



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:41 PM UTC

PDB ID : 7QZG / pdb_00007qzg
Title : SFX structure of dye-type peroxidase DtpB N245A variant in the ferric state
Authors : Lucic, M.; Worrall, J.A.R.; Hough, M.A.; Shilova, A.; Axford, D.A.; Owen, R.L.; Tosha, T.; Sugimoto, H.; Owada, S.
Deposited on : 2022-01-31
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

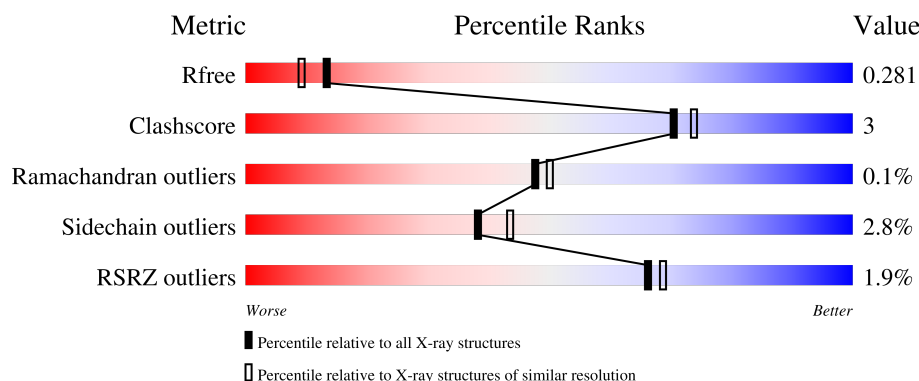
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



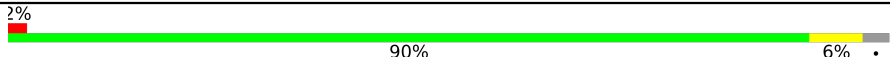
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	316	0% 86% 9% ..
1	B	316	3% 87% 9% ..
1	C	316	0% 89% 8% .
1	D	316	3% 83% 12% ..
1	E	316	2% 89% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	316	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '90%', and a small yellow segment at the end labeled '6%'. A small black dot is located at the far right end of the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15073 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 Dyp-type peroxidase family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	2	0
			2348	1476	406	456	10			
1	B	306	Total	C	N	O	S	0	1	0
			2326	1465	399	453	9			
1	C	306	Total	C	N	O	S	0	4	0
			2355	1481	407	458	9			
1	D	304	Total	C	N	O	S	0	3	0
			2333	1468	402	454	9			
1	E	305	Total	C	N	O	S	0	2	0
			2324	1466	404	445	9			
1	F	306	Total	C	N	O	S	0	2	0
			2334	1470	402	452	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
B	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
C	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
D	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
E	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09
F	245	ALA	ASN	engineered mutation	UNP A0A7U8UU09

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



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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	144	Total O 144 144	0	0

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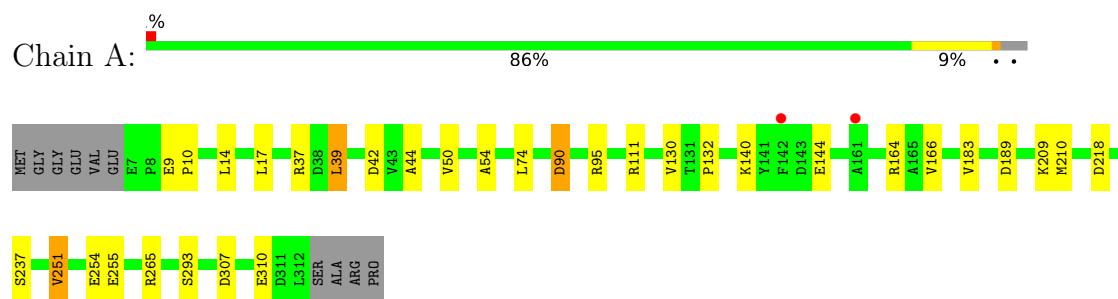
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	123	Total 123	O 123	0	0
4	C	126	Total 126	O 126	0	0
4	D	130	Total 130	O 130	0	0
4	E	143	Total 143	O 143	0	0
4	F	127	Total 127	O 127	0	0

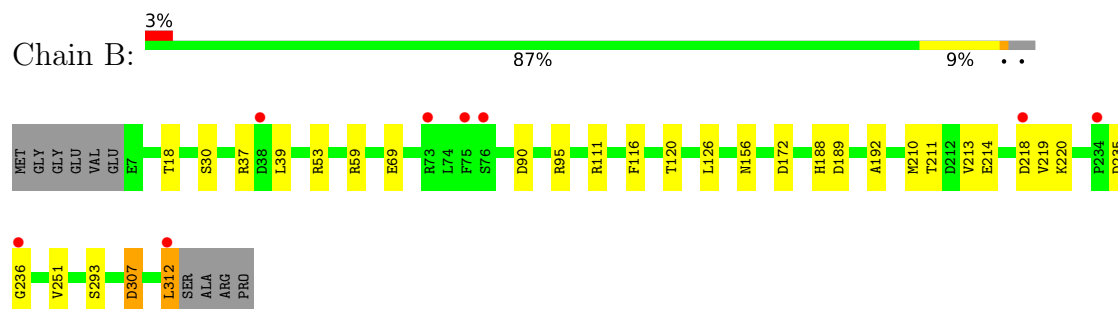
3 Residue-property plots

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.

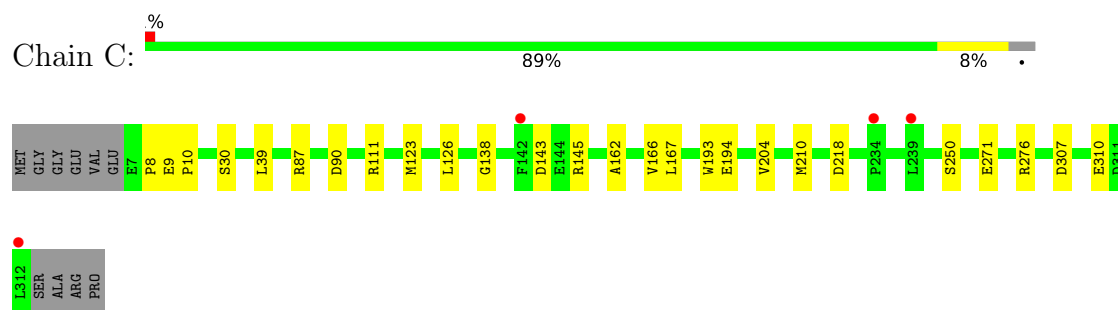
- Molecule 1: Dyp-type peroxidase family



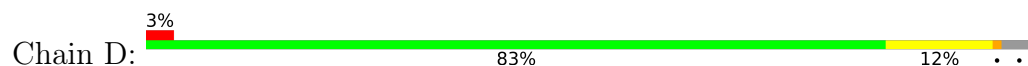
- Molecule 1: Dyp-type peroxidase family

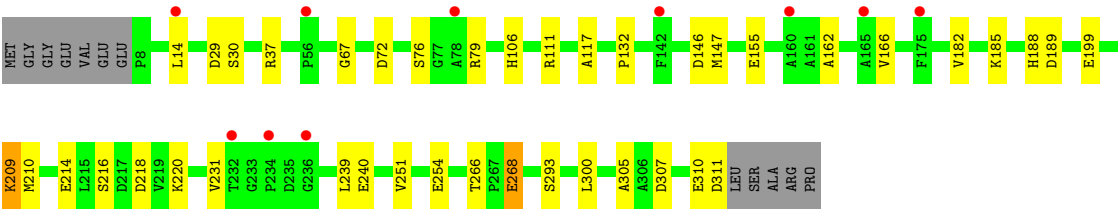


- Molecule 1: Dyp-type peroxidase family

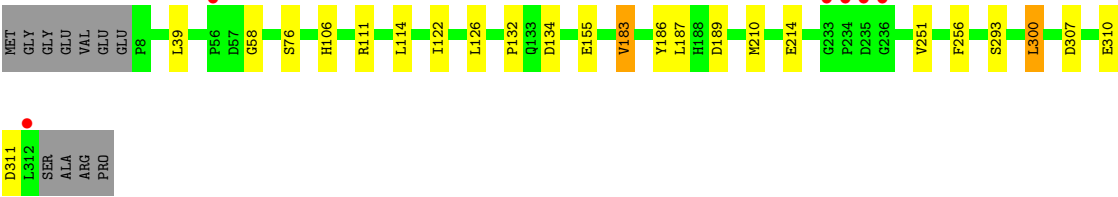
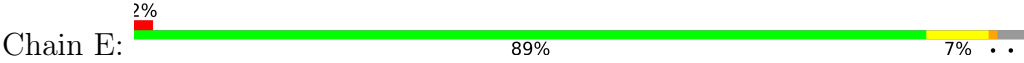


- Molecule 1: Dyp-type peroxidase family

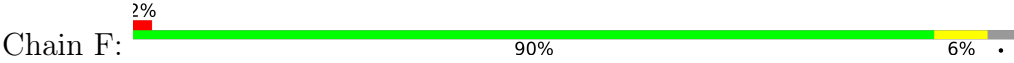




● Molecule 1: Dyp-type peroxidase family



● Molecule 1: Dyp-type peroxidase family



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.95Å 121.83Å 199.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.10 – 2.10 32.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.10-2.10) 99.9 (32.10-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.229 , 0.278 0.236 , 0.281	Depositor DCC
R_{free} test set	6248 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15073	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1.32	6/2398 (0.3%)	1.44	5/3256 (0.2%)
1	B	1.28	3/2376 (0.1%)	1.43	6/3230 (0.2%)
1	C	1.28	3/2405 (0.1%)	1.45	5/3269 (0.2%)
1	D	1.33	7/2383 (0.3%)	1.41	3/3237 (0.1%)
1	E	1.31	6/2374 (0.3%)	1.42	1/3225 (0.0%)
1	F	1.28	1/2384 (0.0%)	1.43	4/3238 (0.1%)
All	All	1.30	26/14320 (0.2%)	1.43	24/19455 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	106	HIS	CE1-NE2	10.03	1.42	1.32
1	D	132	PRO	C-O	-7.59	1.14	1.23
1	E	132	PRO	C-O	-7.30	1.15	1.23
1	D	188	HIS	C-O	6.64	1.31	1.23
1	B	192	ALA	C-O	6.47	1.31	1.24
1	F	72	ASP	C-O	-6.16	1.17	1.24
1	E	189	ASP	C-O	6.08	1.31	1.23
1	D	189	ASP	C-O	5.98	1.30	1.23
1	E	300	LEU	C-O	5.96	1.31	1.24
1	D	305	ALA	C-O	5.93	1.31	1.23
1	E	106	HIS	C-O	5.85	1.31	1.23
1	C	10	PRO	C-O	-5.78	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	HIS	CE1-NE2	5.69	1.38	1.32
1	A	255	GLU	C-O	5.58	1.30	1.24
1	A	54	ALA	C-O	-5.40	1.16	1.24
1	C	138	GLY	C-O	5.37	1.31	1.23
1	C	8	PRO	C-O	-5.32	1.18	1.23
1	E	256	PHE	C-O	-5.26	1.18	1.24
1	A	10	PRO	C-O	-5.25	1.17	1.23
1	E	214	GLU	C-O	-5.25	1.17	1.23
1	B	30	SER	C-O	5.17	1.30	1.23
1	D	67	GLY	C-O	5.15	1.30	1.23
1	A	183	VAL	C-O	5.13	1.29	1.24
1	A	132	PRO	C-O	-5.11	1.17	1.23
1	D	199	GLU	CD-OE2	5.11	1.35	1.25
1	A	130	VAL	N-CA	5.07	1.51	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	38	ASP	CA-CB-CG	10.46	123.06	112.60
1	B	218	ASP	CA-CB-CG	6.42	119.03	112.60
1	C	310	GLU	CA-C-N	6.40	129.15	120.38
1	C	310	GLU	C-N-CA	6.40	129.15	120.38
1	A	189	ASP	CA-C-N	6.19	129.20	120.42
1	A	189	ASP	C-N-CA	6.19	129.20	120.42
1	E	183	VAL	CA-CB-CG1	6.02	120.64	110.40
1	F	9	GLU	CB-CA-C	6.01	116.70	109.85
1	F	115	CYS	N-CA-C	-5.94	104.81	111.28
1	D	37	ARG	CG-CD-NE	-5.82	99.20	112.00
1	B	307	ASP	CB-CA-C	-5.80	99.54	110.67
1	A	218	ASP	CA-CB-CG	5.67	118.27	112.60
1	C	194	GLU	CB-CG-CD	5.56	122.05	112.60
1	C	145	ARG	CB-CA-C	5.53	119.63	109.46
1	D	218	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	189	ASP	CA-C-N	5.41	127.86	120.46
1	B	189	ASP	C-N-CA	5.41	127.86	120.46
1	A	307	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	9	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	9	GLU	CB-CA-C	5.23	116.91	109.38
1	F	88	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	251	VAL	CA-C-N	5.10	125.60	119.94
1	B	251	VAL	C-N-CA	5.10	125.60	119.94
1	D	209	LYS	CA-C-O	-5.02	115.73	120.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	311	ASP	Peptide

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	2348	0	2276	16	0
1	B	2326	0	2246	20	0
1	C	2355	0	2274	16	0
1	D	2333	0	2262	24	0
1	E	2324	0	2256	14	0
1	F	2334	0	2264	12	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
2	C	43	0	30	2	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
4	A	144	0	0	5	0
4	B	123	0	0	10	0
4	C	126	0	0	5	0
4	D	130	0	0	11	0
4	E	143	0	0	6	0
4	F	127	0	0	2	0
All	All	15073	0	13758	95	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 (95) 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:B:210:MET:HB2	1:F:210[A]:MET:HE1	1.39	1.01
1:C:210:MET:HE1	1:E:210:MET:HB2	1.51	0.90
1:A:44:ALA:N	4:A:501:HOH:O	2.06	0.88
1:C:204:VAL:HG11	4:C:625:HOH:O	1.74	0.87
1:A:140:LYS:HD3	1:A:144:GLU:OE1	1.81	0.81
1:A:14:LEU:HD21	1:A:166:VAL:HG21	1.66	0.76
1:B:172:ASP:OD1	4:B:501:HOH:O	2.03	0.75
1:B:116:PHE:O	1:B:120[B]:THR:HG23	1.88	0.74
1:E:114:LEU:HD23	4:E:638:HOH:O	1.86	0.74
1:B:69:GLU:OE1	4:B:502:HOH:O	2.06	0.72
2:B:401:HEM:HMB2	2:B:401:HEM:HBB2	1.70	0.71
1:A:254:GLU:OE1	4:A:502:HOH:O	2.08	0.71
1:B:210:MET:CB	1:F:210[A]:MET:HE1	2.18	0.71
1:E:134:ASP:OD2	4:E:501:HOH:O	2.08	0.70
1:C:210:MET:HE1	1:E:210:MET:CB	2.21	0.69
1:A:42:ASP:C	4:A:501:HOH:O	2.35	0.69
1:D:117:ALA:HA	4:D:623:HOH:O	1.92	0.68
1:D:14:LEU:HD21	1:D:166[A]:VAL:HG21	1.73	0.68
1:C:250:SER:HB2	4:C:520:HOH:O	1.93	0.67
1:F:171:GLU:OE2	4:F:501:HOH:O	2.11	0.67
4:B:605:HOH:O	1:F:210[B]:MET:HE1	1.94	0.67
1:C:193:TRP:CZ3	4:C:625:HOH:O	2.48	0.65
1:D:29:ASP:OD1	4:D:501:HOH:O	2.14	0.65
1:A:209:LYS:HG2	1:A:210[B]:MET:HE2	1.80	0.64
1:A:251:VAL:O	4:A:503:HOH:O	2.15	0.63
1:D:266:THR:OG1	1:D:268:GLU:HG3	1.98	0.63
1:D:79:ARG:NH2	4:D:502:HOH:O	2.19	0.62
1:A:209:LYS:HG2	1:A:210[B]:MET:CE	2.30	0.62
2:C:401:HEM:CMC	2:C:401:HEM:HBC2	2.30	0.62
1:A:164:ARG:NH2	4:A:504:HOH:O	2.33	0.61
1:D:79:ARG:NE	4:D:502:HOH:O	2.16	0.61
1:D:147:MET:O	4:D:503:HOH:O	2.16	0.61
1:C:162:ALA:O	1:C:166[B]:VAL:HG12	2.01	0.60
1:D:251:VAL:HG12	1:F:123:MET:HG3	1.84	0.60
1:B:312:LEU:C	1:B:312:LEU:HD12	2.27	0.59
1:B:53:ARG:HB2	1:C:143[B]:ASP:OD1	2.02	0.59
1:D:231:VAL:HG23	1:D:239:LEU:HB2	1.85	0.59
1:C:39:LEU:HD22	1:C:126:LEU:HD11	1.85	0.59
2:E:401:HEM:HBC2	2:E:401:HEM:HMC2	1.85	0.59
1:B:90:ASP:OD1	1:B:95:ARG:HD2	2.02	0.59
1:B:18:THR:HA	4:B:514:HOH:O	2.02	0.58
1:C:276:ARG:NH1	4:C:509:HOH:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ASP:HB2	4:D:594:HOH:O	2.04	0.57
1:D:155:GLU:O	4:D:504:HOH:O	2.17	0.57
1:E:58:GLY:HA3	4:E:623:HOH:O	2.03	0.57
1:D:239:LEU:HA	4:D:513:HOH:O	2.05	0.56
1:F:79:ARG:NH2	1:F:83:LEU:O	2.37	0.56
1:D:182:VAL:HG22	1:D:300[B]:LEU:HD23	1.87	0.56
1:F:226:VAL:HG12	4:F:538:HOH:O	2.06	0.55
1:B:211:THR:HG23	4:B:556:HOH:O	2.07	0.55
1:E:39:LEU:HD21	1:E:122:ILE:HG23	1.88	0.55
1:B:210:MET:HB2	1:F:210[A]:MET:CE	2.26	0.55
2:B:401:HEM:HBB2	2:B:401:HEM:CMB	2.38	0.54
1:D:185:LYS:NZ	4:D:505:HOH:O	2.29	0.53
1:C:250:SER:CB	4:C:520:HOH:O	2.54	0.53
1:D:72:ASP:OD2	1:D:79:ARG:NH1	2.43	0.52
1:D:240:GLU:OE2	4:D:504:HOH:O	2.19	0.52
1:B:213:VAL:HG12	4:B:515:HOH:O	2.09	0.52
1:B:156:ASN:O	4:B:504:HOH:O	2.18	0.50
1:A:90:ASP:OD1	1:A:95:ARG:HD2	2.11	0.50
2:C:401:HEM:HBC2	2:C:401:HEM:HMC2	1.93	0.50
1:A:37:ARG:NH1	1:A:74:LEU:O	2.43	0.50
1:C:143[B]:ASP:OD1	1:C:143[B]:ASP:O	2.30	0.50
1:D:266:THR:OG1	1:D:268:GLU:CG	2.60	0.49
1:C:166[B]:VAL:HG13	1:C:167:LEU:HG	1.94	0.49
1:C:87:ARG:NH2	1:C:271:GLU:OE1	2.45	0.49
1:C:210:MET:CE	1:E:210:MET:HB2	2.32	0.49
1:A:251:VAL:CG1	1:C:123:MET:HG3	2.43	0.48
2:E:401:HEM:HBD1	4:E:519:HOH:O	2.14	0.48
1:B:213:VAL:CG1	4:B:515:HOH:O	2.60	0.47
1:D:254:GLU:OE2	1:F:127:ARG:HD2	2.15	0.47
1:B:39:LEU:HD22	1:B:126:LEU:HD11	1.96	0.46
1:B:59:ARG:NH1	4:B:514:HOH:O	2.40	0.46
1:A:210[A]:MET:HE1	1:D:209:LYS:HE2	1.98	0.45
1:B:120[B]:THR:HG22	1:E:251:VAL:HG12	1.98	0.45
1:D:214:GLU:OE2	1:D:220:LYS:NZ	2.40	0.45
1:B:37:ARG:O	1:B:312:LEU:HD11	2.16	0.45
1:E:186:TYR:C	1:E:187:LEU:HD12	2.42	0.45
1:A:50:VAL:HA	4:E:610:HOH:O	2.17	0.44
1:E:39:LEU:HD22	1:E:126:LEU:HG	1.99	0.44
1:F:88:GLU:HG3	1:F:96:ALA:O	2.18	0.44
1:A:209:LYS:CG	1:A:210[B]:MET:CE	2.96	0.44
1:C:210:MET:HE1	1:E:210:MET:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLU:OE2	1:B:220:LYS:NZ	2.38	0.43
1:E:155:GLU:O	4:E:502:HOH:O	2.21	0.42
1:A:39:LEU:HD22	1:A:39:LEU:O	2.20	0.42
1:D:72:ASP:CG	1:D:79:ARG:HH11	2.27	0.41
1:E:187:LEU:HD12	1:E:187:LEU:N	2.35	0.41
1:E:300:LEU:C	1:E:300:LEU:HD23	2.45	0.41
4:B:605:HOH:O	1:F:210[B]:MET:CE	2.63	0.41
1:F:300:LEU:HD23	1:F:301:PHE:N	2.36	0.41
1:D:162:ALA:O	1:D:166[A]:VAL:HG22	2.21	0.40
1:D:14:LEU:HD21	1:D:166[A]:VAL:CG2	2.46	0.40
1:B:213:VAL:HG21	4:D:506:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/316 (97%)	302 (99%)	4 (1%)	0	100	100
1	B	305/316 (96%)	297 (97%)	6 (2%)	2 (1%)	18	15
1	C	308/316 (98%)	303 (98%)	5 (2%)	0	100	100
1	D	305/316 (96%)	301 (99%)	4 (1%)	0	100	100
1	E	305/316 (96%)	300 (98%)	5 (2%)	0	100	100
1	F	306/316 (97%)	301 (98%)	5 (2%)	0	100	100
All	All	1835/1896 (97%)	1804 (98%)	29 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	GLY
1	B	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	246/251 (98%)	236 (96%)	10 (4%)	27	29
1	B	242/251 (96%)	237 (98%)	5 (2%)	47	54
1	C	246/251 (98%)	241 (98%)	5 (2%)	48	56
1	D	245/251 (98%)	235 (96%)	10 (4%)	27	29
1	E	240/251 (96%)	234 (98%)	6 (2%)	42	48
1	F	244/251 (97%)	238 (98%)	6 (2%)	42	48
All	All	1463/1506 (97%)	1421 (97%)	42 (3%)	38	42

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	39	LEU
1	A	90	ASP
1	A	111	ARG
1	A	237	SER
1	A	251	VAL
1	A	265[A]	ARG
1	A	265[B]	ARG
1	A	293	SER
1	A	310	GLU
1	B	111	ARG
1	B	219	VAL
1	B	293	SER
1	B	307	ASP
1	B	312	LEU
1	C	30	SER
1	C	90	ASP
1	C	111	ARG
1	C	218	ASP
1	C	307	ASP
1	D	30	SER
1	D	76	SER

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Mol	Chain	Res	Type
1	D	111	ARG
1	D	210	MET
1	D	216	SER
1	D	268	GLU
1	D	293	SER
1	D	307	ASP
1	D	310	GLU
1	D	311	ASP
1	E	76	SER
1	E	111	ARG
1	E	183	VAL
1	E	293	SER
1	E	307	ASP
1	E	310	GLU
1	F	57	ASP
1	F	87	ARG
1	F	111	ARG
1	F	254	GLU
1	F	307	ASP
1	F	313	SER

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

Mol	Chain	Res	Type
1	C	55	GLN

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

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	B	401	1	50,50,50	1.90	12 (24%)	67,82,82	2.02	22 (32%)
2	HEM	C	401	1	50,50,50	2.25	19 (38%)	67,82,82	1.83	16 (23%)
2	HEM	A	401	1	50,50,50	1.56	10 (20%)	67,82,82	2.21	24 (35%)
2	HEM	D	401	1	50,50,50	2.10	13 (26%)	67,82,82	2.07	23 (34%)
2	HEM	F	401	1	50,50,50	1.98	13 (26%)	67,82,82	2.17	20 (29%)
2	HEM	E	401	1	50,50,50	1.96	17 (34%)	67,82,82	2.10	26 (38%)

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	-	4/14/54/54	-
2	HEM	C	401	1	-	4/14/54/54	-
2	HEM	A	401	1	-	6/14/54/54	-
2	HEM	D	401	1	-	4/14/54/54	-
2	HEM	F	401	1	-	4/14/54/54	-
2	HEM	E	401	1	-	5/14/54/54	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	HEM	C1C-NC	-6.00	1.28	1.39
2	D	401	HEM	FE-NB	5.75	2.12	1.94
2	D	401	HEM	C1A-C2A	-5.55	1.33	1.44
2	A	401	HEM	FE-NB	5.46	2.11	1.94
2	C	401	HEM	C3B-C4B	5.26	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C4C-NC	-5.08	1.30	1.39
2	F	401	HEM	C1B-NB	-4.98	1.31	1.40
2	F	401	HEM	CHC-C1C	-4.97	1.28	1.38
2	C	401	HEM	C1B-NB	-4.94	1.31	1.40
2	D	401	HEM	FE-NC	4.83	2.11	1.95
2	B	401	HEM	FE-NC	4.55	2.10	1.95
2	C	401	HEM	FE-NC	4.29	2.09	1.95
2	C	401	HEM	C4D-ND	-4.15	1.33	1.40
2	B	401	HEM	C4A-NA	-4.04	1.32	1.39
2	D	401	HEM	C1B-NB	-3.94	1.33	1.40
2	E	401	HEM	FE-NB	3.92	2.07	1.94
2	E	401	HEM	FE-NC	3.90	2.08	1.95
2	A	401	HEM	FE-NC	3.87	2.07	1.95
2	C	401	HEM	C3B-C2B	-3.87	1.29	1.37
2	B	401	HEM	C4D-ND	-3.76	1.33	1.40
2	B	401	HEM	C1B-NB	-3.74	1.33	1.40
2	E	401	HEM	C1B-NB	-3.68	1.33	1.40
2	E	401	HEM	C4D-C3D	3.66	1.51	1.45
2	D	401	HEM	C1D-C2D	3.64	1.51	1.44
2	F	401	HEM	O1D-CGD	3.63	1.33	1.22
2	D	401	HEM	CHC-C1C	3.62	1.45	1.38
2	C	401	HEM	O1A-CGA	3.58	1.33	1.22
2	E	401	HEM	C1C-C2C	-3.57	1.38	1.45
2	C	401	HEM	O1D-CGD	3.55	1.33	1.22
2	E	401	HEM	O1A-CGA	3.51	1.33	1.22
2	C	401	HEM	C4B-NB	-3.50	1.32	1.38
2	F	401	HEM	FE-NC	3.47	2.06	1.95
2	C	401	HEM	CMC-C2C	3.33	1.57	1.50
2	E	401	HEM	C1D-C2D	3.32	1.51	1.44
2	F	401	HEM	C1D-ND	-3.21	1.32	1.38
2	D	401	HEM	CHB-C1B	3.20	1.44	1.38
2	C	401	HEM	C3C-C4C	-3.13	1.40	1.46
2	E	401	HEM	C3D-C2D	-3.09	1.30	1.36
2	E	401	HEM	C1A-NA	-3.04	1.33	1.39
2	E	401	HEM	C3B-C4B	2.96	1.50	1.44
2	C	401	HEM	CBD-CAD	2.96	1.62	1.51
2	A	401	HEM	C3B-C4B	2.89	1.50	1.44
2	B	401	HEM	CAC-C3C	2.89	1.55	1.47
2	E	401	HEM	C3C-C4C	-2.84	1.41	1.46
2	C	401	HEM	C4A-NA	-2.80	1.34	1.39
2	B	401	HEM	C3C-C4C	2.78	1.50	1.46
2	F	401	HEM	C4C-NC	-2.75	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEM	C3C-C4C	-2.69	1.41	1.46
2	B	401	HEM	FE-NB	2.68	2.03	1.94
2	B	401	HEM	CMD-C2D	2.67	1.56	1.50
2	E	401	HEM	FE-NA	2.59	2.03	1.95
2	F	401	HEM	CBD-CGD	2.54	1.56	1.50
2	D	401	HEM	O1A-CGA	2.52	1.30	1.22
2	E	401	HEM	CBD-CGD	2.51	1.56	1.50
2	A	401	HEM	CHC-C1C	2.49	1.43	1.38
2	D	401	HEM	CMB-C2B	2.49	1.55	1.50
2	F	401	HEM	CBA-CGA	-2.44	1.44	1.50
2	C	401	HEM	FE-NB	2.44	2.02	1.94
2	F	401	HEM	CMC-C2C	-2.41	1.45	1.50
2	C	401	HEM	CMB-C2B	2.41	1.55	1.50
2	E	401	HEM	CHB-C4A	-2.40	1.34	1.39
2	D	401	HEM	C1C-NC	-2.38	1.35	1.39
2	C	401	HEM	C1B-C2B	2.37	1.49	1.44
2	F	401	HEM	FE-NA	2.32	2.02	1.95
2	F	401	HEM	CMD-C2D	2.25	1.55	1.50
2	E	401	HEM	C1A-C2A	2.22	1.49	1.44
2	C	401	HEM	C4D-C3D	2.21	1.48	1.45
2	C	401	HEM	CBD-CGD	2.21	1.55	1.50
2	A	401	HEM	C1A-C2A	-2.21	1.40	1.44
2	C	401	HEM	CBA-CGA	2.17	1.55	1.50
2	B	401	HEM	C4B-NB	-2.16	1.34	1.38
2	A	401	HEM	O2D-CGD	-2.15	1.23	1.30
2	A	401	HEM	CMB-C2B	2.15	1.55	1.50
2	E	401	HEM	CHA-C4D	2.13	1.42	1.38
2	B	401	HEM	O2D-CGD	-2.11	1.23	1.30
2	F	401	HEM	FE-ND	-2.09	1.88	1.94
2	A	401	HEM	C4A-C3A	-2.09	1.38	1.43
2	D	401	HEM	CHD-C1D	-2.08	1.34	1.39
2	B	401	HEM	O1A-CGA	2.05	1.28	1.22
2	A	401	HEM	C4B-NB	-2.05	1.34	1.38
2	A	401	HEM	C1B-NB	-2.03	1.36	1.40
2	C	401	HEM	C2A-C3A	-2.02	1.33	1.38
2	E	401	HEM	CHC-C1C	2.01	1.42	1.38
2	D	401	HEM	O2D-CGD	-2.01	1.24	1.30

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	CHC-C4B-NB	9.15	134.27	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	CHC-C4B-NB	5.78	130.65	124.42
2	C	401	HEM	CHD-C1D-ND	5.54	130.39	124.42
2	A	401	HEM	CMB-C2B-C1B	5.21	133.18	125.03
2	A	401	HEM	CMD-C2D-C1D	5.10	133.00	125.03
2	A	401	HEM	O2A-CGA-CBA	5.06	130.00	114.00
2	E	401	HEM	CHD-C4C-NC	4.97	129.86	124.45
2	A	401	HEM	O2D-CGD-CBD	4.53	128.33	114.00
2	B	401	HEM	C1A-CHA-C4D	-4.44	115.80	126.25
2	F	401	HEM	CHB-C1B-NB	4.44	129.86	124.37
2	E	401	HEM	C1B-NB-C4B	4.39	110.40	105.21
2	C	401	HEM	C4C-CHD-C1D	-4.24	117.00	126.02
2	F	401	HEM	C1B-NB-C4B	4.22	110.20	105.21
2	D	401	HEM	CHD-C1D-ND	4.21	128.95	124.42
2	E	401	HEM	CHB-C1B-NB	4.21	129.57	124.37
2	C	401	HEM	CHD-C1D-C2D	-4.15	118.47	125.03
2	D	401	HEM	C3C-C2C-C1C	4.13	110.95	107.05
2	D	401	HEM	CHC-C4B-NB	4.11	128.85	124.42
2	C	401	HEM	CAD-C3D-C4D	4.11	131.86	124.70
2	F	401	HEM	C4A-CHB-C1B	-4.04	116.76	126.25
2	F	401	HEM	C4C-C3C-C2C	-4.01	103.34	106.81
2	D	401	HEM	CHD-C1D-C2D	-3.97	118.76	125.03
2	B	401	HEM	CHD-C1D-C2D	-3.96	118.78	125.03
2	E	401	HEM	CHD-C1D-ND	3.95	128.67	124.42
2	A	401	HEM	CHD-C4C-NC	3.94	128.75	124.45
2	E	401	HEM	C4C-CHD-C1D	-3.89	117.75	126.02
2	C	401	HEM	CMD-C2D-C1D	3.86	131.07	125.03
2	F	401	HEM	C3B-C2B-C1B	3.86	109.31	106.41
2	D	401	HEM	C1B-NB-C4B	3.85	109.77	105.21
2	E	401	HEM	O2D-CGD-CBD	3.84	126.15	114.00
2	A	401	HEM	CHA-C1A-NA	3.81	130.77	123.86
2	E	401	HEM	CHD-C1D-C2D	-3.80	119.03	125.03
2	A	401	HEM	C2A-C1A-NA	-3.79	105.94	110.15
2	A	401	HEM	O2A-CGA-O1A	-3.78	113.60	123.33
2	B	401	HEM	CHC-C1C-NC	-3.65	120.48	124.45
2	D	401	HEM	CMD-C2D-C1D	3.59	130.64	125.03
2	A	401	HEM	CMB-C2B-C3B	-3.52	119.90	128.43
2	F	401	HEM	CHC-C4B-C3B	-3.48	118.12	125.07
2	B	401	HEM	O1A-CGA-CBA	-3.42	112.26	123.09
2	A	401	HEM	CAD-C3D-C4D	3.39	130.61	124.70
2	A	401	HEM	CAB-C3B-C2B	-3.39	117.42	128.43
2	B	401	HEM	CHA-C4D-ND	3.37	128.54	124.37
2	A	401	HEM	CAA-CBA-CGA	-3.37	104.74	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	C4C-C3C-C2C	-3.36	103.90	106.81
2	A	401	HEM	O2D-CGD-O1D	-3.33	114.77	123.33
2	B	401	HEM	C1D-C2D-C3D	-3.30	103.51	106.98
2	D	401	HEM	CMB-C2B-C1B	-3.27	119.93	125.03
2	E	401	HEM	O2D-CGD-O1D	-3.26	114.96	123.33
2	B	401	HEM	C1B-NB-C4B	3.25	109.06	105.21
2	B	401	HEM	C2D-C1D-ND	3.21	113.61	109.90
2	D	401	HEM	CHA-C4D-ND	3.21	128.34	124.37
2	F	401	HEM	CHD-C4C-NC	3.21	127.95	124.45
2	A	401	HEM	C1A-CHA-C4D	-3.18	118.76	126.25
2	E	401	HEM	CAB-C3B-C2B	-3.18	118.09	128.43
2	E	401	HEM	CAA-C2A-C1A	3.17	131.12	124.94
2	D	401	HEM	CHA-C4D-C3D	-3.16	119.40	125.23
2	D	401	HEM	CHB-C1B-NB	3.13	128.24	124.37
2	E	401	HEM	CMA-C3A-C4A	3.06	130.08	125.42
2	C	401	HEM	C4C-C3C-C2C	3.03	109.44	106.81
2	B	401	HEM	C3C-C2C-C1C	-3.03	104.18	107.05
2	B	401	HEM	CAA-CBA-CGA	-3.02	105.65	113.67
2	E	401	HEM	C3B-C4B-NB	-3.00	107.31	109.47
2	F	401	HEM	C4B-C3B-C2B	-2.96	104.56	107.28
2	C	401	HEM	CHA-C4D-ND	2.93	128.00	124.37
2	E	401	HEM	CHA-C4D-ND	2.92	127.98	124.37
2	D	401	HEM	C4A-C3A-C2A	2.91	110.15	106.82
2	B	401	HEM	CMB-C2B-C1B	2.88	129.53	125.03
2	C	401	HEM	CAD-C3D-C2D	-2.87	122.49	127.87
2	C	401	HEM	C2B-C1B-NB	2.85	113.12	109.84
2	B	401	HEM	CHD-C1D-ND	2.85	127.48	124.42
2	E	401	HEM	C1A-CHA-C4D	-2.83	119.60	126.25
2	B	401	HEM	O2A-CGA-CBA	2.76	122.73	114.00
2	B	401	HEM	CMD-C2D-C1D	2.74	129.32	125.03
2	C	401	HEM	CHA-C4D-C3D	-2.74	120.18	125.23
2	D	401	HEM	CHD-C4C-NC	2.72	127.42	124.45
2	E	401	HEM	C4B-C3B-C2B	-2.72	104.78	107.28
2	D	401	HEM	C4C-CHD-C1D	-2.69	120.31	126.02
2	D	401	HEM	CMC-C2C-C1C	-2.68	120.02	124.73
2	F	401	HEM	C3B-C4B-NB	-2.65	107.56	109.47
2	C	401	HEM	CHC-C4B-NB	2.65	127.27	124.42
2	E	401	HEM	CAB-C3B-C4B	2.65	136.08	124.39
2	F	401	HEM	CHC-C1C-NC	-2.62	121.60	124.45
2	B	401	HEM	CHA-C1A-NA	2.56	128.51	123.86
2	A	401	HEM	CAB-C3B-C4B	2.55	135.65	124.39
2	E	401	HEM	CHC-C4B-NB	2.52	127.13	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	CHA-C1A-NA	2.50	128.39	123.86
2	D	401	HEM	CHC-C1C-NC	2.48	127.16	124.45
2	C	401	HEM	C3B-C2B-C1B	-2.47	104.55	106.41
2	E	401	HEM	CAA-C2A-C3A	-2.46	121.56	127.07
2	F	401	HEM	C1A-CHA-C4D	-2.42	120.55	126.25
2	A	401	HEM	CAD-C3D-C2D	-2.42	123.34	127.87
2	C	401	HEM	C3C-C2C-C1C	-2.40	104.78	107.05
2	F	401	HEM	CHA-C1A-NA	2.40	128.20	123.86
2	D	401	HEM	C4C-NC-C1C	2.38	109.70	105.82
2	F	401	HEM	CHA-C4D-C3D	-2.37	120.85	125.23
2	B	401	HEM	O2D-CGD-CBD	2.37	121.49	114.00
2	E	401	HEM	C4C-NC-C1C	2.36	109.67	105.82
2	E	401	HEM	CHA-C4D-C3D	-2.35	120.89	125.23
2	C	401	HEM	C4A-C3A-C2A	2.35	109.50	106.82
2	B	401	HEM	CMB-C2B-C3B	-2.32	122.80	128.43
2	A	401	HEM	CMD-C2D-C3D	-2.32	119.86	126.15
2	A	401	HEM	CHA-C4D-C3D	-2.30	120.99	125.23
2	D	401	HEM	C1D-C2D-C3D	-2.29	104.58	106.98
2	C	401	HEM	CHB-C1B-C2B	-2.26	120.52	126.95
2	B	401	HEM	C2C-C1C-NC	2.25	113.81	109.64
2	A	401	HEM	C4C-NC-C1C	2.22	109.45	105.82
2	F	401	HEM	CMB-C2B-C3B	-2.22	123.05	128.43
2	A	401	HEM	CHA-C4D-ND	2.22	127.12	124.37
2	F	401	HEM	CHB-C4A-NA	2.22	127.89	123.86
2	D	401	HEM	CAC-C3C-C2C	2.19	135.56	128.43
2	B	401	HEM	CHC-C4B-C3B	-2.18	120.71	125.07
2	F	401	HEM	CHA-C4D-ND	2.18	127.06	124.37
2	D	401	HEM	O2A-CGA-O1A	2.18	128.93	123.33
2	A	401	HEM	CBD-CAD-C3D	-2.17	106.54	112.53
2	F	401	HEM	CHD-C4C-C3C	-2.17	121.56	125.21
2	B	401	HEM	C4A-C3A-C2A	2.14	109.27	106.82
2	D	401	HEM	CMA-C3A-C2A	-2.14	121.09	125.62
2	E	401	HEM	C3B-C2B-C1B	2.14	108.02	106.41
2	A	401	HEM	O1A-CGA-CBA	-2.13	116.33	123.09
2	D	401	HEM	C4B-C3B-C2B	-2.13	105.32	107.28
2	A	401	HEM	C4A-NA-C1A	2.12	109.28	105.82
2	E	401	HEM	CHB-C1B-C2B	-2.10	120.99	126.95
2	B	401	HEM	CHA-C1A-C2A	-2.09	120.72	125.30
2	F	401	HEM	C2D-C1D-ND	2.09	112.32	109.90
2	F	401	HEM	CAC-C3C-C2C	2.08	135.19	128.43
2	E	401	HEM	C2D-C1D-ND	2.06	112.29	109.90
2	D	401	HEM	C2C-C1C-NC	-2.06	105.83	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	CBD-CAD-C3D	-2.03	106.91	112.53
2	C	401	HEM	CMB-C2B-C3B	2.02	133.31	128.43
2	E	401	HEM	CHB-C4A-C3A	-2.01	121.58	127.43
2	A	401	HEM	CBB-CAB-C3B	-2.01	117.48	127.53

There are no chirality outliers.

All (27) torsion outliers are listed below:

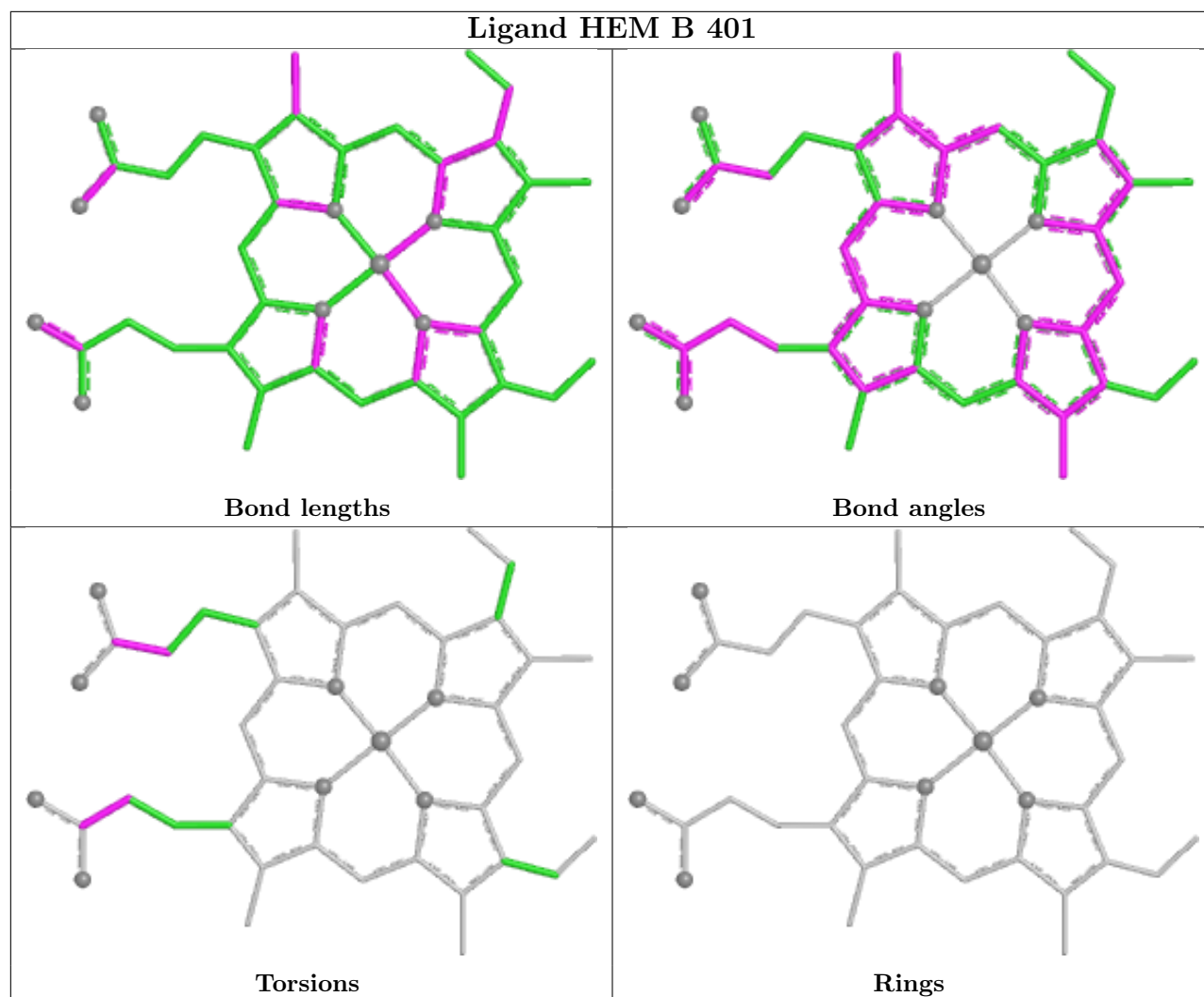
Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C4B-C3B-CAB-CBB
2	E	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAA-CBA-CGA-O2A
2	E	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAA-CBA-CGA-O1A
2	F	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAA-CBA-CGA-O1A
2	F	401	HEM	CAA-CBA-CGA-O1A
2	F	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAD-CBD-CGD-O2D
2	E	401	HEM	CAA-CBA-CGA-O1A
2	E	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A

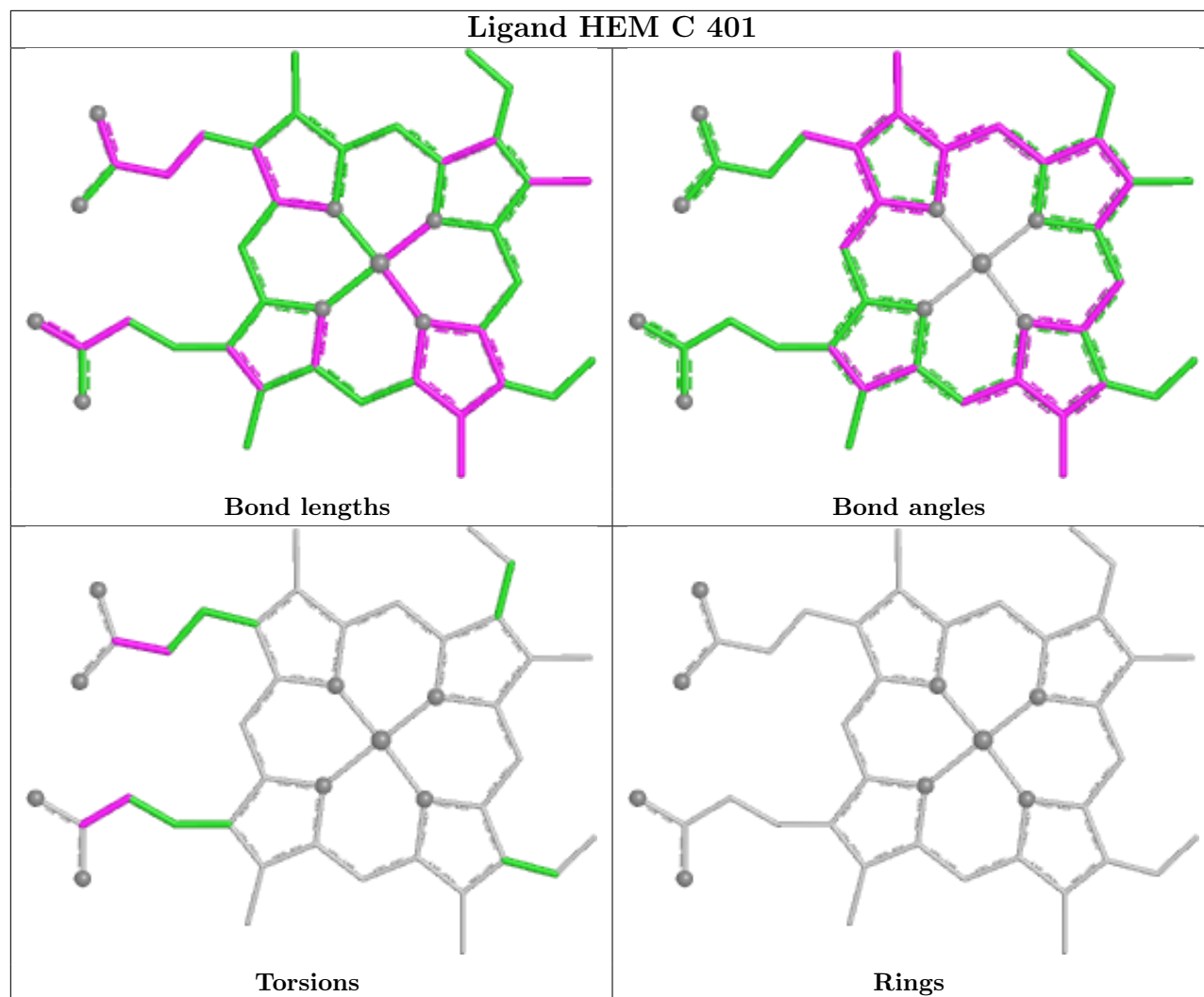
There are no ring outliers.

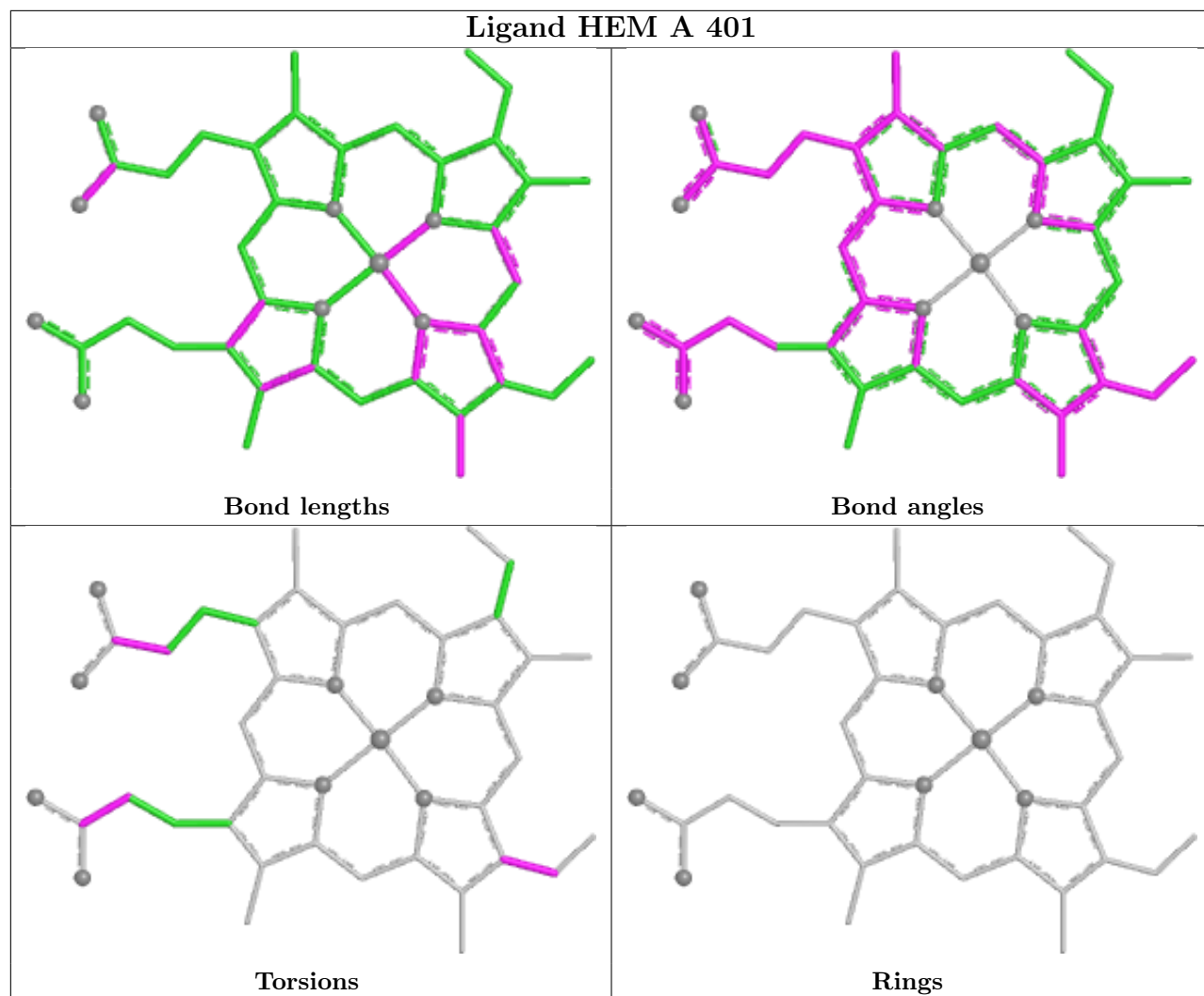
3 monomers are involved in 6 short contacts:

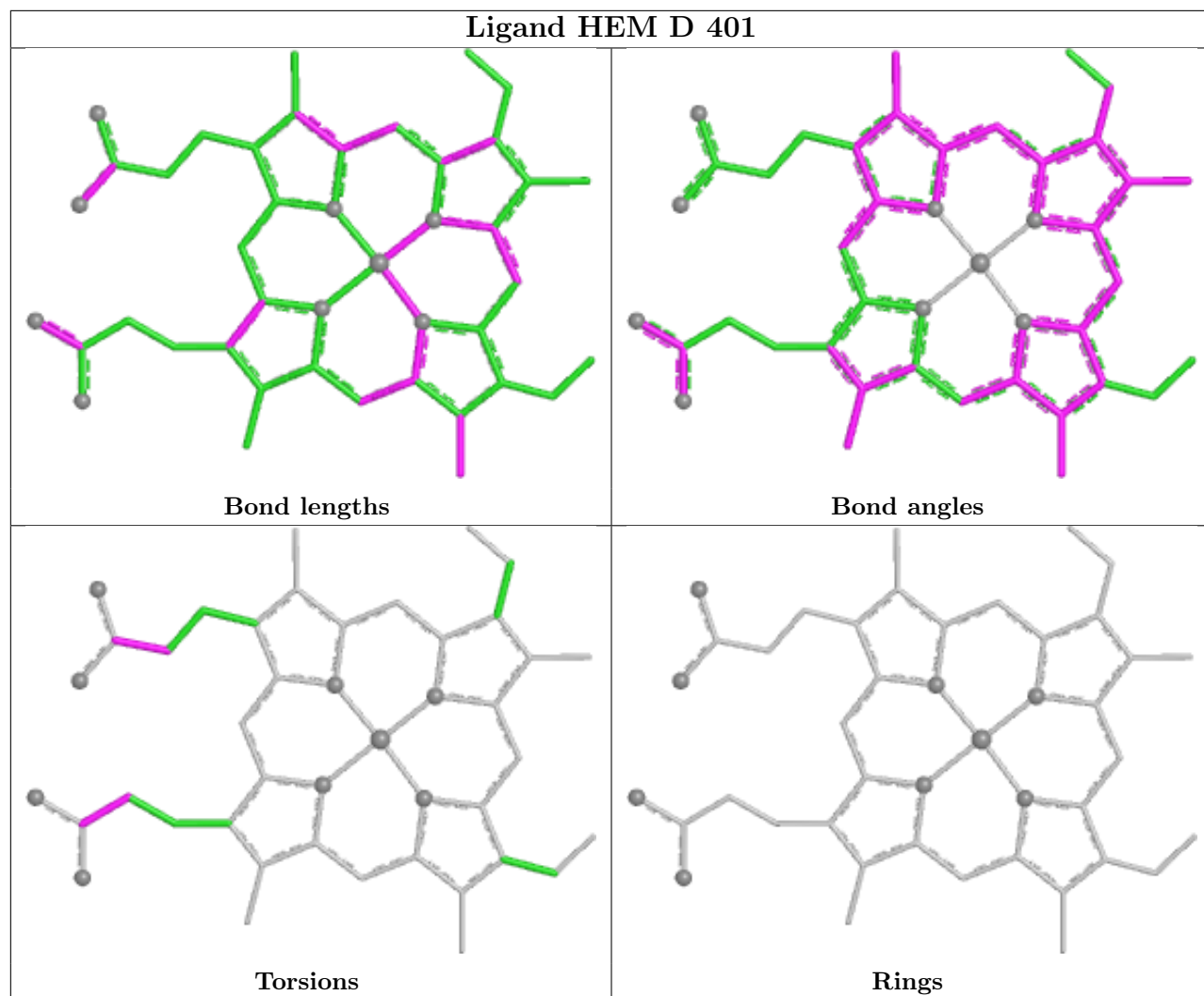
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	2	0
2	C	401	HEM	2	0
2	E	401	HEM	2	0

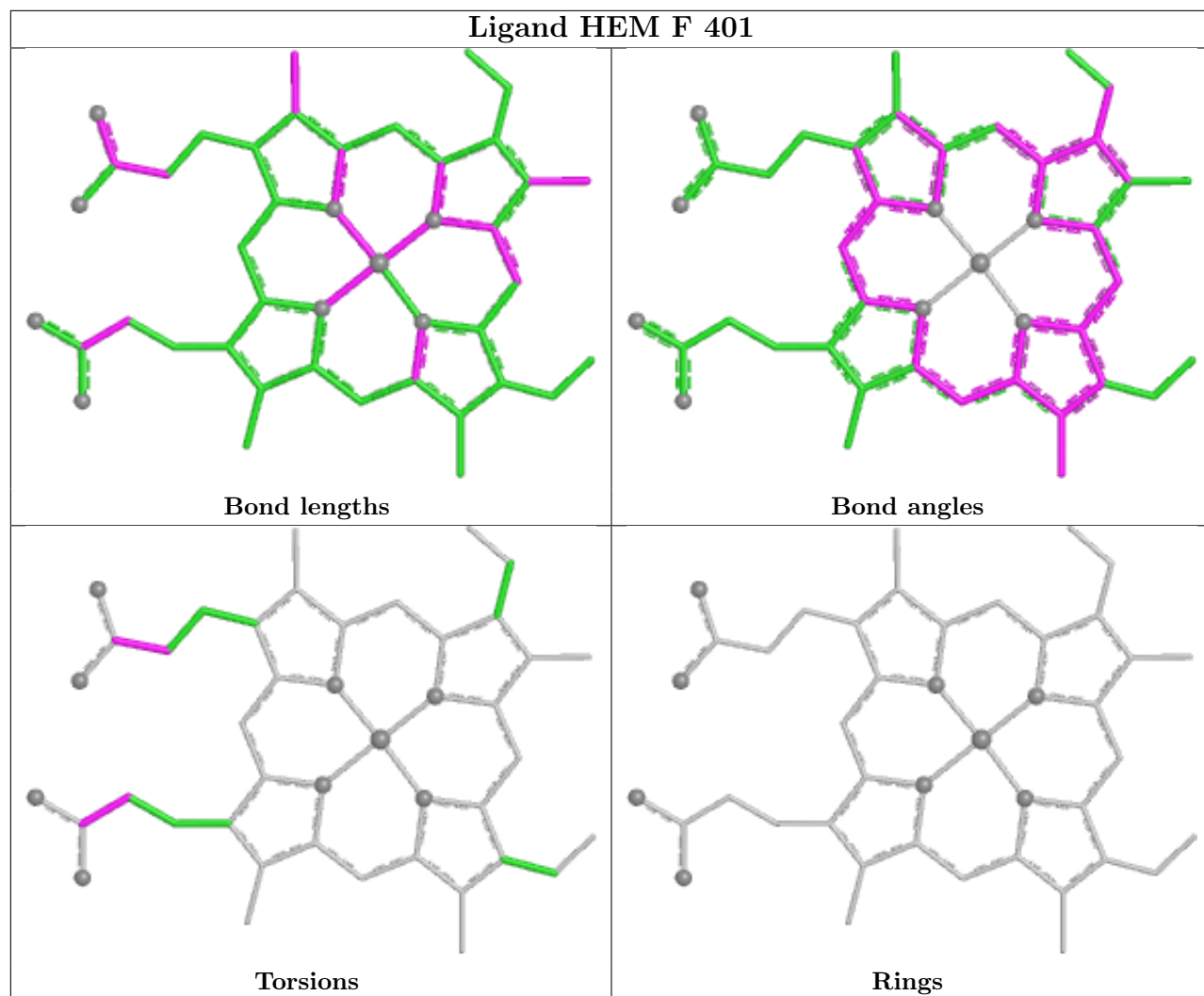
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

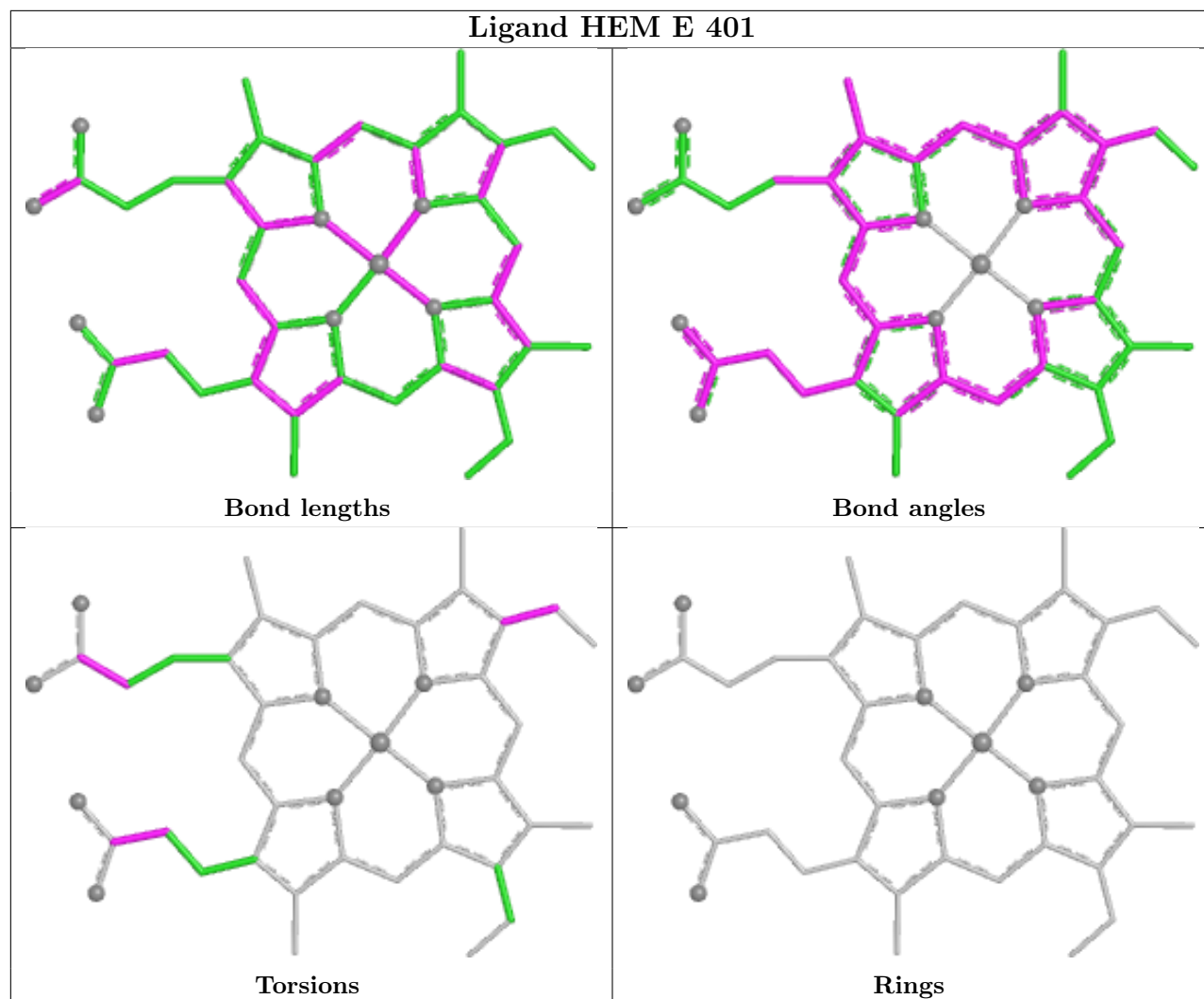












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	306/316 (96%)	0.17	2 (0%) 84 86	13, 28, 49, 68	2 (0%)
1	B	306/316 (96%)	0.34	8 (2%) 57 60	14, 31, 54, 74	1 (0%)
1	C	306/316 (96%)	0.34	4 (1%) 75 77	10, 30, 54, 74	4 (1%)
1	D	304/316 (96%)	0.26	10 (3%) 49 51	10, 29, 52, 74	3 (0%)
1	E	305/316 (96%)	0.21	6 (1%) 65 67	13, 29, 49, 94	2 (0%)
1	F	306/316 (96%)	0.18	5 (1%) 70 73	11, 29, 51, 88	2 (0%)
All	All	1833/1896 (96%)	0.25	35 (1%) 66 69	10, 29, 52, 94	14 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	LEU	4.2
1	F	234	PRO	4.1
1	C	312	LEU	3.4
1	E	234	PRO	3.3
1	A	142	PHE	3.1
1	C	142	PHE	3.0
1	E	56	PRO	3.0
1	B	236	GLY	3.0
1	E	233	GLY	2.9
1	E	236	GLY	2.9
1	E	235	ASP	2.7
1	B	38	ASP	2.7
1	C	239	LEU	2.6
1	D	14	LEU	2.6
1	D	232	THR	2.6
1	C	234	PRO	2.6
1	B	76	SER	2.5
1	D	175	PHE	2.5
1	F	233	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	234	PRO	2.4
1	E	312	LEU	2.4
1	D	236	GLY	2.4
1	D	160	ALA	2.3
1	B	234	PRO	2.3
1	B	75	PHE	2.2
1	B	73	ARG	2.2
1	D	142	PHE	2.2
1	B	218	ASP	2.2
1	F	8	PRO	2.2
1	F	235	ASP	2.1
1	D	165	ALA	2.1
1	D	78	ALA	2.1
1	F	236	GLY	2.1
1	A	161	ALA	2.1
1	D	56	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

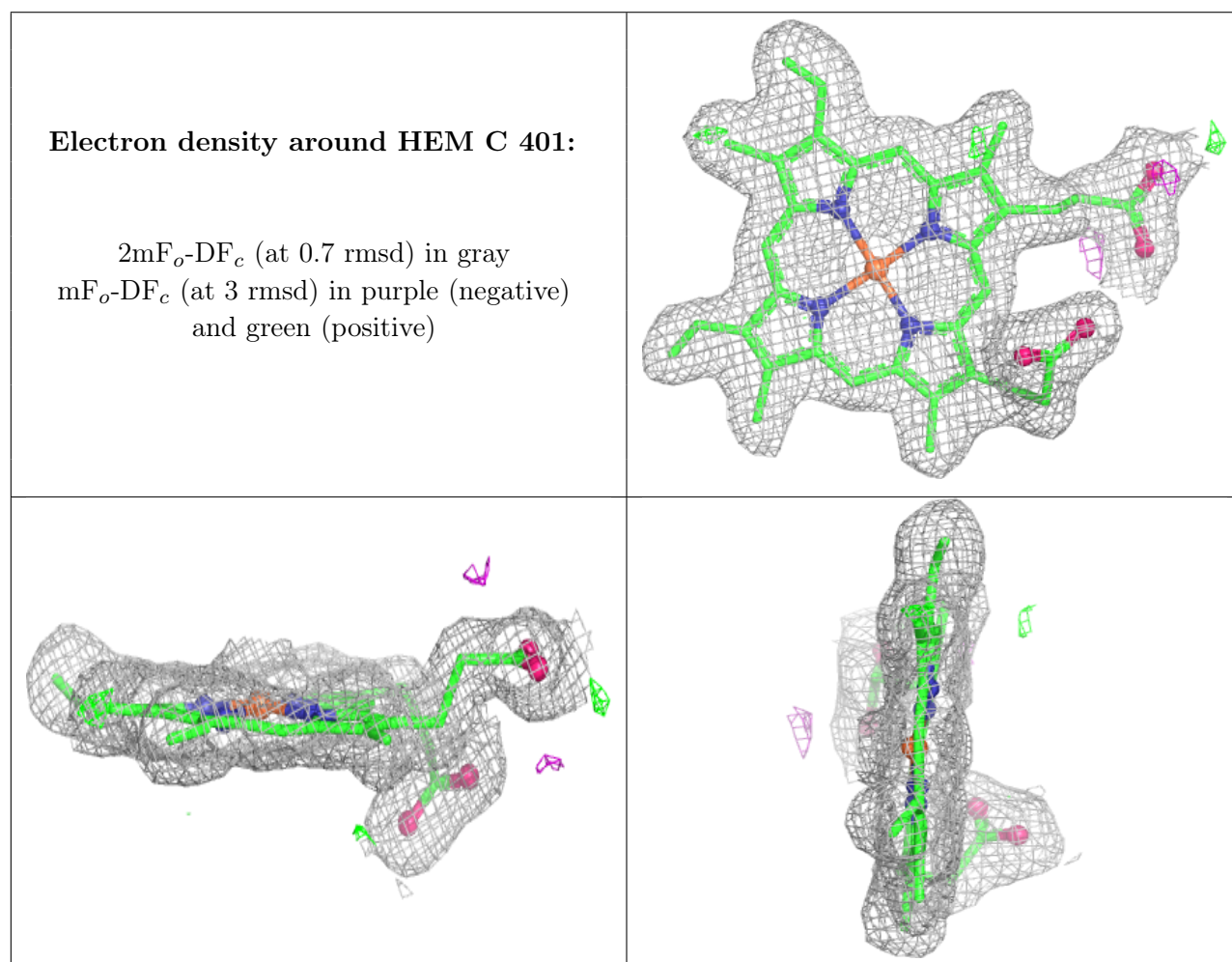
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	402	1/1	0.95	0.05	42,42,42,42	0
2	HEM	C	401	43/43	0.97	0.07	17,21,28,29	0
2	HEM	E	401	43/43	0.97	0.07	18,23,29,37	0
2	HEM	A	401	43/43	0.97	0.06	18,21,26,29	0
2	HEM	B	401	43/43	0.98	0.07	17,23,29,36	0
2	HEM	F	401	43/43	0.98	0.06	18,21,27,32	0
3	MG	A	402	1/1	0.98	0.04	25,25,25,25	0

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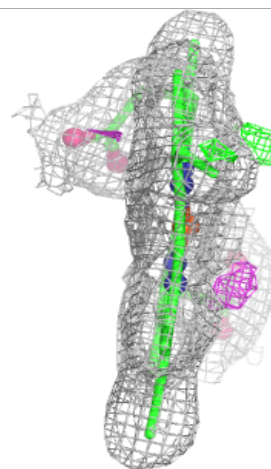
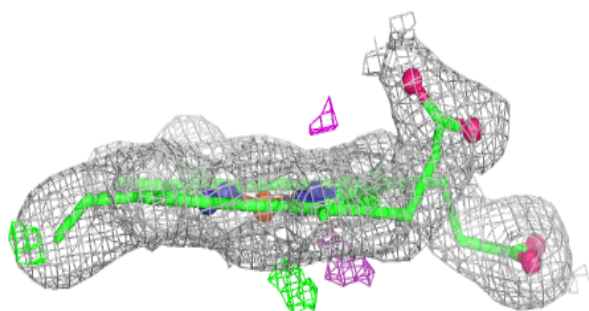
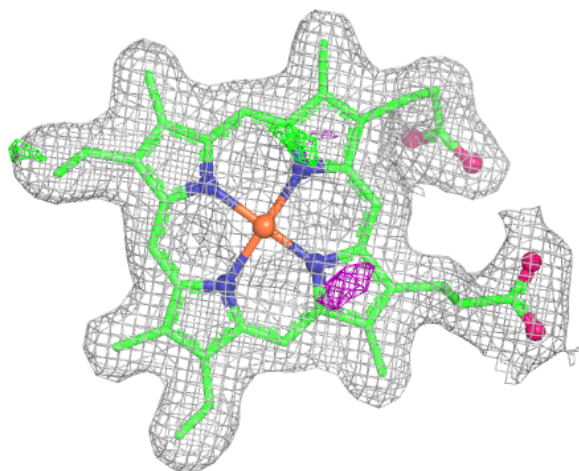
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	D	401	43/43	0.98	0.06	16,23,27,31	0

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.



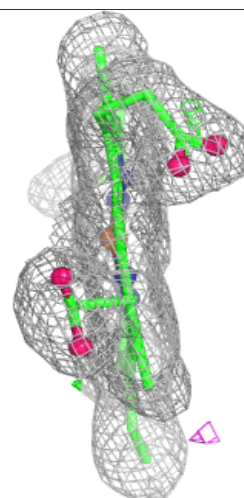
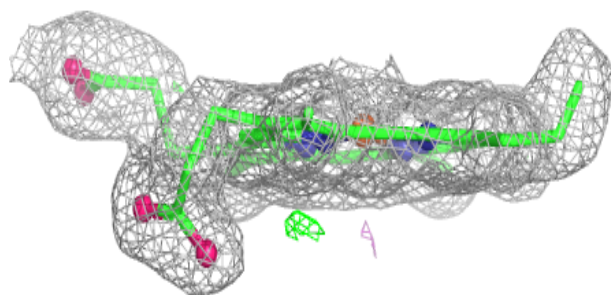
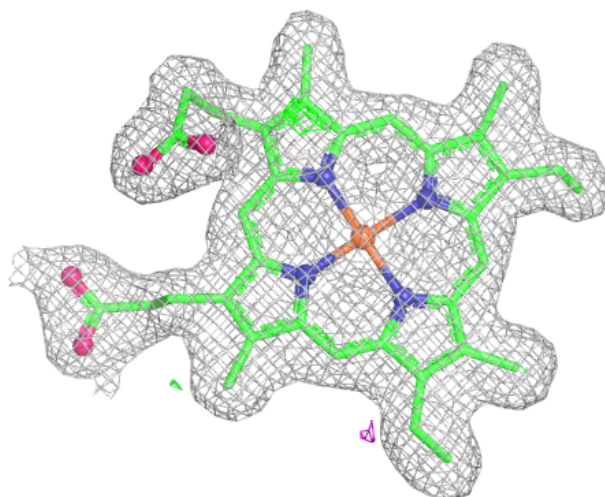
Electron density around HEM E 401:

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



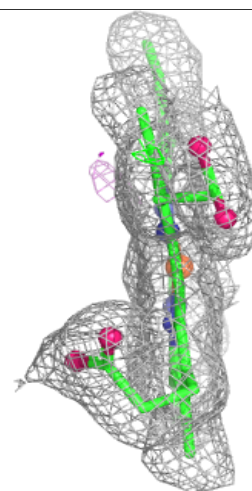
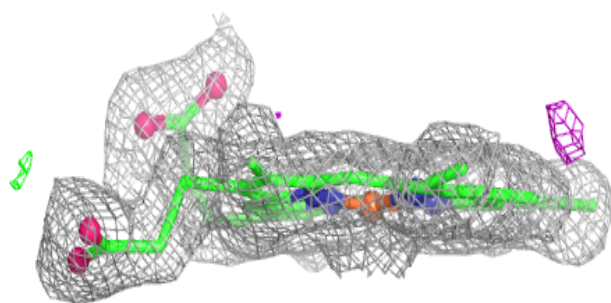
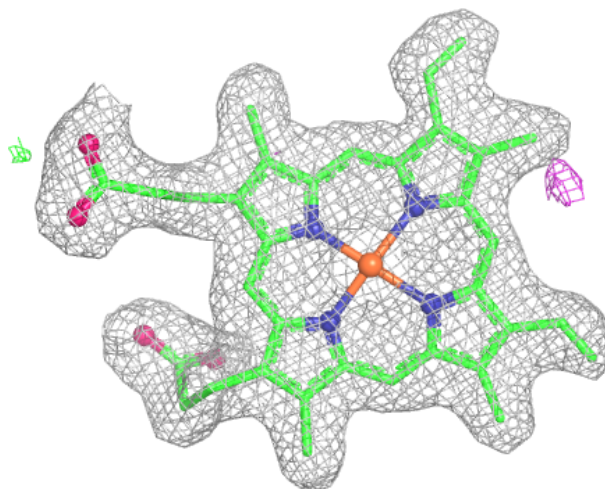
Electron density around HEM A 401:

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



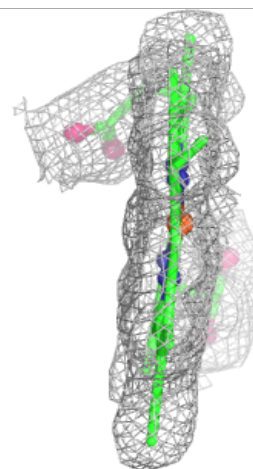
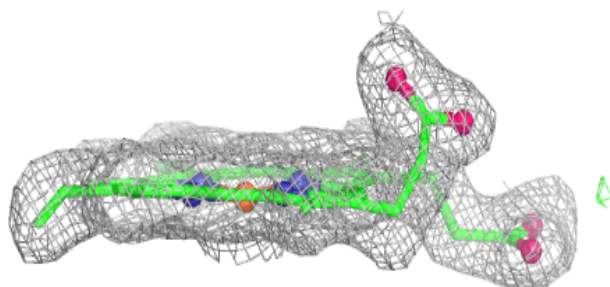
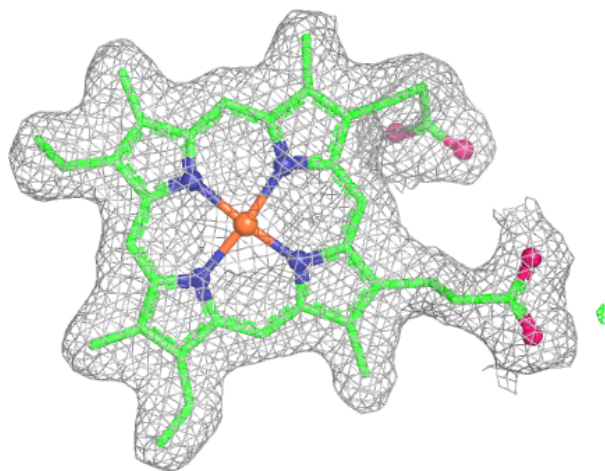
Electron density around HEM B 401:

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



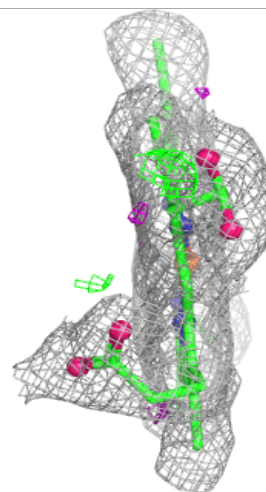
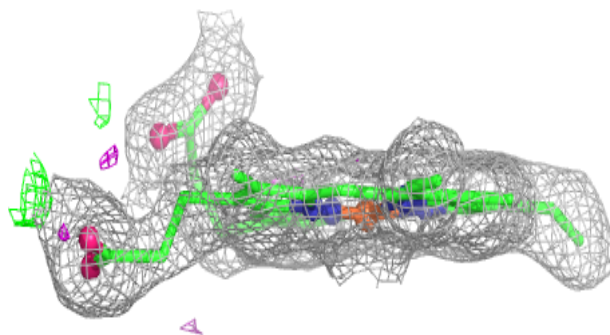
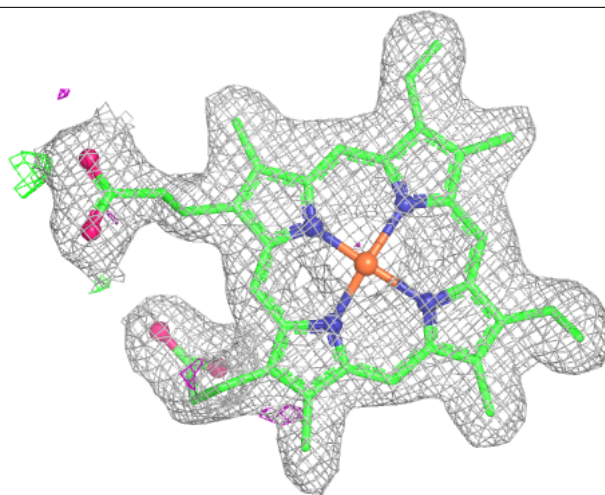
Electron density around HEM F 401:

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



Electron density around HEM D 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.