA	1:B:309:LEU:O	2.21	0.40
1:B:168:VAL:HG12	1:B:176:ALA:HA	2.02	0.40
1:C:162:ALA:O	1:C:163:ARG:C	2.64	0.40
1:F:57:ASP:O	1:F:110:SER:OG	2.38	0.40
1:F:212:ASP:CG	1:F:212:ASP:O	2.64	0.40
1:F:13:VAL:HG12	1:F:14:LEU:HD23	2.04	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	303/313 (97%)	286 (94%)	16 (5%)	1 (0%)	37	60
1	B	303/313 (97%)	290 (96%)	13 (4%)	0	100	100
1	C	304/313 (97%)	282 (93%)	21 (7%)	1 (0%)	37	60
1	D	304/313 (97%)	287 (94%)	17 (6%)	0	100	100
1	E	304/313 (97%)	284 (93%)	19 (6%)	1 (0%)	37	60
1	F	303/313 (97%)	273 (90%)	28 (9%)	2 (1%)	19	40
All	All	1821/1878 (97%)	1702 (94%)	114 (6%)	5 (0%)	37	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ASP

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Mol	Chain	Res	Type
1	F	76	SER
1	F	254	GLU
1	C	235	ASP
1	E	235	ASP

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	239/250 (96%)	224 (94%)	15 (6%)	15	34
1	B	230/250 (92%)	218 (95%)	12 (5%)	19	42
1	C	234/250 (94%)	226 (97%)	8 (3%)	32	59
1	D	236/250 (94%)	220 (93%)	16 (7%)	13	31
1	E	237/250 (95%)	224 (94%)	13 (6%)	18	40
1	F	235/250 (94%)	216 (92%)	19 (8%)	9	22
All	All	1411/1500 (94%)	1328 (94%)	83 (6%)	16	37

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	19	SER
1	A	30	SER
1	A	45	SER
1	A	53	ARG
1	A	76	SER
1	A	95	ARG
1	A	163	ARG
1	A	166	VAL
1	A	216	SER
1	A	226	VAL
1	A	230	SER
1	A	258	THR
1	A	266	THR

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Mol	Chain	Res	Type
1	A	307	ASP
1	B	24	LEU
1	B	30	SER
1	B	53	ARG
1	B	76	SER
1	B	88	GLU
1	B	125	ARG
1	B	216	SER
1	B	219	VAL
1	B	226	VAL
1	B	230	SER
1	B	258	THR
1	B	311	ASP
1	C	19	SER
1	C	53	ARG
1	C	76	SER
1	C	111	ARG
1	C	226	VAL
1	C	231	VAL
1	C	245	ASN
1	C	258	THR
1	D	19	SER
1	D	39	LEU
1	D	53	ARG
1	D	69	GLU
1	D	76	SER
1	D	88	GLU
1	D	95	ARG
1	D	140	LYS
1	D	143	ASP
1	D	203	ARG
1	D	216	SER
1	D	226	VAL
1	D	230	SER
1	D	251	VAL
1	D	258	THR
1	D	312	LEU
1	E	19	SER
1	E	53	ARG
1	E	76	SER
1	E	140	LYS
1	E	210	MET

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Mol	Chain	Res	Type
1	E	216	SER
1	E	217	ASP
1	E	219	VAL
1	E	226	VAL
1	E	256	PHE
1	E	258	THR
1	E	266	THR
1	E	307	ASP
1	F	14	LEU
1	F	30	SER
1	F	37	ARG
1	F	39	LEU
1	F	53	ARG
1	F	56	PRO
1	F	90	ASP
1	F	140	LYS
1	F	166	VAL
1	F	194	GLU
1	F	199	GLU
1	F	216	SER
1	F	226	VAL
1	F	237	SER
1	F	251	VAL
1	F	253	ARG
1	F	258	THR
1	F	268	GLU
1	F	296	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	286	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	B	401	1	41,50,50	2.05	10 (24%)	45,82,82	2.64	20 (44%)
2	HEM	D	401	1	41,50,50	2.32	10 (24%)	45,82,82	3.37	22 (48%)
2	HEM	C	401	1	41,50,50	2.30	15 (36%)	45,82,82	3.27	25 (55%)
2	HEM	E	401	1	41,50,50	1.88	13 (31%)	45,82,82	2.80	25 (55%)
2	HEM	A	401	1	41,50,50	1.88	11 (26%)	45,82,82	2.82	21 (46%)
2	HEM	F	401	1	41,50,50	1.81	8 (19%)	45,82,82	2.52	23 (51%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	401	1	-	6/12/54/54	-
2	HEM	D	401	1	-	5/12/54/54	-
2	HEM	C	401	1	-	6/12/54/54	-
2	HEM	E	401	1	-	6/12/54/54	-
2	HEM	A	401	1	-	7/12/54/54	-
2	HEM	F	401	1	-	6/12/54/54	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C4D-C3D	7.63	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	CBD-CGD	6.73	1.66	1.50
2	D	401	HEM	C4D-C3D	6.05	1.55	1.45
2	C	401	HEM	C4D-C3D	5.47	1.54	1.45
2	D	401	HEM	C1B-NB	-5.41	1.31	1.40
2	F	401	HEM	C4D-C3D	5.22	1.54	1.45
2	F	401	HEM	C1D-C2D	5.08	1.54	1.44
2	D	401	HEM	O2D-CGD	4.94	1.47	1.30
2	C	401	HEM	C4B-NB	-4.78	1.29	1.38
2	D	401	HEM	CBD-CGD	4.66	1.61	1.50
2	E	401	HEM	C4B-NB	-4.59	1.29	1.38
2	D	401	HEM	C4B-NB	-4.50	1.29	1.38
2	D	401	HEM	C1D-C2D	4.45	1.53	1.44
2	E	401	HEM	C1B-NB	-4.33	1.32	1.40
2	C	401	HEM	C1B-NB	-4.30	1.32	1.40
2	A	401	HEM	C1D-ND	-4.23	1.30	1.38
2	A	401	HEM	CBD-CGD	4.23	1.60	1.50
2	A	401	HEM	C1B-NB	-3.88	1.33	1.40
2	A	401	HEM	C4D-C3D	3.70	1.51	1.45
2	A	401	HEM	O1D-CGD	3.61	1.34	1.22
2	B	401	HEM	CAD-C3D	3.59	1.60	1.51
2	C	401	HEM	CBD-CAD	3.38	1.62	1.52
2	F	401	HEM	C1B-NB	-3.29	1.34	1.40
2	C	401	HEM	CAD-C3D	3.29	1.59	1.51
2	B	401	HEM	C1D-C2D	3.17	1.50	1.44
2	B	401	HEM	CBD-CAD	3.12	1.61	1.52
2	F	401	HEM	O1D-CGD	3.11	1.32	1.22
2	D	401	HEM	O1A-CGA	3.10	1.32	1.22
2	E	401	HEM	C3B-C4B	3.06	1.51	1.44
2	C	401	HEM	C4D-ND	-3.04	1.35	1.40
2	E	401	HEM	CAD-C3D	2.96	1.59	1.51
2	D	401	HEM	CHC-C4B	-2.94	1.32	1.41
2	C	401	HEM	C1D-C2D	2.87	1.50	1.44
2	B	401	HEM	CBD-CGD	2.82	1.57	1.50
2	B	401	HEM	C3B-C4B	2.76	1.50	1.44
2	A	401	HEM	CBD-CAD	2.73	1.60	1.52
2	B	401	HEM	O1D-CGD	2.70	1.31	1.22
2	F	401	HEM	FE-NB	2.70	2.10	1.96
2	B	401	HEM	FE-NB	2.68	2.10	1.96
2	B	401	HEM	CHA-C4D	2.66	1.41	1.35
2	A	401	HEM	C4B-NB	-2.64	1.33	1.38
2	F	401	HEM	CHB-C1B	2.63	1.41	1.35
2	C	401	HEM	CHC-C4B	-2.62	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C3B-C4B	-2.60	1.39	1.44
2	B	401	HEM	C1B-NB	-2.60	1.35	1.40
2	E	401	HEM	O1A-CGA	2.58	1.30	1.22
2	E	401	HEM	C1D-ND	-2.50	1.33	1.38
2	A	401	HEM	FE-NB	2.49	2.09	1.96
2	E	401	HEM	C4D-C3D	2.49	1.49	1.45
2	A	401	HEM	C1D-C2D	2.45	1.49	1.44
2	F	401	HEM	C1A-NA	2.42	1.41	1.36
2	C	401	HEM	C1B-C2B	-2.40	1.39	1.44
2	C	401	HEM	O1A-CGA	2.38	1.30	1.22
2	A	401	HEM	CAD-C3D	2.38	1.57	1.51
2	E	401	HEM	O1D-CGD	2.33	1.29	1.22
2	F	401	HEM	C3C-C2C	-2.31	1.37	1.40
2	E	401	HEM	CMC-C2C	2.28	1.57	1.51
2	C	401	HEM	CAB-C3B	-2.18	1.41	1.47
2	E	401	HEM	C4D-ND	-2.16	1.36	1.40
2	E	401	HEM	C3B-C2B	-2.14	1.33	1.37
2	E	401	HEM	CBD-CGD	2.12	1.55	1.50
2	E	401	HEM	CMD-C2D	2.11	1.55	1.50
2	C	401	HEM	C4A-CHB	-2.09	1.35	1.41
2	D	401	HEM	C4A-NA	-2.08	1.31	1.36
2	D	401	HEM	C1D-ND	-2.05	1.34	1.38
2	A	401	HEM	C3B-C2B	-2.04	1.33	1.37
2	C	401	HEM	O2D-CGD	2.03	1.37	1.30

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	HEM	O1D-CGD-CBD	-10.55	89.18	123.08
2	D	401	HEM	O2D-CGD-CBD	9.27	143.81	114.03
2	C	401	HEM	CHC-C4B-NB	6.68	131.69	124.43
2	E	401	HEM	CMB-C2B-C1B	6.40	134.79	125.04
2	A	401	HEM	C3D-C4D-ND	6.33	117.22	110.17
2	C	401	HEM	O2D-CGD-CBD	6.04	133.45	114.03
2	E	401	HEM	C2C-C3C-C4C	6.02	111.10	106.90
2	C	401	HEM	CBD-CAD-C3D	6.00	129.29	112.63
2	C	401	HEM	C3D-C4D-ND	5.96	116.80	110.17
2	F	401	HEM	CHC-C4B-NB	5.96	130.90	124.43
2	C	401	HEM	C2C-C3C-C4C	5.78	110.94	106.90
2	B	401	HEM	CAD-C3D-C4D	5.70	134.63	124.66
2	D	401	HEM	C3D-C4D-ND	5.65	116.46	110.17
2	E	401	HEM	C3D-C4D-ND	5.56	116.36	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CBD-CAD-C3D	5.46	127.79	112.63
2	B	401	HEM	CBD-CAD-C3D	5.45	127.78	112.63
2	C	401	HEM	C3B-C2B-C1B	-5.41	102.47	106.49
2	A	401	HEM	C2D-C1D-ND	5.37	116.32	109.88
2	B	401	HEM	CHB-C1B-NB	5.23	130.84	124.38
2	D	401	HEM	CHC-C4B-NB	5.20	130.08	124.43
2	A	401	HEM	CAA-CBA-CGA	-5.13	99.39	113.76
2	A	401	HEM	C4D-C3D-C2D	-5.04	99.55	106.90
2	A	401	HEM	C4D-ND-C1D	-5.02	99.88	105.07
2	B	401	HEM	C2C-C3C-C4C	-5.01	103.40	106.90
2	F	401	HEM	C4C-CHD-C1D	5.01	129.17	122.56
2	A	401	HEM	CBD-CAD-C3D	5.01	126.54	112.63
2	D	401	HEM	C3B-C2B-C1B	-4.87	102.87	106.49
2	D	401	HEM	CAD-C3D-C4D	4.83	133.10	124.66
2	D	401	HEM	C4D-ND-C1D	-4.76	100.15	105.07
2	F	401	HEM	C2D-C1D-ND	4.72	115.53	109.88
2	C	401	HEM	C4D-ND-C1D	-4.65	100.27	105.07
2	E	401	HEM	CHC-C4B-NB	4.61	129.44	124.43
2	C	401	HEM	C2D-C1D-ND	4.48	115.24	109.88
2	B	401	HEM	O1D-CGD-CBD	-4.47	108.71	123.08
2	B	401	HEM	CHC-C4B-NB	4.43	129.24	124.43
2	A	401	HEM	C4C-CHD-C1D	4.39	128.35	122.56
2	B	401	HEM	O2D-CGD-CBD	4.38	128.09	114.03
2	D	401	HEM	C2D-C1D-ND	4.33	115.07	109.88
2	A	401	HEM	CMB-C2B-C1B	4.31	131.60	125.04
2	C	401	HEM	O2D-CGD-O1D	-4.29	112.62	123.30
2	E	401	HEM	CAB-C3B-C2B	-4.27	114.55	128.60
2	B	401	HEM	CMD-C2D-C1D	4.25	131.51	125.04
2	E	401	HEM	O2A-CGA-O1A	4.21	133.78	123.30
2	A	401	HEM	C4A-C3A-C2A	4.20	109.92	107.00
2	F	401	HEM	CMD-C2D-C1D	4.14	131.35	125.04
2	E	401	HEM	C2D-C1D-ND	4.13	114.83	109.88
2	E	401	HEM	C4D-C3D-C2D	-4.12	100.90	106.90
2	C	401	HEM	C4D-C3D-C2D	-4.10	100.92	106.90
2	D	401	HEM	CHA-C4D-ND	-4.05	119.38	124.38
2	F	401	HEM	C1B-NB-C4B	4.01	109.22	105.07
2	D	401	HEM	C4D-C3D-C2D	-4.01	101.06	106.90
2	F	401	HEM	O1A-CGA-CBA	-3.97	110.34	123.08
2	A	401	HEM	CAD-CBD-CGD	3.96	122.12	113.60
2	C	401	HEM	CHB-C1B-NB	3.94	129.25	124.38
2	B	401	HEM	C1B-NB-C4B	3.91	109.11	105.07
2	C	401	HEM	CAD-C3D-C4D	3.89	131.45	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	C3D-C4D-ND	3.76	114.35	110.17
2	C	401	HEM	C1B-NB-C4B	3.67	108.86	105.07
2	B	401	HEM	C4A-C3A-C2A	-3.66	104.45	107.00
2	C	401	HEM	CMC-C2C-C3C	3.63	131.48	124.68
2	D	401	HEM	CHC-C4B-C3B	-3.63	119.01	124.57
2	E	401	HEM	C4D-ND-C1D	-3.62	101.34	105.07
2	A	401	HEM	CAD-C3D-C4D	3.54	130.84	124.66
2	A	401	HEM	C1B-NB-C4B	3.51	108.70	105.07
2	E	401	HEM	C3B-C2B-C1B	-3.50	103.89	106.49
2	F	401	HEM	O1D-CGD-CBD	-3.42	112.11	123.08
2	C	401	HEM	CHA-C4D-ND	-3.41	120.17	124.38
2	A	401	HEM	CHD-C1D-ND	-3.37	120.77	124.43
2	C	401	HEM	O1A-CGA-CBA	-3.36	112.28	123.08
2	B	401	HEM	CAD-C3D-C2D	-3.34	121.66	127.88
2	C	401	HEM	CMD-C2D-C1D	3.32	130.10	125.04
2	B	401	HEM	C4C-CHD-C1D	3.28	126.88	122.56
2	C	401	HEM	C3C-C4C-NC	-3.27	104.77	110.94
2	F	401	HEM	C4D-ND-C1D	-3.24	101.73	105.07
2	F	401	HEM	CHD-C1D-ND	-3.24	120.92	124.43
2	C	401	HEM	CHD-C1D-ND	-3.22	120.93	124.43
2	C	401	HEM	CAD-CBD-CGD	3.20	120.50	113.60
2	D	401	HEM	CMC-C2C-C3C	3.18	130.62	124.68
2	D	401	HEM	C2C-C3C-C4C	3.18	109.12	106.90
2	E	401	HEM	CHB-C1B-NB	3.16	128.28	124.38
2	E	401	HEM	CMC-C2C-C3C	3.14	130.56	124.68
2	C	401	HEM	CHC-C4B-C3B	-3.10	119.83	124.57
2	E	401	HEM	CBD-CAD-C3D	3.08	121.18	112.63
2	B	401	HEM	CHB-C1B-C2B	-3.06	118.27	126.72
2	D	401	HEM	C3C-C4C-NC	-2.94	105.40	110.94
2	A	401	HEM	CAB-C3B-C2B	-2.90	119.03	128.60
2	E	401	HEM	CAB-C3B-C4B	2.89	137.94	124.47
2	F	401	HEM	CAD-C3D-C4D	2.86	129.66	124.66
2	C	401	HEM	O1D-CGD-CBD	-2.85	113.91	123.08
2	E	401	HEM	CMB-C2B-C3B	-2.85	121.32	128.30
2	E	401	HEM	CHB-C1B-C2B	-2.83	118.89	126.72
2	F	401	HEM	CAD-CBD-CGD	-2.83	107.52	113.60
2	F	401	HEM	CHB-C1B-NB	2.78	127.81	124.38
2	E	401	HEM	C3C-C4C-NC	-2.75	105.75	110.94
2	F	401	HEM	CMA-C3A-C4A	-2.67	124.36	128.46
2	E	401	HEM	CHA-C4D-C3D	-2.65	120.36	125.33
2	B	401	HEM	C2D-C1D-ND	2.64	113.05	109.88
2	C	401	HEM	CHB-C1B-C2B	-2.62	119.48	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	C1B-NB-C4B	2.61	107.77	105.07
2	A	401	HEM	C3C-C4C-NC	-2.61	106.01	110.94
2	F	401	HEM	O2D-CGD-O1D	2.56	129.67	123.30
2	A	401	HEM	CHA-C4D-C3D	-2.52	120.60	125.33
2	D	401	HEM	CMB-C2B-C1B	2.52	128.87	125.04
2	F	401	HEM	CBD-CAD-C3D	2.51	119.61	112.63
2	E	401	HEM	C2B-C1B-NB	2.46	112.75	109.84
2	D	401	HEM	CMD-C2D-C1D	2.45	128.76	125.04
2	A	401	HEM	CMB-C2B-C3B	-2.42	122.39	128.30
2	F	401	HEM	CMA-C3A-C2A	2.39	129.44	124.94
2	A	401	HEM	O2A-CGA-O1A	2.38	129.24	123.30
2	A	401	HEM	CHC-C4B-NB	2.35	126.99	124.43
2	A	401	HEM	CHB-C1B-NB	2.35	127.28	124.38
2	E	401	HEM	O2A-CGA-CBA	-2.35	106.49	114.03
2	B	401	HEM	CAA-CBA-CGA	-2.32	107.25	113.76
2	D	401	HEM	CHD-C1D-ND	-2.32	121.92	124.43
2	C	401	HEM	C4B-C3B-C2B	2.31	108.95	107.11
2	E	401	HEM	CMD-C2D-C1D	2.30	128.54	125.04
2	F	401	HEM	O2A-CGA-O1A	2.29	129.01	123.30
2	A	401	HEM	O1A-CGA-CBA	-2.29	115.72	123.08
2	F	401	HEM	CAA-CBA-CGA	-2.29	107.34	113.76
2	C	401	HEM	CMB-C2B-C3B	2.26	133.83	128.30
2	E	401	HEM	CAD-C3D-C2D	2.24	132.06	127.88
2	F	401	HEM	C4D-C3D-C2D	-2.24	103.63	106.90
2	D	401	HEM	CBA-CAA-C2A	-2.24	108.80	112.62
2	B	401	HEM	CAB-C3B-C2B	-2.22	121.30	128.60
2	B	401	HEM	CMB-C2B-C1B	2.19	128.38	125.04
2	B	401	HEM	C4D-C3D-C2D	-2.19	103.71	106.90
2	D	401	HEM	C1B-NB-C4B	2.18	107.33	105.07
2	D	401	HEM	CAA-C2A-C3A	-2.18	120.98	127.25
2	E	401	HEM	CHD-C1D-ND	-2.17	122.08	124.43
2	B	401	HEM	CBB-CAB-C3B	-2.16	116.89	127.62
2	F	401	HEM	C1D-C2D-C3D	-2.13	104.71	106.96
2	D	401	HEM	CBB-CAB-C3B	-2.06	117.35	127.62
2	F	401	HEM	O2A-CGA-CBA	2.05	120.63	114.03
2	E	401	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
2	B	401	HEM	CHD-C1D-C2D	-2.02	121.82	124.98
2	F	401	HEM	C3C-C4C-NC	-2.01	107.15	110.94

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	HEM	C4D-C3D-CAD-CBD
2	C	401	HEM	C2D-C3D-CAD-CBD
2	E	401	HEM	C4D-C3D-CAD-CBD
2	E	401	HEM	C2D-C3D-CAD-CBD
2	F	401	HEM	C4D-C3D-CAD-CBD
2	A	401	HEM	C4D-C3D-CAD-CBD
2	F	401	HEM	C2D-C3D-CAD-CBD
2	B	401	HEM	C2D-C3D-CAD-CBD
2	B	401	HEM	C4D-C3D-CAD-CBD
2	F	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	C4D-C3D-CAD-CBD
2	E	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAD-CBD-CGD-O2D
2	E	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	F	401	HEM	CAA-CBA-CGA-O1A
2	E	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	C2D-C3D-CAD-CBD
2	E	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAD-CBD-CGD-O1D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	C4B-C3B-CAB-CBB
2	B	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	1	0
2	D	401	HEM	4	0

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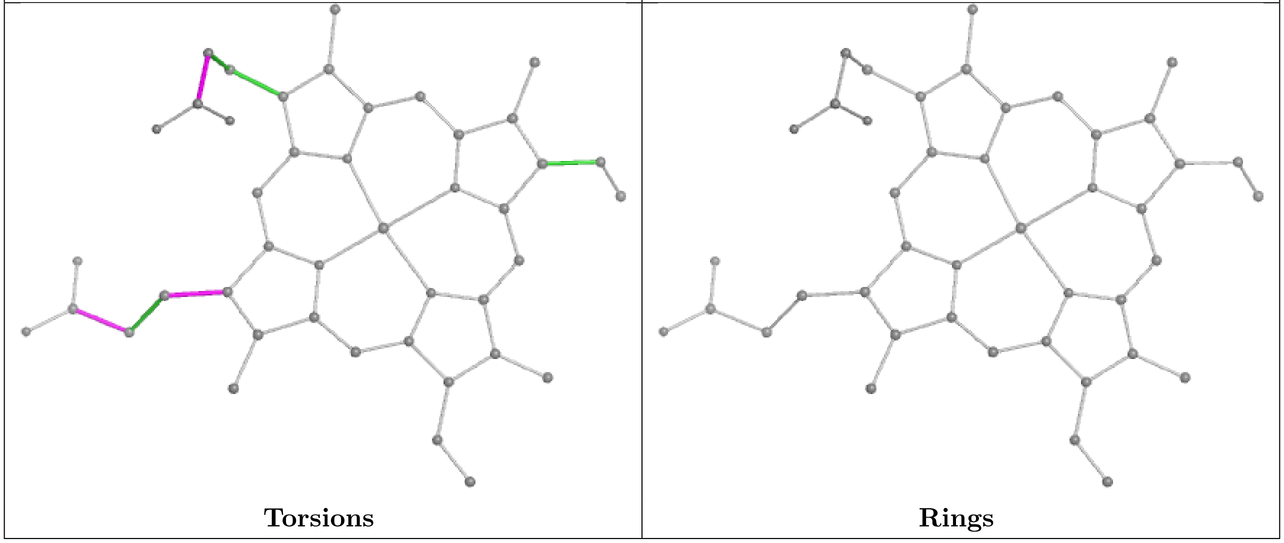
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	HEM	2	0
2	E	401	HEM	2	0
2	A	401	HEM	2	0
2	F	401	HEM	3	0

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 then 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 B 401

Bond lengths

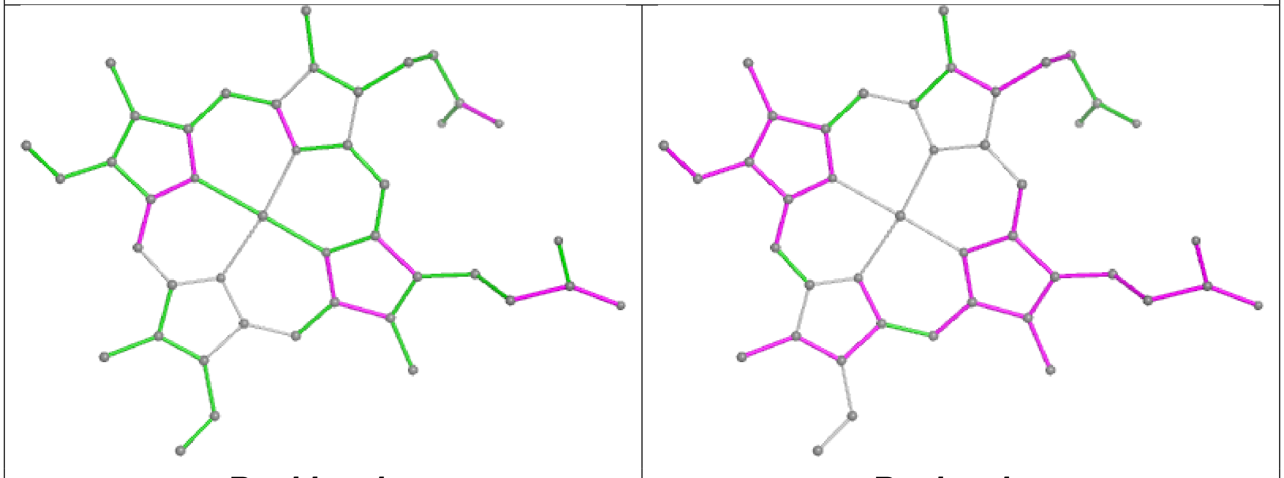
Bond angles



Torsions

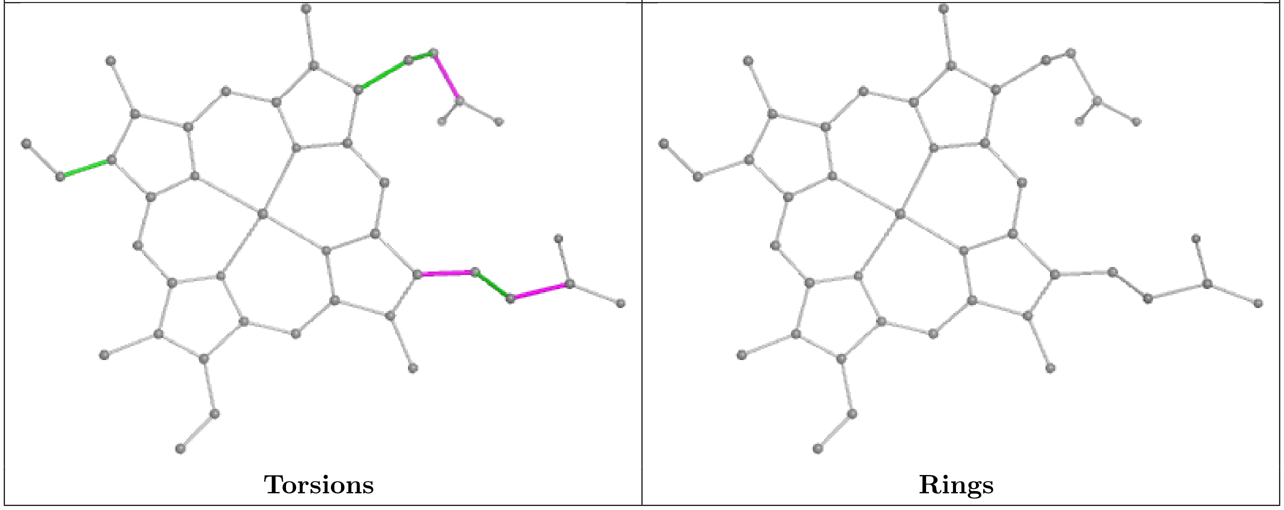
Rings

Ligand HEM D 401



Bond lengths

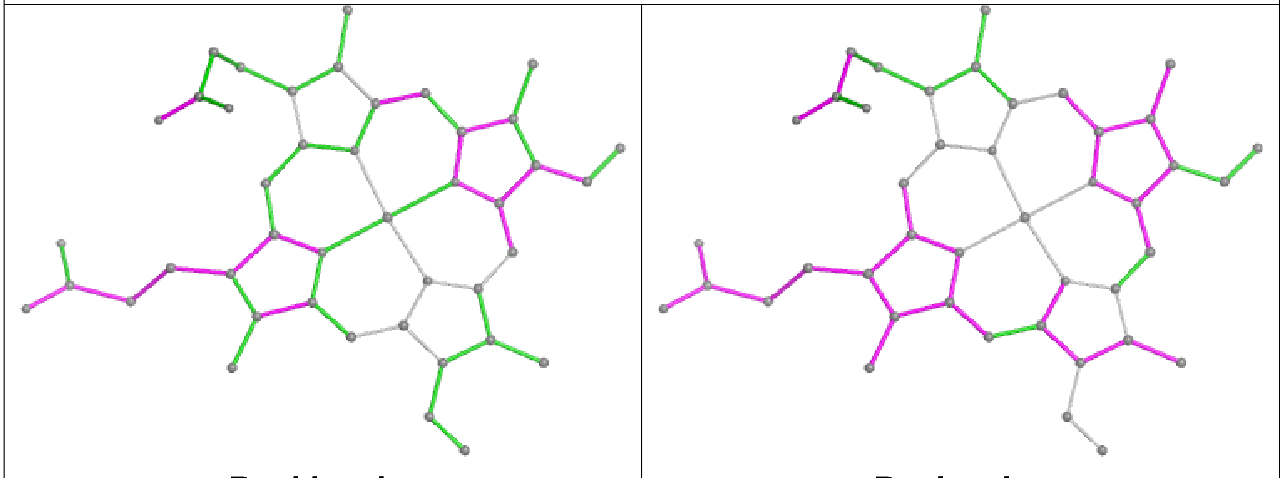
Bond angles



Torsions

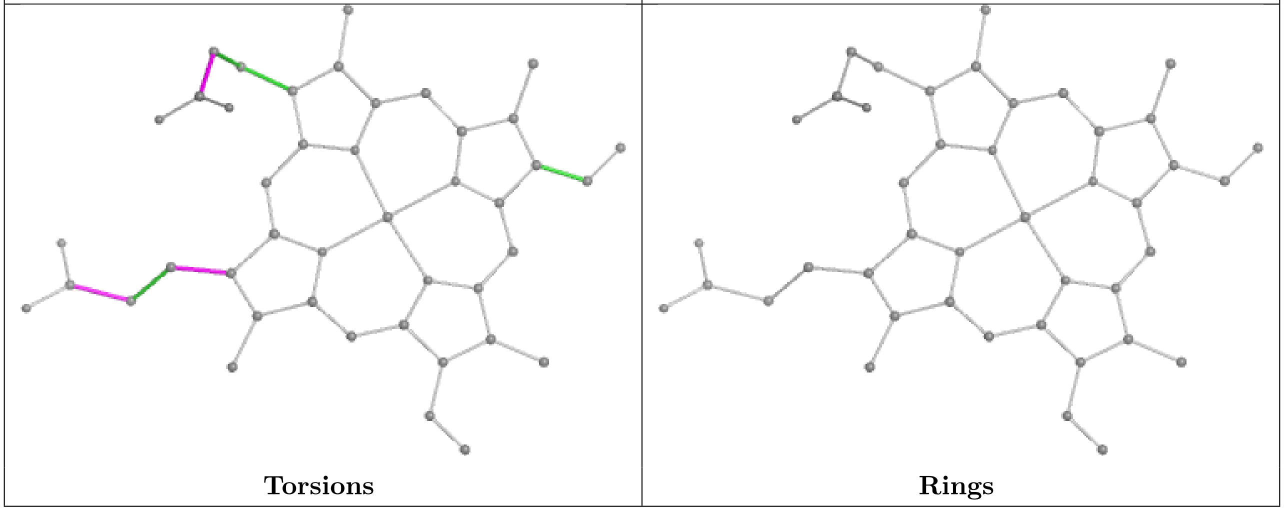
Rings

Ligand HEM C 401



Bond lengths

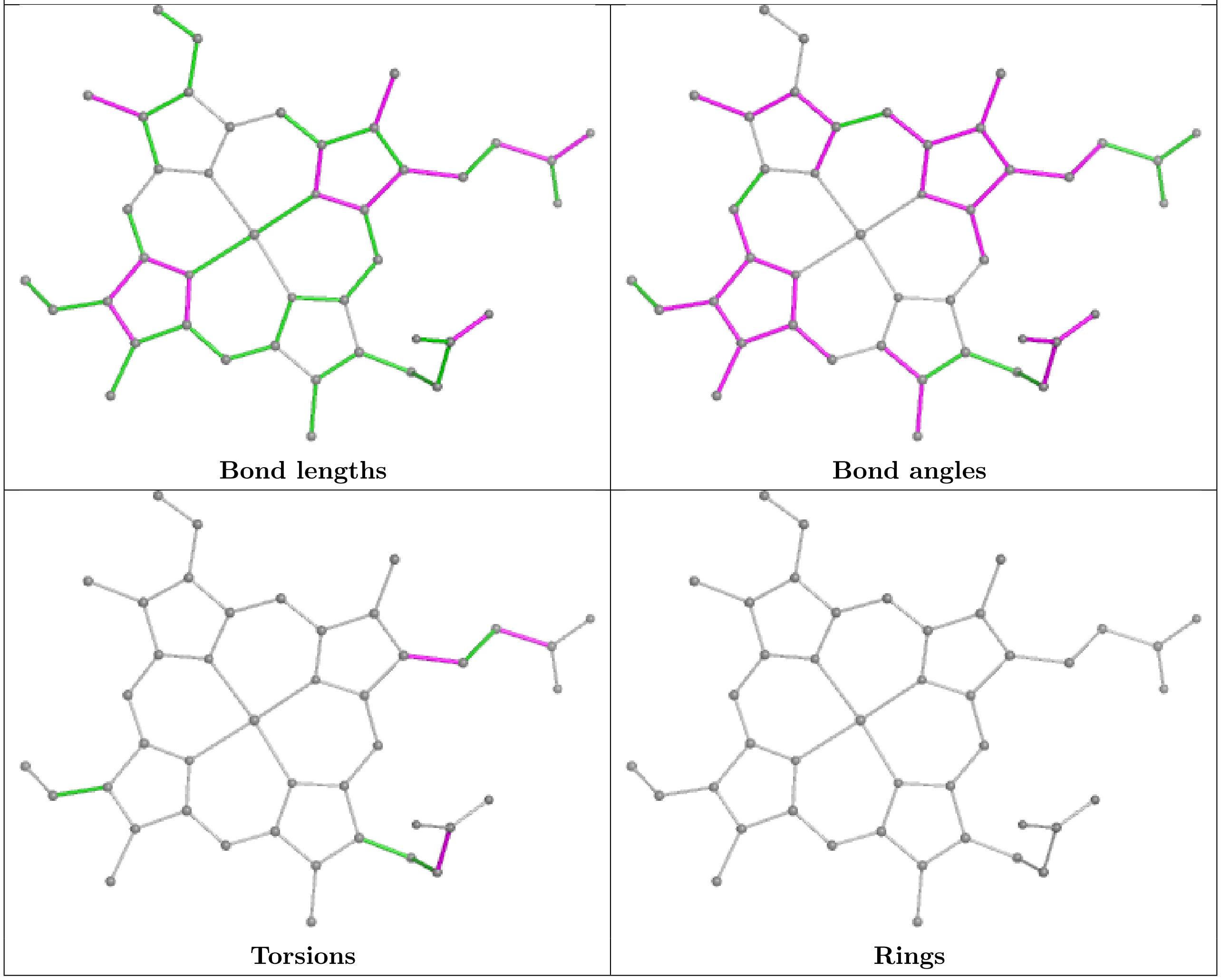
Bond angles



Torsions

Rings

Ligand HEM E 401



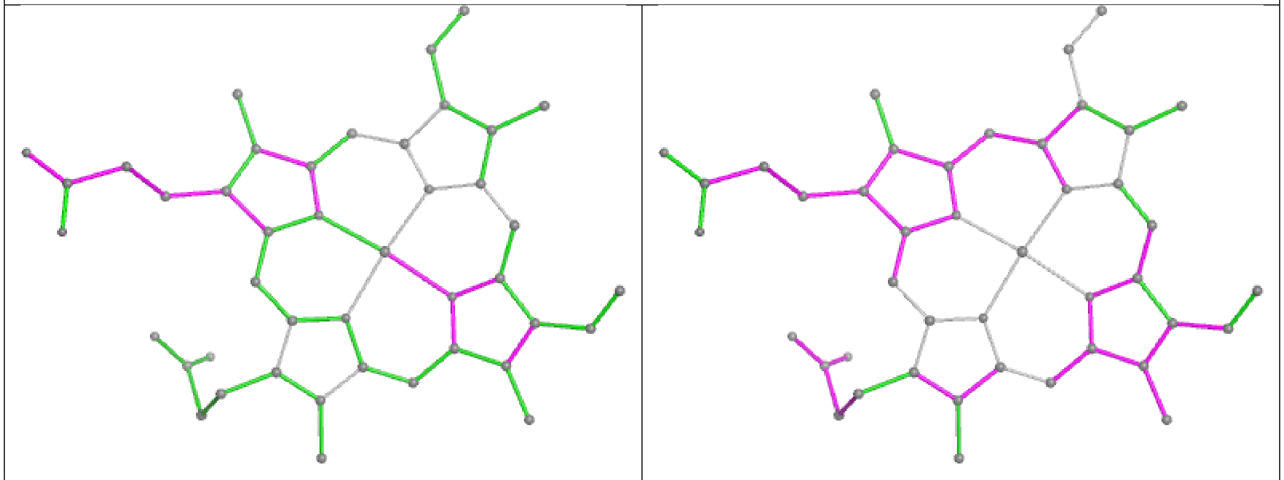
Bond lengths

Bond angles

Torsions

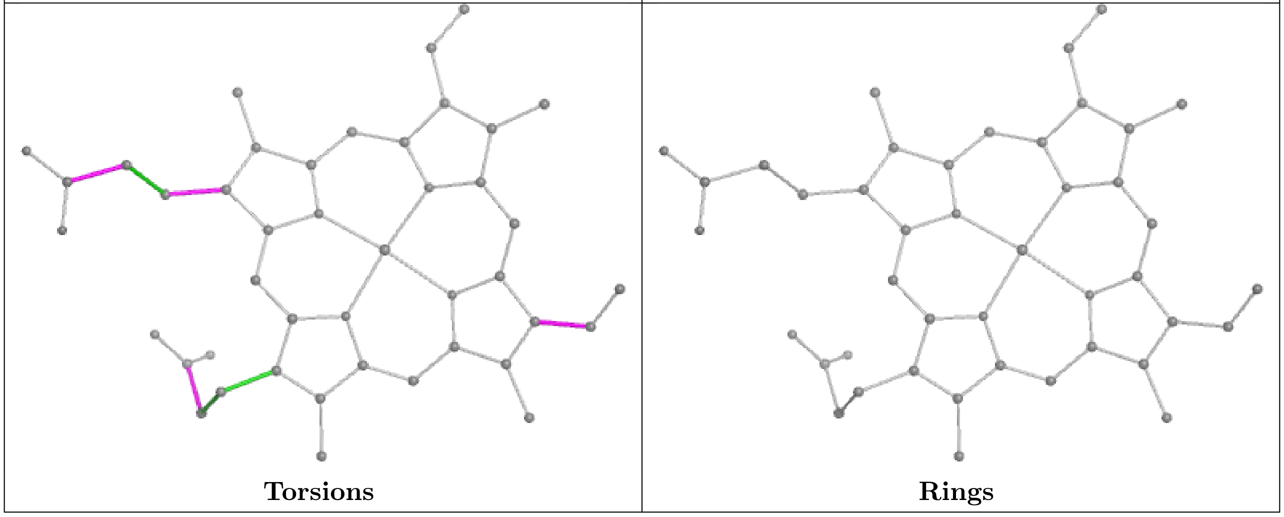
Rings

Ligand HEM A 401



Bond lengths

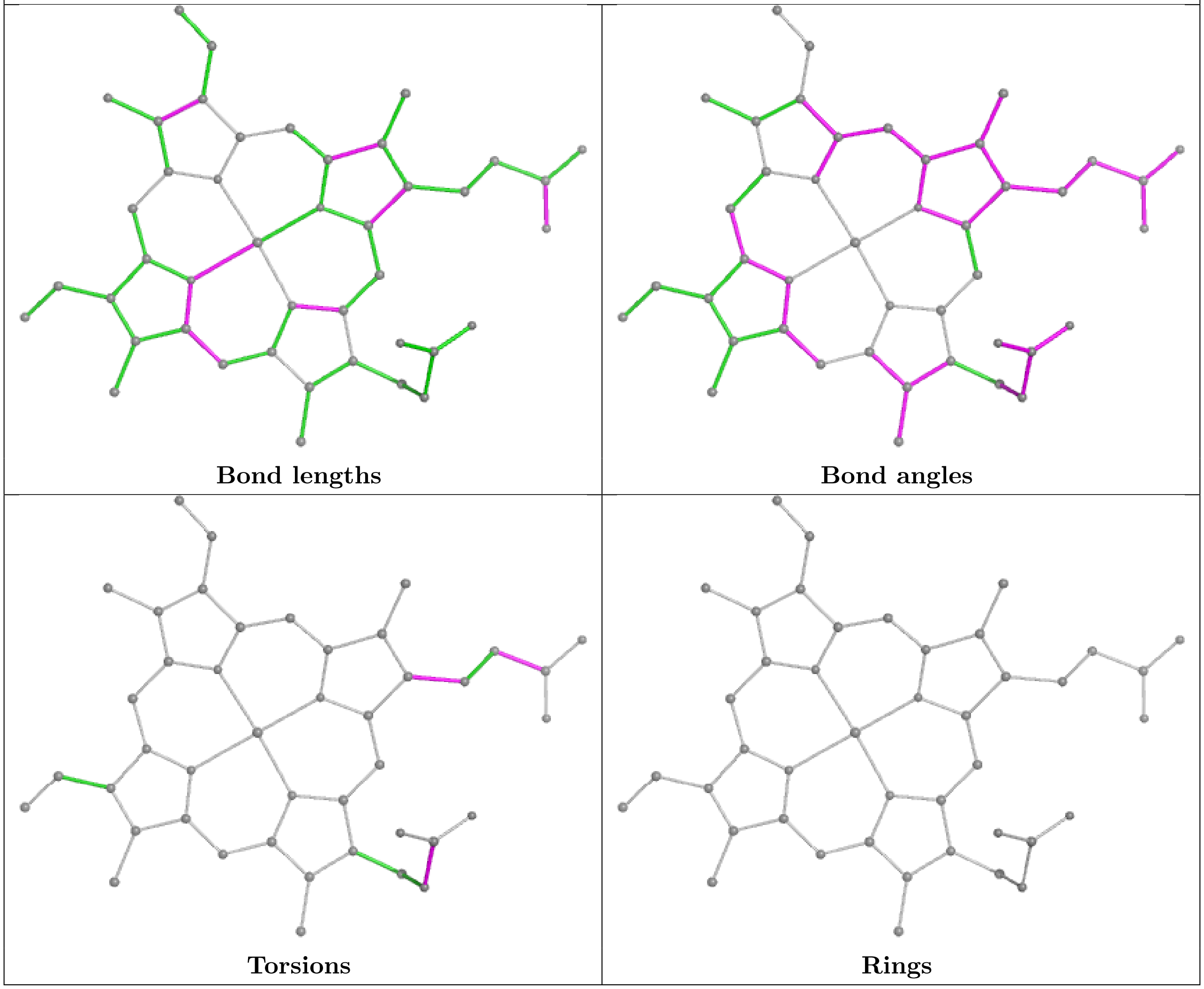
Bond angles



Torsions

Rings

Ligand HEM F 401



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	305/313 (97%)	-1.39	0	100	100	26, 50, 80, 102	0
1	B	305/313 (97%)	-1.32	0	100	100	33, 62, 93, 118	0
1	C	306/313 (97%)	-1.37	0	100	100	26, 56, 90, 125	0
1	D	306/313 (97%)	-1.33	0	100	100	29, 51, 89, 115	0
1	E	306/313 (97%)	-1.33	0	100	100	35, 55, 93, 130	0
1	F	305/313 (97%)	-1.42	0	100	100	32, 54, 83, 122	0
All	All	1833/1878 (97%)	-1.36	0	100	100	26, 55, 90, 130	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	HEM	A	401	43/43	0.99	0.04	40,53,59,70	0

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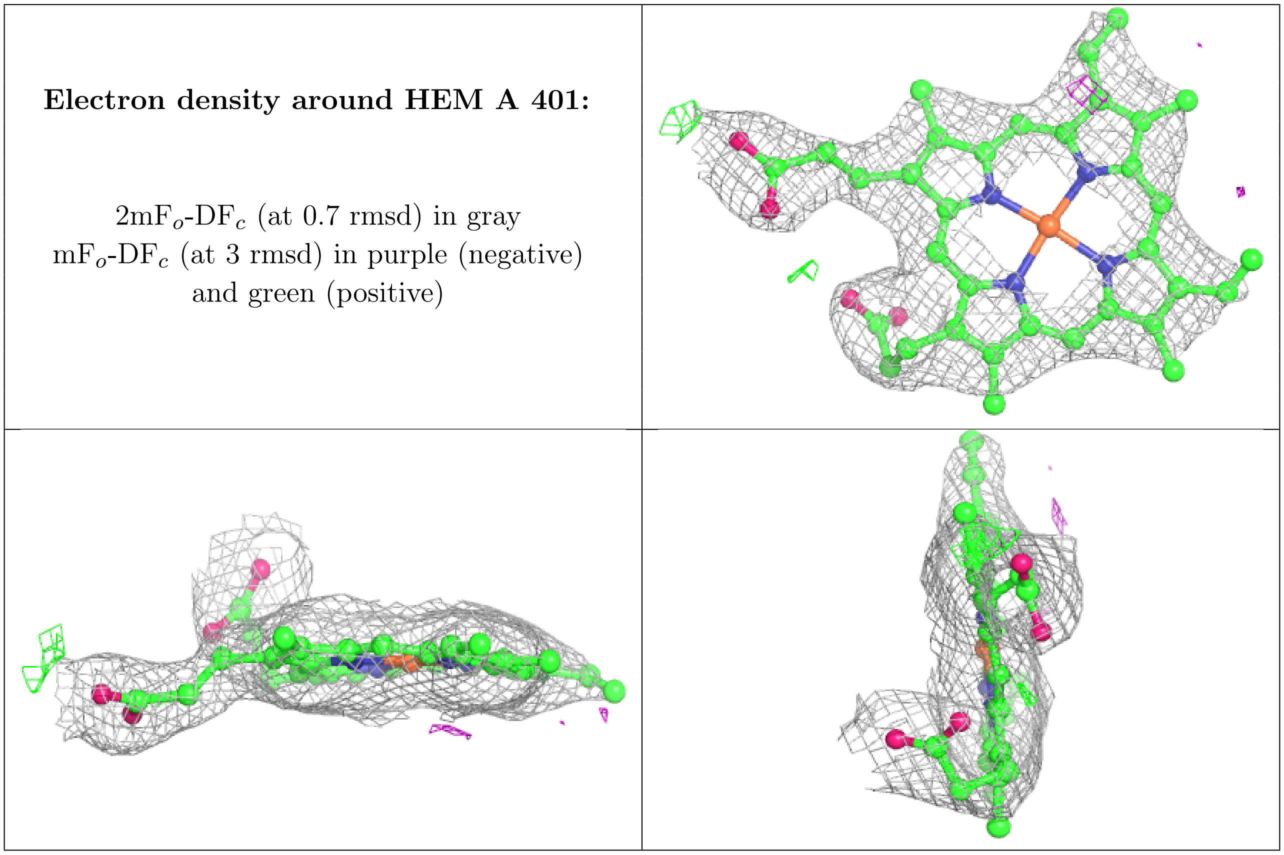
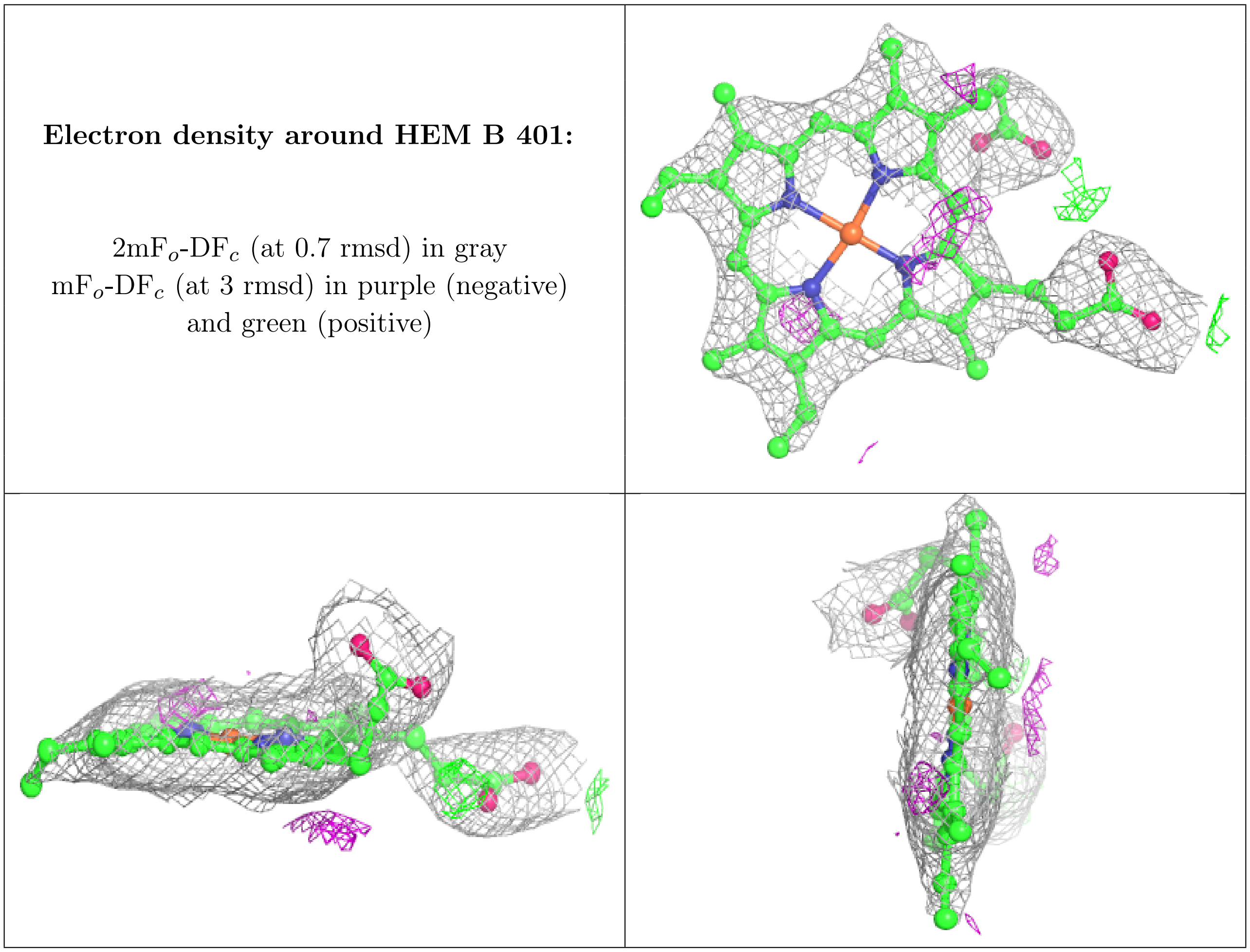
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	HEM	B	401	43/43	0.99	0.04	33,46,58,70	0
2	HEM	C	401	43/43	0.99	0.05	31,52,63,73	0
2	HEM	D	401	43/43	0.99	0.04	29,42,50,54	0
2	HEM	E	401	43/43	0.99	0.04	32,44,55,61	0
2	HEM	F	401	43/43	0.99	0.04	30,41,58,68	0

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 A 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

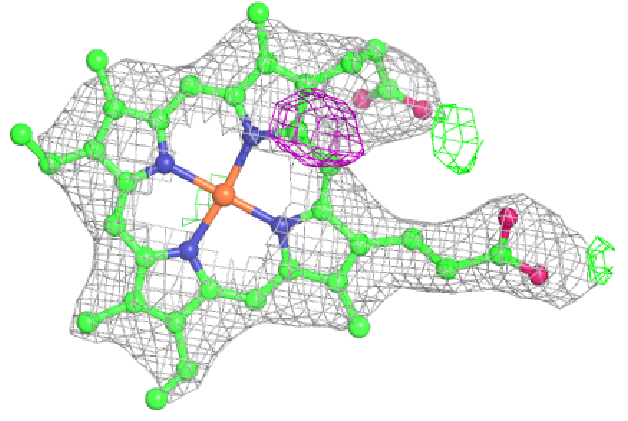


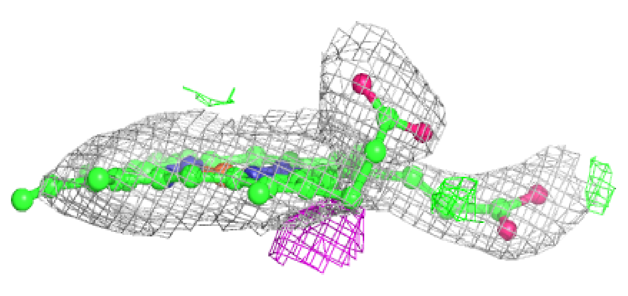
Electron density around HEM B 401:

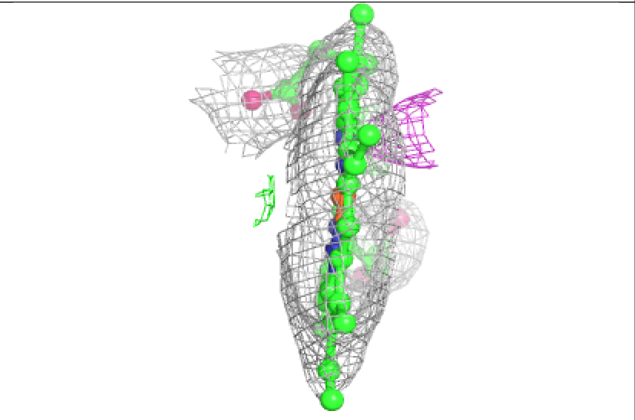
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM 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)

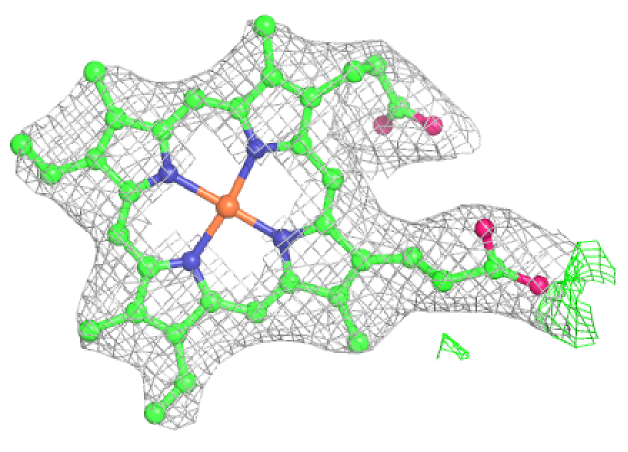


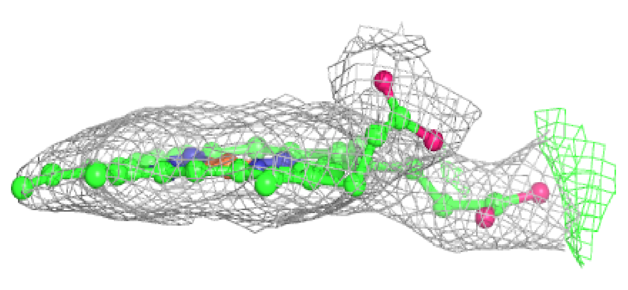


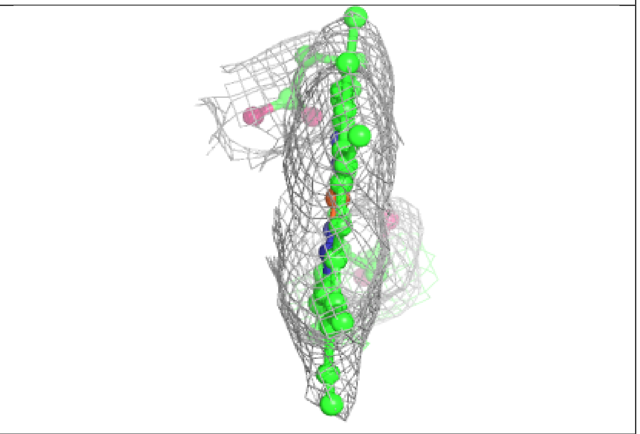


Electron density around HEM D 401:

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

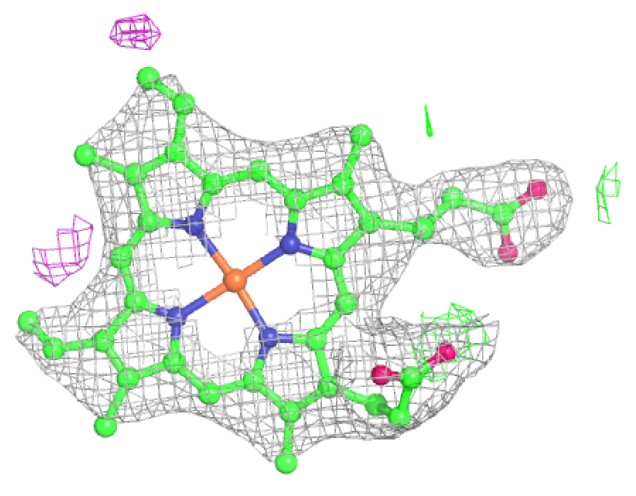


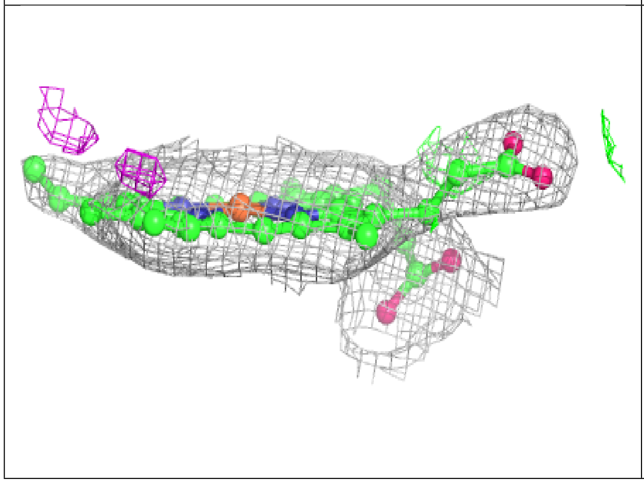


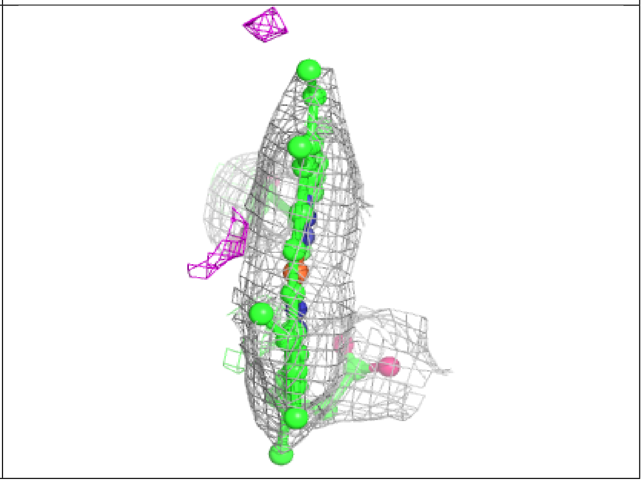


Electron density around HEM E 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

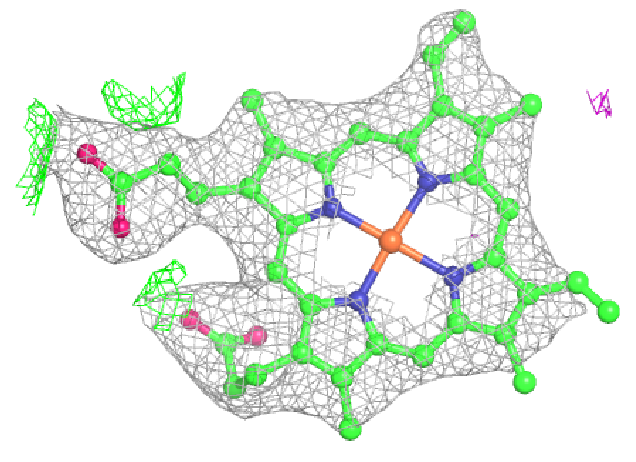


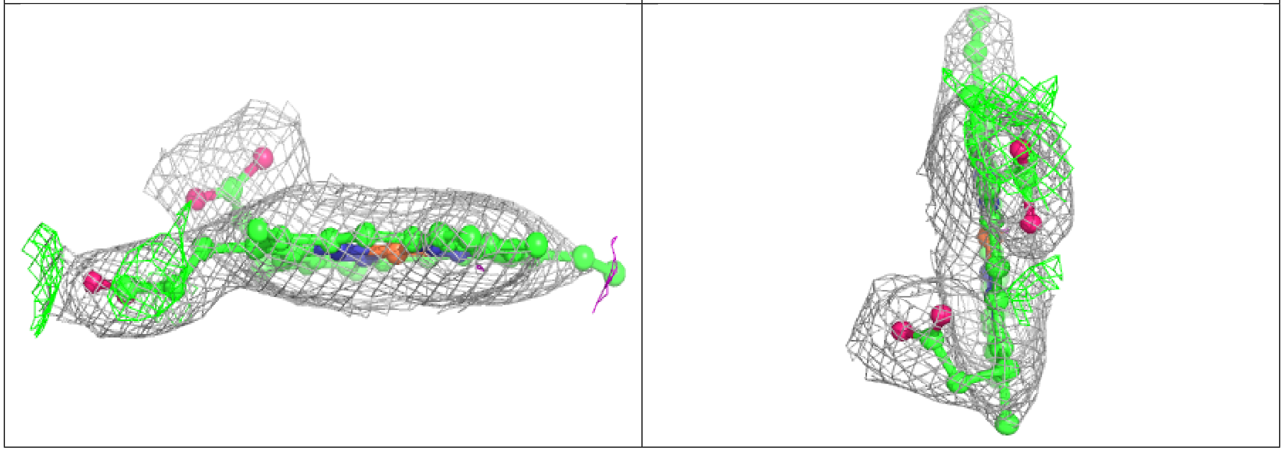




Electron density around HEM F 401:

$2mF_o$-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 ⓘ

There are no such residues in this entry.