



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 01:23 am BST

PDB ID : 9HXX / pdb_00009hxx
Title : DtpB in complex with photocaged nitric oxide, 100 microsecond, 30 microjoule, SFX
Authors : Smyth, P.; Williams, L.J.; Hough, M.A.; Worrall, J.A.R.; Owen, R.L.
Deposited on : 2025-01-08
Resolution : 1.52 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:

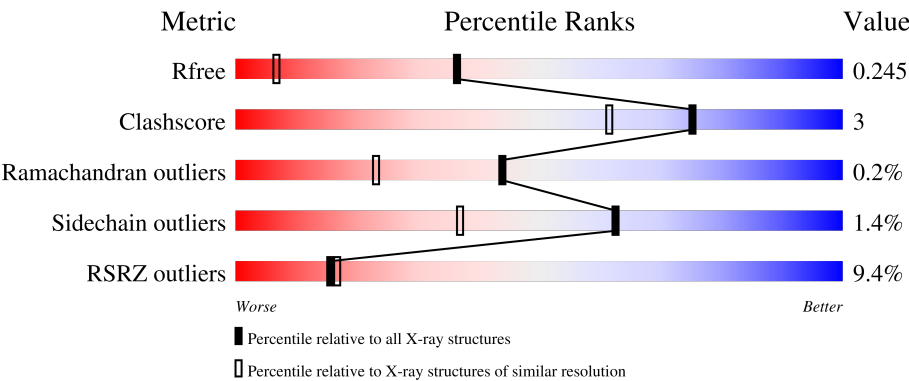
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.52 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.



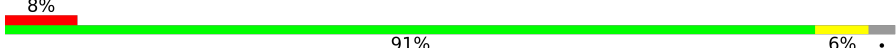
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5293 (1.54-1.50)
Clashscore	180529	5759 (1.54-1.50)
Ramachandran outliers	177936	5653 (1.54-1.50)
Sidechain outliers	177891	5650 (1.54-1.50)
RSRZ outliers	164620	5293 (1.54-1.50)

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	<div><div>7%</div><div>91%</div><div>...</div></div>
1	B	316	<div><div>7%</div><div>88%</div><div>8%</div><div>...</div></div>
1	C	316	<div><div>16%</div><div>89%</div><div>7%</div><div>...</div></div>
1	D	316	<div><div>9%</div><div>89%</div><div>7%</div><div>...</div></div>
1	E	316	<div><div>9%</div><div>89%</div><div>6%</div><div>...</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	316	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO	B	402	-	-	X	-
3	NO	D	402	-	-	X	-
3	NO	F	402	-	-	X	-

2 Entry composition [i](#)

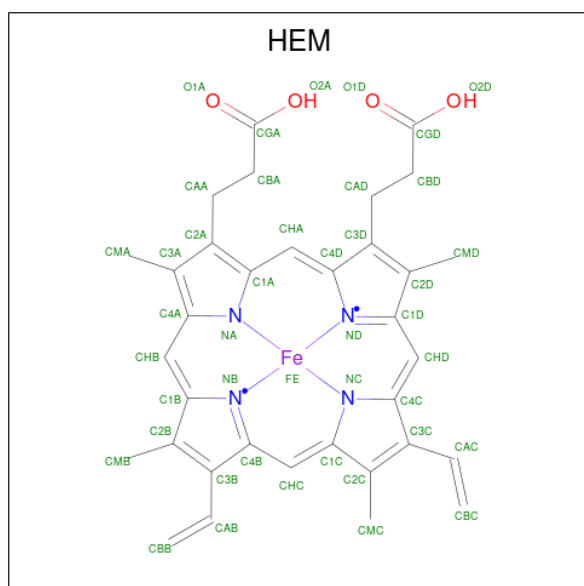
There are 4 unique types of molecules in this entry. The entry contains 15479 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dye-decolorizing peroxidase (DyP), encapsulated subgroup.

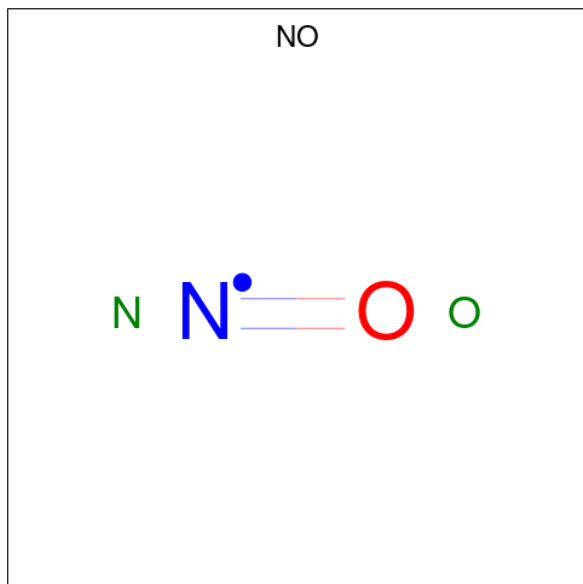
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	2	0
			2346	1474	404	458	10			
1	B	306	Total	C	N	O	S	0	9	0
			2398	1506	414	469	9			
1	C	306	Total	C	N	O	S	0	2	0
			2336	1470	402	454	10			
1	D	306	Total	C	N	O	S	0	5	0
			2365	1488	409	459	9			
1	E	305	Total	C	N	O	S	0	2	0
			2323	1466	401	447	9			
1	F	305	Total	C	N	O	S	0	6	0
			2363	1487	408	458	10			

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

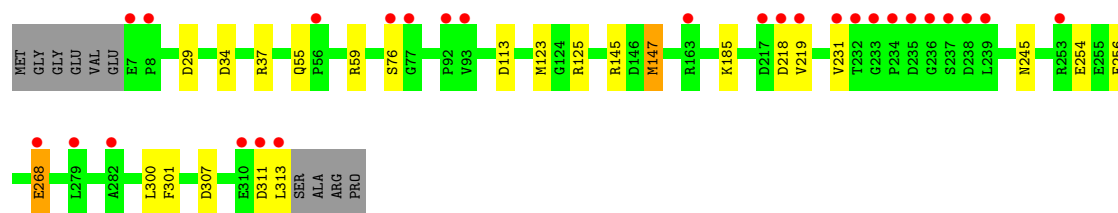
- Molecule 3 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



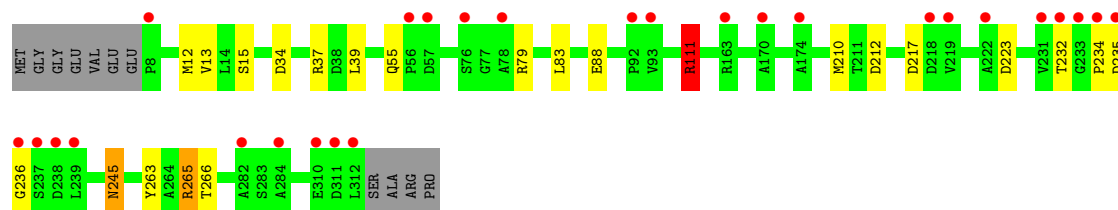
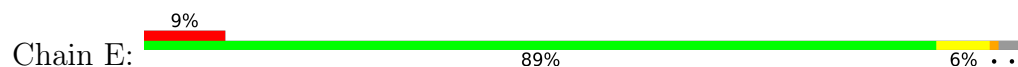
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			2	1	1		
3	B	1	Total	N	O	0	0
			2	1	1		
3	C	1	Total	N	O	0	0
			2	1	1		
3	D	1	Total	N	O	0	0
			2	1	1		
3	E	1	Total	N	O	0	0
			2	1	1		
3	F	1	Total	N	O	0	0
			2	1	1		

- Molecule 4 is water.

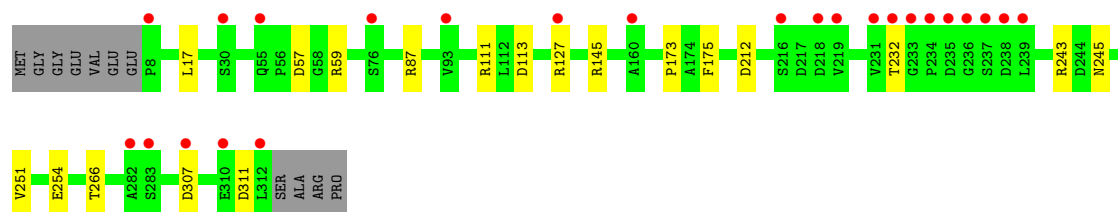
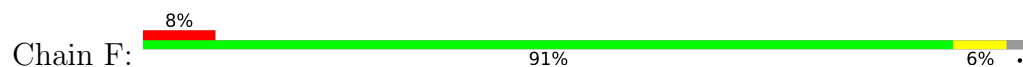
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total 174	O 174	0	0
4	B	181	Total 181	O 181	0	0
4	C	148	Total 148	O 148	0	0
4	D	189	Total 189	O 189	0	0
4	E	188	Total 188	O 188	0	0
4	F	198	Total 198	O 198	0	0



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



- Molecule 1: 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	87.47Å 124.39Å 193.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.13 – 1.52 45.13 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.13-1.52) 99.9 (45.13-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.209 , 0.235 0.220 , 0.245	Depositor DCC
R_{free} test set	2084 reflections (0.65%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15479	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NO

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	0.73	0/2396	1.19	8/3255 (0.2%)
1	B	0.78	0/2455	1.16	11/3338 (0.3%)
1	C	0.71	0/2392	1.17	6/3250 (0.2%)
1	D	0.78	0/2420	1.14	6/3286 (0.2%)
1	E	0.76	0/2376	1.16	6/3229 (0.2%)
1	F	0.75	0/2419	1.15	11/3284 (0.3%)
All	All	0.75	0/14458	1.16	48/19642 (0.2%)

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	2
1	B	0	3
1	C	0	1
1	E	0	2
1	F	0	1
All	All	0	9

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLN	CB-CA-C	10.99	126.67	109.42
1	F	254	GLU	CB-CG-CD	8.54	127.11	112.60
1	A	232	THR	CA-CB-OG1	-8.44	96.93	109.60
1	B	93	VAL	N-CA-CB	-8.31	104.82	111.64
1	D	147	MET	CG-SD-CE	7.88	118.23	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	254	GLU	CB-CA-C	7.10	121.97	111.89
1	E	265	ARG	N-CA-CB	-6.95	98.86	110.39
1	F	175	PHE	CA-CB-CG	-6.76	107.04	113.80
1	C	113	ASP	CA-CB-CG	6.68	119.28	112.60
1	B	113	ASP	CA-CB-CG	6.46	119.06	112.60
1	F	232	THR	CA-CB-OG1	-6.35	100.07	109.60
1	C	212	ASP	CA-CB-CG	6.33	118.93	112.60
1	D	29	ASP	CA-CB-CG	6.33	118.92	112.60
1	F	212	ASP	CA-CB-CG	6.26	118.86	112.60
1	D	268	GLU	CB-CG-CD	6.22	123.17	112.60
1	A	212	ASP	CA-CB-CG	6.18	118.78	112.60
1	F	113	ASP	CA-CB-CG	6.17	118.77	112.60
1	B	232	THR	CA-CB-OG1	-6.04	100.54	109.60
1	E	210	MET	CG-SD-CE	-6.01	87.68	100.90
1	B	55	GLN	O-C-N	-5.93	115.14	121.42
1	E	232	THR	CA-CB-OG1	-5.84	100.83	109.60
1	C	194	GLU	CB-CG-CD	5.83	122.51	112.60
1	B	55	GLN	CB-CA-C	5.79	118.79	109.41
1	A	56	PRO	N-CA-CB	-5.72	96.31	102.60
1	D	113	ASP	CA-CB-CG	5.67	118.27	112.60
1	E	212	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	143	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	307	ASP	CB-CA-C	-5.52	100.08	110.67
1	E	223	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	212	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	223	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	238	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	294	THR	CA-CB-OG1	-5.39	101.51	109.60
1	F	173	PRO	N-CA-C	5.39	120.92	113.65
1	D	145	ARG	CA-CB-CG	-5.29	103.52	114.10
1	D	185	LYS	CG-CD-CE	5.27	123.42	111.30
1	F	266	THR	CA-CB-OG1	-5.22	101.77	109.60
1	B	243	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	F	145	ARG	CA-CB-CG	-5.14	103.83	114.10
1	E	111	ARG	CG-CD-NE	5.12	123.26	112.00
1	F	111	ARG	CG-CD-NE	5.10	123.23	112.00
1	C	95	ARG	N-CA-CB	-5.08	102.14	110.68
1	B	294	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	287	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	218	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	29	ASP	CA-CB-CG	5.02	117.62	112.60
1	F	311	ASP	CA-CB-CG	5.00	117.61	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	ARG	NE-CZ-NH1	-5.00	116.50	121.50

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	37	ARG	Sidechain
1	B	37	ARG	Sidechain
1	B	55	GLN	Mainchain,Peptide
1	C	111	ARG	Sidechain
1	E	111	ARG	Sidechain
1	E	265	ARG	Sidechain
1	F	59	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	2346	0	2270	7	0
1	B	2398	0	2313	19	0
1	C	2336	0	2267	15	0
1	D	2365	0	2294	16	0
1	E	2323	0	2256	13	0
1	F	2363	0	2300	6	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
2	E	43	0	30	1	0
2	F	43	0	30	2	0
3	A	2	0	0	1	0
3	B	2	0	0	2	0
3	C	2	0	0	1	0
3	D	2	0	0	2	0
3	E	2	0	0	0	0
3	F	2	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	174	0	0	1	0
4	B	181	0	0	4	0
4	C	148	0	0	1	0
4	D	189	0	0	3	0
4	E	188	0	0	2	0
4	F	198	0	0	2	0
All	All	15479	0	13880	81	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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ASP:C	1:D:313:LEU:N	2.10	1.09
4:B:562:HOH:O	1:C:210[A]:MET:HE3	1.77	0.85
1:E:12:MET:HG3	1:E:15:SER:OG	1.80	0.81
1:D:300[B]:LEU:HD13	1:D:300[B]:LEU:C	2.09	0.77
1:E:55:GLN:HB3	4:F:687:HOH:O	1.85	0.76
1:B:121:GLU:O	1:B:125[B]:ARG:NE	2.19	0.75
1:D:34:ASP:OD1	1:D:37[B]:ARG:NH1	2.20	0.72
1:C:215:LEU:HB3	1:C:219:VAL:HG23	1.71	0.72
1:B:245:ASN:ND2	3:B:402:NO:O	2.25	0.70
1:E:34:ASP:OD1	1:E:37:ARG:NH2	2.26	0.68
2:D:401:HEM:NB	3:D:402:NO:N	2.43	0.66
1:C:300:LEU:C	1:C:300:LEU:HD23	2.21	0.65
1:D:55[B]:GLN:NE2	4:D:501:HOH:O	2.28	0.65
2:F:401:HEM:NB	3:F:402:NO:O	2.30	0.65
1:C:300:LEU:HD23	1:C:301:PHE:N	2.13	0.64
2:C:401:HEM:HMC2	2:C:401:HEM:HBC2	1.79	0.64
1:A:34:ASP:OD1	1:A:37:ARG:NH2	2.30	0.62
2:F:401:HEM:C1B	3:F:402:NO:O	2.52	0.62
1:F:245:ASN:ND2	3:F:402:NO:N	2.47	0.62
1:D:245:ASN:ND2	3:D:402:NO:O	2.34	0.61
1:D:55[A]:GLN:HA	1:D:55[A]:GLN:OE1	2.00	0.59
1:E:245:ASN:ND2	4:E:502:HOH:O	2.33	0.59
1:E:234:PRO:C	1:E:236:GLY:H	2.12	0.58
1:C:245:ASN:ND2	3:C:402:NO:O	2.37	0.57
1:B:237:SER:O	1:B:238:ASP:HB2	2.05	0.56
1:C:79:ARG:NH2	1:C:83:LEU:O	2.40	0.55
1:B:125[B]:ARG:N	1:B:125[B]:ARG:HE	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASN:ND2	3:A:402:NO:O	2.40	0.54
1:C:231:VAL:HG23	1:C:239:LEU:HB2	1.90	0.54
1:A:214:GLU:OE2	1:A:220:LYS:NZ	2.30	0.53
1:E:245:ASN:ND2	1:E:245:ASN:H	2.07	0.52
1:C:215:LEU:HB3	1:C:219:VAL:CG2	2.38	0.51
1:E:13[A]:VAL:HG13	1:E:263:TYR:CD1	2.46	0.50
1:D:147:MET:CG	1:D:256:PHE:HB3	2.42	0.50
1:D:147:MET:HG2	1:D:256:PHE:HB3	1.94	0.50
1:E:39:LEU:C	1:E:39:LEU:HD13	2.37	0.49
1:D:59:ARG:HD2	4:D:604:HOH:O	2.11	0.49
1:D:123:MET:HG3	1:F:251[B]:VAL:HG12	1.94	0.49
2:B:401:HEM:HBC2	2:B:401:HEM:HMC2	1.95	0.48
2:E:401:HEM:HMC1	2:E:401:HEM:HBC2	1.94	0.48
1:D:125[B]:ARG:HE	1:D:125[B]:ARG:N	2.11	0.48
1:E:234:PRO:O	1:E:236:GLY:N	2.47	0.48
1:E:217:ASP:O	4:E:501:HOH:O	2.20	0.48
1:B:84[A]:HIS:HD2	1:B:85:PRO:O	1.97	0.48
1:C:39:LEU:HD22	1:C:126:LEU:CG	2.44	0.47
1:B:34:ASP:OD1	1:B:37:ARG:NH2	2.47	0.47
1:B:214:GLU:OE2	1:B:220:LYS:NZ	2.36	0.47
1:B:121:GLU:O	1:B:125[B]:ARG:CZ	2.63	0.47
1:B:116:PHE:O	1:B:120[B]:THR:HG23	2.14	0.46
1:D:300[B]:LEU:C	1:D:300[B]:LEU:CD1	2.82	0.46
1:B:95:ARG:HG3	4:B:513:HOH:O	2.15	0.46
1:D:300[B]:LEU:HD13	1:D:301:PHE:N	2.30	0.46
1:A:251:VAL:HG12	1:C:123:MET:HG3	1.97	0.46
1:B:312:LEU:C	1:B:312:LEU:HD12	2.41	0.46
1:D:125[B]:ARG:HD3	4:D:650:HOH:O	2.15	0.45
1:C:39:LEU:HD22	1:C:126:LEU:HG	1.99	0.45
1:E:234:PRO:C	1:E:236:GLY:N	2.72	0.45
1:C:218:ASP:N	1:C:218:ASP:OD1	2.48	0.44
1:B:125[B]:ARG:HD3	4:B:602:HOH:O	2.18	0.44
1:C:37:ARG:HD3	4:C:633:HOH:O	2.19	0.43
1:C:300:LEU:C	1:C:300:LEU:CD2	2.91	0.43
1:B:125[B]:ARG:HE	1:B:125[B]:ARG:H	1.66	0.43
1:E:79:ARG:NH2	1:E:83:LEU:O	2.51	0.43
1:B:237:SER:O	1:B:238:ASP:CB	2.66	0.43
1:D:218:ASP:OD2	1:D:219:VAL:HG23	2.18	0.43
1:A:39:LEU:C	1:A:39:LEU:HD13	2.44	0.43
2:A:401:HEM:HMC2	2:A:401:HEM:HBC2	2.00	0.43
1:F:57:ASP:HB2	4:F:544:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:HA	1:A:56:PRO:HA	1.83	0.42
1:F:243:ARG:HD2	3:F:402:NO:N	2.35	0.42
1:C:219:VAL:O	1:C:221:PRO:HD3	2.20	0.41
1:A:210[A]:MET:HG2	4:A:620:HOH:O	2.20	0.41
2:D:401:HEM:HMC2	2:D:401:HEM:HBC2	2.01	0.41
1:F:87[A]:ARG:HA	1:F:87[A]:ARG:HE	1.85	0.41
1:D:254:GLU:HG2	1:F:127:ARG:CZ	2.50	0.41
1:E:245:ASN:H	1:E:245:ASN:HD22	1.67	0.41
1:B:163:ARG:HG3	1:B:167:LEU:HD12	2.02	0.41
1:B:95:ARG:CG	4:B:513:HOH:O	2.69	0.41
1:B:39:LEU:C	1:B:39:LEU:HD13	2.45	0.40
1:B:243:ARG:HD2	3:B:402:NO:N	2.37	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	306/316 (97%)	299 (98%)	7 (2%)	0	100	100
1	B	313/316 (99%)	307 (98%)	4 (1%)	2 (1%)	22	6
1	C	306/316 (97%)	301 (98%)	5 (2%)	0	100	100
1	D	308/316 (98%)	301 (98%)	7 (2%)	0	100	100
1	E	305/316 (96%)	298 (98%)	6 (2%)	1 (0%)	37	18
1	F	309/316 (98%)	304 (98%)	5 (2%)	0	100	100
All	All	1847/1896 (97%)	1810 (98%)	34 (2%)	3 (0%)	44	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	235	ASP
1	B	56	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/252 (98%)	241 (98%)	6 (2%)	44	15
1	B	253/252 (100%)	251 (99%)	2 (1%)	79	62
1	C	246/252 (98%)	244 (99%)	2 (1%)	79	62
1	D	249/252 (99%)	245 (98%)	4 (2%)	58	31
1	E	242/252 (96%)	238 (98%)	4 (2%)	56	28
1	F	250/252 (99%)	248 (99%)	2 (1%)	79	62
All	All	1487/1512 (98%)	1467 (99%)	20 (1%)	62	39

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	56	PRO
1	A	111	ARG
1	A	218	ASP
1	A	219	VAL
1	A	310	GLU
1	B	55	GLN
1	B	307	ASP
1	C	218	ASP
1	C	307	ASP
1	D	76	SER
1	D	231	VAL
1	D	268	GLU
1	D	307	ASP
1	E	88	GLU
1	E	111	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	245	ASN
1	E	266	THR
1	F	17	LEU
1	F	307	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	E	245	ASN

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 ⓘ

12 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	F	401	1	41,50,50	1.20	3 (7%)	45,82,82	2.08	16 (35%)
3	NO	C	402	2	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NO	A	402	2	0,1,1	-	-	-		
2	HEM	C	401	3,1	41,50,50	1.42	7 (17%)	45,82,82	2.25	13 (28%)
2	HEM	D	401	3,1	41,50,50	1.42	7 (17%)	45,82,82	2.05	18 (40%)
2	HEM	A	401	3,1	41,50,50	1.27	6 (14%)	45,82,82	2.23	18 (40%)
3	NO	B	402	2	0,1,1	-	-	-		
2	HEM	E	401	3,1	41,50,50	1.36	8 (19%)	45,82,82	2.40	14 (31%)
3	NO	F	402	-	0,1,1	-	-	-		
3	NO	D	402	2	0,1,1	-	-	-		
2	HEM	B	401	3,1	41,50,50	1.28	6 (14%)	45,82,82	2.09	17 (37%)
3	NO	E	402	2	0,1,1	-	-	-		

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	F	401	1	-	5/12/54/54	-
2	HEM	C	401	3,1	-	5/12/54/54	-
2	HEM	D	401	3,1	-	5/12/54/54	-
2	HEM	A	401	3,1	-	6/12/54/54	-
2	HEM	E	401	3,1	-	5/12/54/54	-
2	HEM	B	401	3,1	-	6/12/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEM	C3C-C2C	-3.84	1.35	1.40
2	E	401	HEM	C1B-NB	-3.55	1.34	1.40
2	B	401	HEM	C3C-C2C	-3.31	1.35	1.40
2	C	401	HEM	C4D-ND	-3.15	1.34	1.40
2	E	401	HEM	C4D-ND	-3.01	1.35	1.40
2	D	401	HEM	C4D-C3D	3.00	1.50	1.45
2	B	401	HEM	O1A-CGA	2.80	1.31	1.22
2	A	401	HEM	C3C-C2C	-2.71	1.36	1.40
2	A	401	HEM	CHA-C4D	2.69	1.41	1.35
2	A	401	HEM	C3B-C4B	2.68	1.50	1.44
2	C	401	HEM	C4B-NB	-2.65	1.33	1.38
2	F	401	HEM	C1B-NB	-2.59	1.35	1.40
2	A	401	HEM	C1B-NB	-2.54	1.35	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEM	C4D-ND	-2.53	1.35	1.40
2	C	401	HEM	O2A-CGA	-2.52	1.22	1.30
2	C	401	HEM	C1D-ND	-2.51	1.33	1.38
2	E	401	HEM	O2D-CGD	-2.48	1.22	1.30
2	E	401	HEM	C4B-NB	-2.45	1.33	1.38
2	D	401	HEM	C3C-CAC	2.35	1.52	1.47
2	F	401	HEM	C3C-C2C	-2.32	1.37	1.40
2	A	401	HEM	C4D-ND	-2.31	1.36	1.40
2	D	401	HEM	O2D-CGD	-2.29	1.23	1.30
2	A	401	HEM	C4A-NA	2.29	1.40	1.36
2	B	401	HEM	CHA-C4D	2.29	1.40	1.35
2	D	401	HEM	CHA-C4D	2.28	1.40	1.35
2	C	401	HEM	FE-NB	2.25	2.08	1.96
2	E	401	HEM	C1A-NA	2.24	1.40	1.36
2	B	401	HEM	CHB-C1B	2.20	1.40	1.35
2	E	401	HEM	FE-NB	2.17	2.07	1.96
2	E	401	HEM	C4D-C3D	2.16	1.48	1.45
2	C	401	HEM	CHB-C1B	2.11	1.40	1.35
2	B	401	HEM	O2A-CGA	-2.09	1.23	1.30
2	E	401	HEM	C3B-C4B	2.08	1.49	1.44
2	B	401	HEM	C3C-CAC	-2.08	1.43	1.47
2	D	401	HEM	C1A-CHA	-2.07	1.35	1.41
2	F	401	HEM	CAA-C2A	2.03	1.55	1.52
2	C	401	HEM	C4D-C3D	2.01	1.48	1.45

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	C1B-NB-C4B	6.38	111.67	105.07
2	E	401	HEM	CHC-C4B-NB	6.02	130.97	124.43
2	C	401	HEM	C1B-NB-C4B	5.91	111.17	105.07
2	B	401	HEM	C4D-ND-C1D	-5.21	99.69	105.07
2	C	401	HEM	CHC-C4B-NB	5.04	129.91	124.43
2	E	401	HEM	C2C-C3C-C4C	4.86	110.29	106.90
2	B	401	HEM	C2D-C1D-ND	4.67	115.48	109.88
2	D	401	HEM	C3D-C4D-ND	4.51	115.18	110.17
2	A	401	HEM	C1B-NB-C4B	4.50	109.72	105.07
2	C	401	HEM	C4A-C3A-C2A	4.50	110.13	107.00
2	B	401	HEM	C3D-C4D-ND	4.42	115.08	110.17
2	C	401	HEM	CHB-C1B-NB	4.35	129.75	124.38
2	C	401	HEM	C4D-ND-C1D	4.31	109.53	105.07
2	C	401	HEM	CHD-C1D-ND	4.30	129.10	124.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	CMA-C3A-C4A	-4.24	121.94	128.46
2	A	401	HEM	C3B-C2B-C1B	4.21	109.61	106.49
2	F	401	HEM	C2D-C1D-ND	4.17	114.88	109.88
2	E	401	HEM	CHD-C1D-C2D	-4.16	118.48	124.98
2	C	401	HEM	CHA-C4D-ND	4.12	129.47	124.38
2	A	401	HEM	C4A-C3A-C2A	4.12	109.86	107.00
2	F	401	HEM	C3D-C4D-ND	4.02	114.64	110.17
2	E	401	HEM	C2D-C1D-ND	3.98	114.65	109.88
2	F	401	HEM	C4D-ND-C1D	-3.98	100.96	105.07
2	A	401	HEM	C4B-C3B-C2B	-3.97	103.96	107.11
2	E	401	HEM	CHB-C1B-NB	3.95	129.26	124.38
2	D	401	HEM	C4D-ND-C1D	-3.92	101.02	105.07
2	A	401	HEM	CHC-C4B-NB	3.84	128.60	124.43
2	F	401	HEM	CHD-C1D-C2D	-3.58	119.39	124.98
2	E	401	HEM	CMC-C2C-C3C	3.52	131.27	124.68
2	A	401	HEM	CHD-C1D-C2D	-3.48	119.55	124.98
2	A	401	HEM	C3D-C4D-ND	3.47	114.03	110.17
2	B	401	HEM	CAD-C3D-C4D	3.29	130.41	124.66
2	D	401	HEM	C2D-C1D-ND	3.29	113.82	109.88
2	D	401	HEM	C2C-C3C-C4C	3.26	109.17	106.90
2	D	401	HEM	CMC-C2C-C3C	3.19	130.64	124.68
2	A	401	HEM	CHA-C4D-C3D	-3.17	119.37	125.33
2	B	401	HEM	C3C-C4C-NC	-3.10	105.09	110.94
2	A	401	HEM	CHD-C1D-ND	3.06	127.76	124.43
2	E	401	HEM	C3C-C4C-NC	-3.02	105.24	110.94
2	F	401	HEM	CHA-C4D-C3D	-3.02	119.67	125.33
2	C	401	HEM	CMA-C3A-C4A	-3.01	123.84	128.46
2	F	401	HEM	O2A-CGA-CBA	2.99	123.64	114.03
2	A	401	HEM	CMD-C2D-C1D	2.97	129.56	125.04
2	E	401	HEM	CHA-C4D-C3D	-2.94	119.80	125.33
2	A	401	HEM	CMC-C2C-C3C	2.94	130.17	124.68
2	B	401	HEM	C4B-CHC-C1C	2.92	126.42	122.56
2	F	401	HEM	CHC-C4B-NB	2.91	127.59	124.43
2	A	401	HEM	CHB-C1B-NB	2.91	127.97	124.38
2	F	401	HEM	C3C-C4C-NC	-2.89	105.49	110.94
2	E	401	HEM	CHA-C4D-ND	2.87	127.93	124.38
2	D	401	HEM	C4A-C3A-C2A	2.86	108.99	107.00
2	A	401	HEM	C3C-C4C-NC	-2.86	105.55	110.94
2	B	401	HEM	C4B-C3B-C2B	2.83	109.36	107.11
2	D	401	HEM	CHC-C4B-NB	2.82	127.50	124.43
2	C	401	HEM	CMC-C2C-C3C	2.80	129.92	124.68
2	B	401	HEM	CHA-C4D-C3D	-2.79	120.08	125.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	C3B-C2B-C1B	2.78	108.55	106.49
2	D	401	HEM	C4D-C3D-C2D	-2.78	102.84	106.90
2	B	401	HEM	CHD-C1D-C2D	-2.78	120.64	124.98
2	B	401	HEM	C3B-C2B-C1B	-2.74	104.45	106.49
2	D	401	HEM	CHD-C1D-C2D	-2.73	120.72	124.98
2	A	401	HEM	C4D-ND-C1D	-2.72	102.26	105.07
2	D	401	HEM	C3C-C4C-NC	-2.68	105.88	110.94
2	D	401	HEM	C4B-C3B-C2B	-2.68	104.99	107.11
2	D	401	HEM	O2D-CGD-O1D	-2.66	116.67	123.30
2	C	401	HEM	O2A-CGA-CBA	2.62	122.44	114.03
2	D	401	HEM	CAD-CBD-CGD	-2.59	108.04	113.60
2	B	401	HEM	CAD-CBD-CGD	-2.57	108.06	113.60
2	F	401	HEM	CMA-C3A-C2A	2.57	129.79	124.94
2	D	401	HEM	CMA-C3A-C4A	-2.50	124.62	128.46
2	F	401	HEM	CAD-C3D-C4D	2.49	129.01	124.66
2	E	401	HEM	C4B-C3B-C2B	-2.41	105.20	107.11
2	B	401	HEM	CMB-C2B-C1B	2.39	128.68	125.04
2	D	401	HEM	CHB-C1B-NB	2.39	127.33	124.38
2	A	401	HEM	C2D-C1D-ND	2.28	112.61	109.88
2	E	401	HEM	CAD-CBD-CGD	-2.26	108.75	113.60
2	A	401	HEM	C2C-C3C-C4C	2.24	108.46	106.90
2	F	401	HEM	O1D-CGD-CBD	-2.24	115.88	123.08
2	F	401	HEM	CMD-C2D-C1D	2.21	128.40	125.04
2	C	401	HEM	C2B-C1B-NB	-2.20	107.23	109.84
2	B	401	HEM	CMA-C3A-C4A	-2.19	125.10	128.46
2	A	401	HEM	O1D-CGD-CBD	-2.18	116.08	123.08
2	C	401	HEM	C3D-C4D-ND	-2.16	107.76	110.17
2	B	401	HEM	C4D-C3D-C2D	-2.15	103.77	106.90
2	C	401	HEM	CHD-C1D-C2D	-2.11	121.69	124.98
2	B	401	HEM	O2D-CGD-CBD	2.09	120.76	114.03
2	D	401	HEM	O2D-CGD-CBD	2.09	120.75	114.03
2	F	401	HEM	CMC-C2C-C3C	2.08	128.58	124.68
2	E	401	HEM	C3B-C2B-C1B	2.07	108.03	106.49
2	E	401	HEM	CHD-C1D-ND	2.06	126.67	124.43
2	D	401	HEM	CBA-CAA-C2A	2.06	116.13	112.62
2	F	401	HEM	O2D-CGD-CBD	2.05	120.62	114.03
2	B	401	HEM	CBD-CAD-C3D	-2.04	106.95	112.63
2	B	401	HEM	CMD-C2D-C1D	2.02	128.12	125.04
2	F	401	HEM	C3B-C2B-C1B	-2.02	104.99	106.49
2	A	401	HEM	CMA-C3A-C4A	-2.01	125.37	128.46

There are no chirality outliers.

All (32) torsion outliers are listed below:

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

There are no ring outliers.

11 monomers are involved in 15 short contacts:

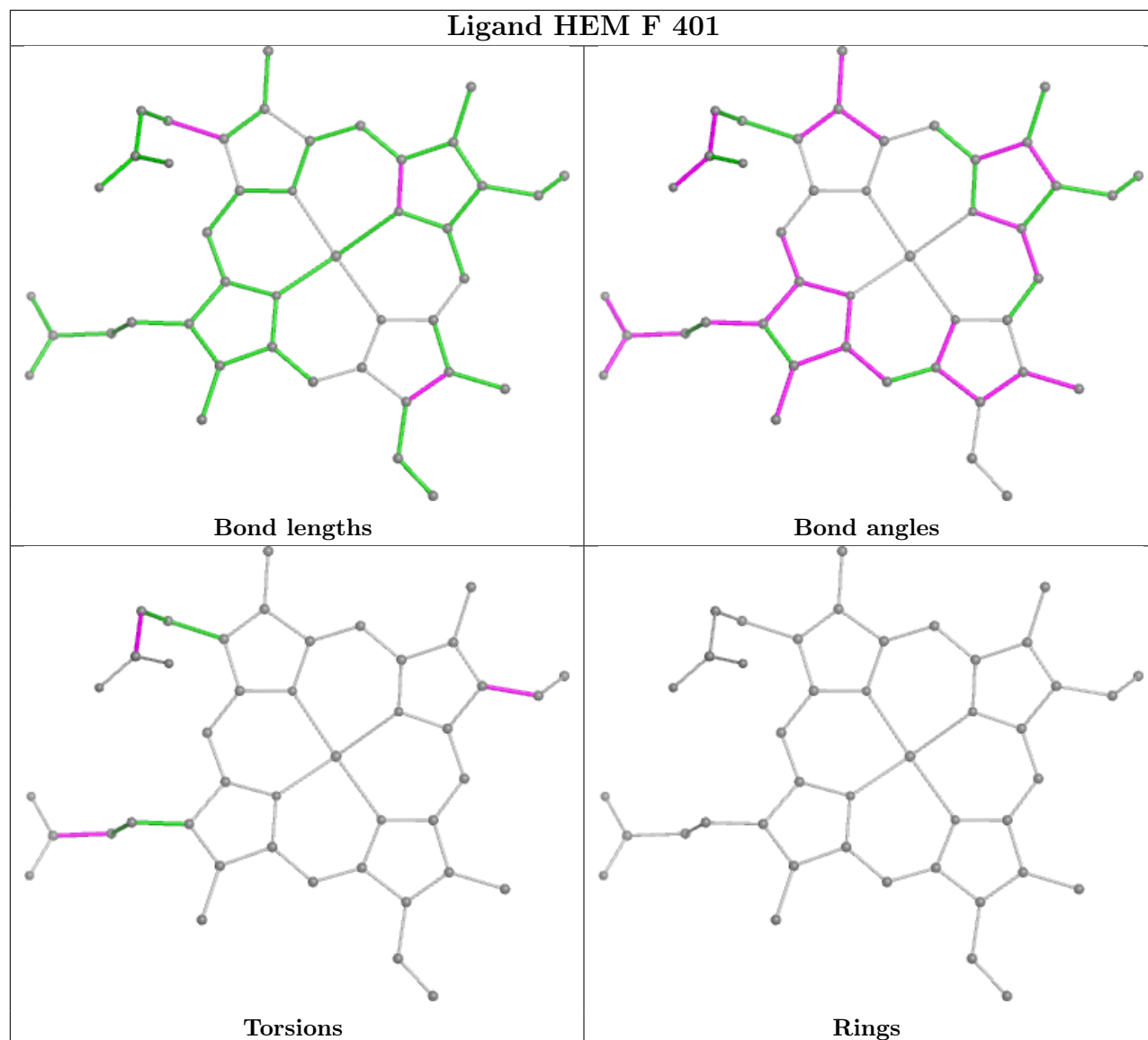
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	HEM	2	0
3	C	402	NO	1	0
3	A	402	NO	1	0
2	C	401	HEM	1	0

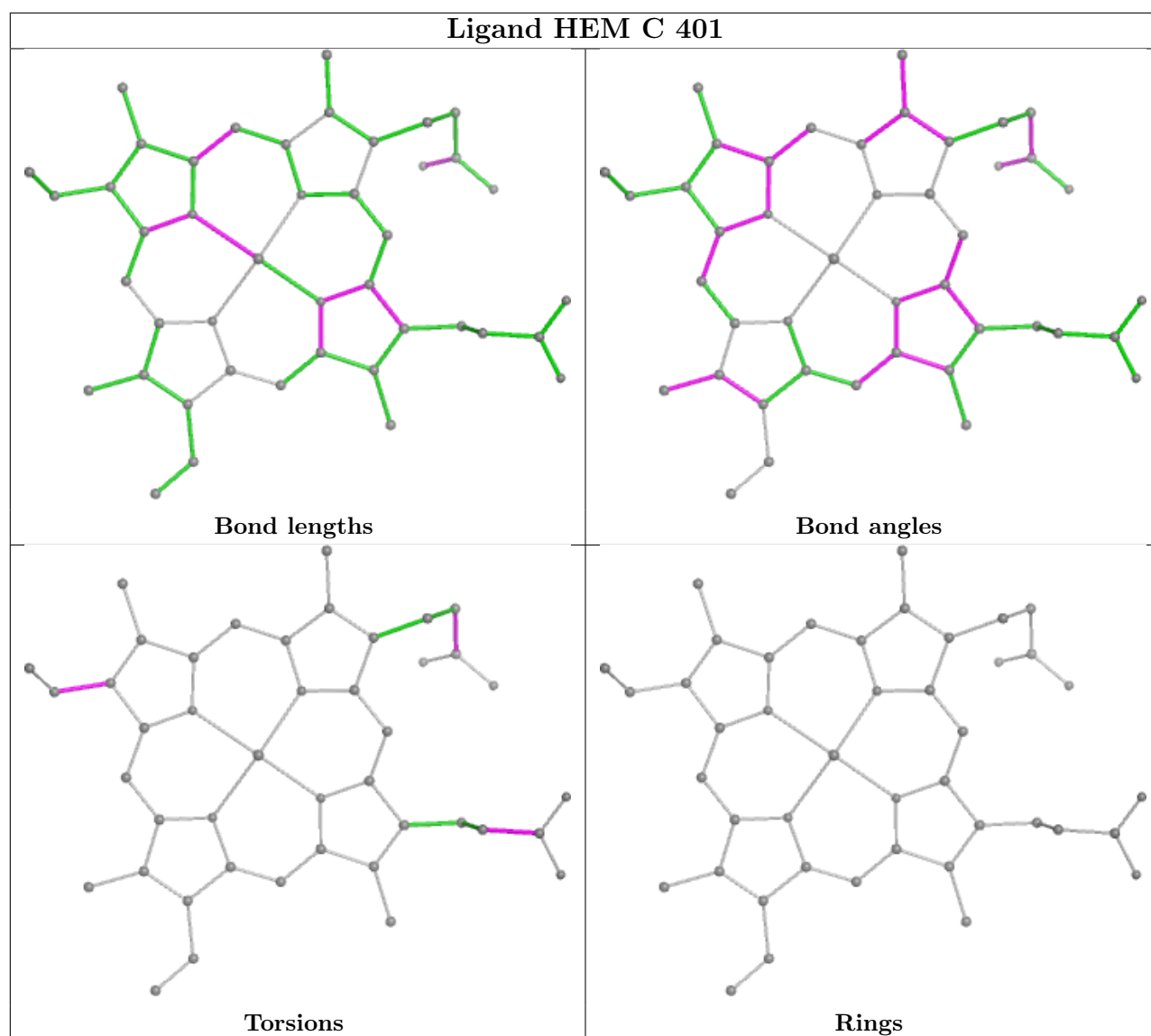
Continued on next page...

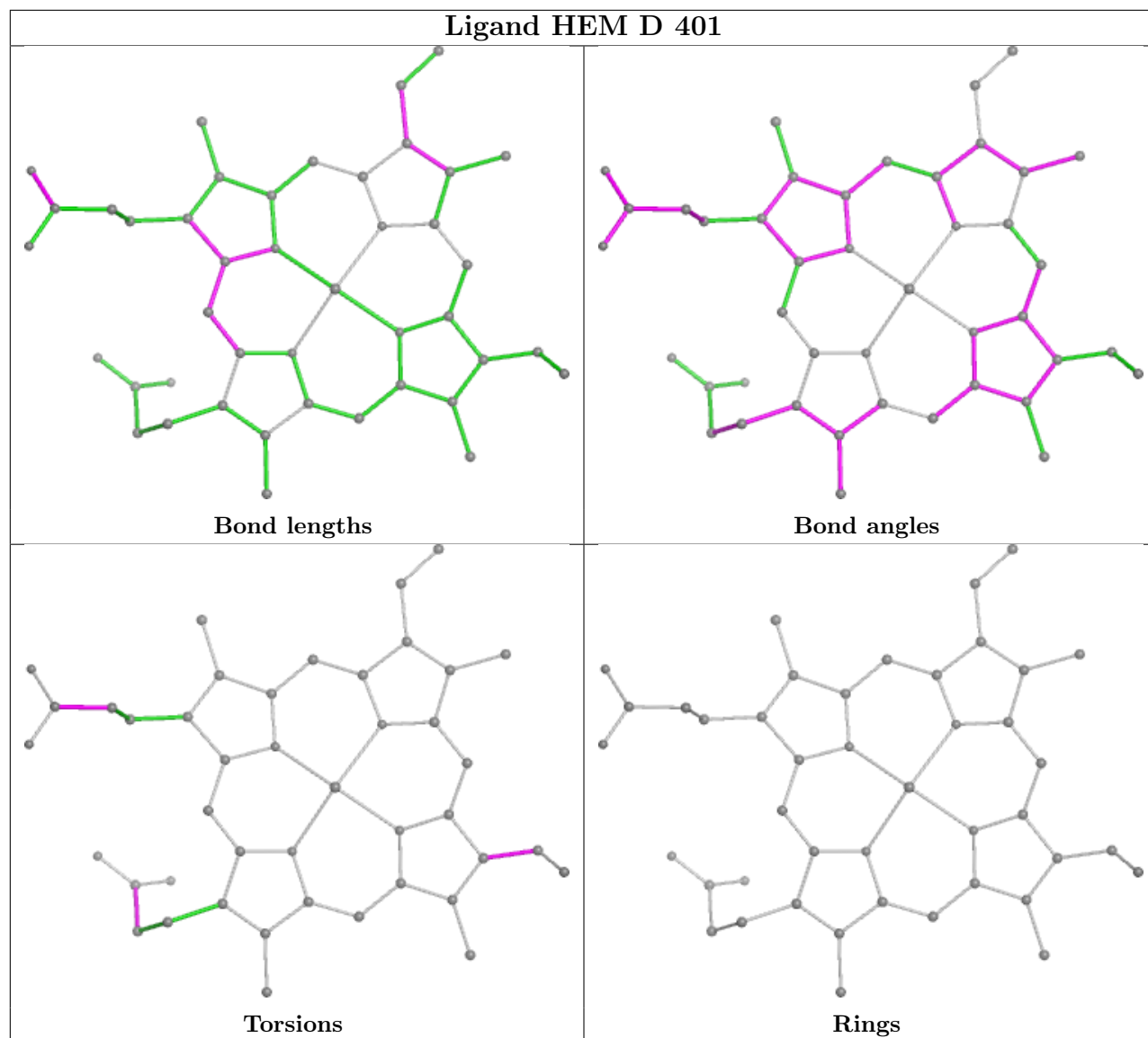
Continued from previous page...

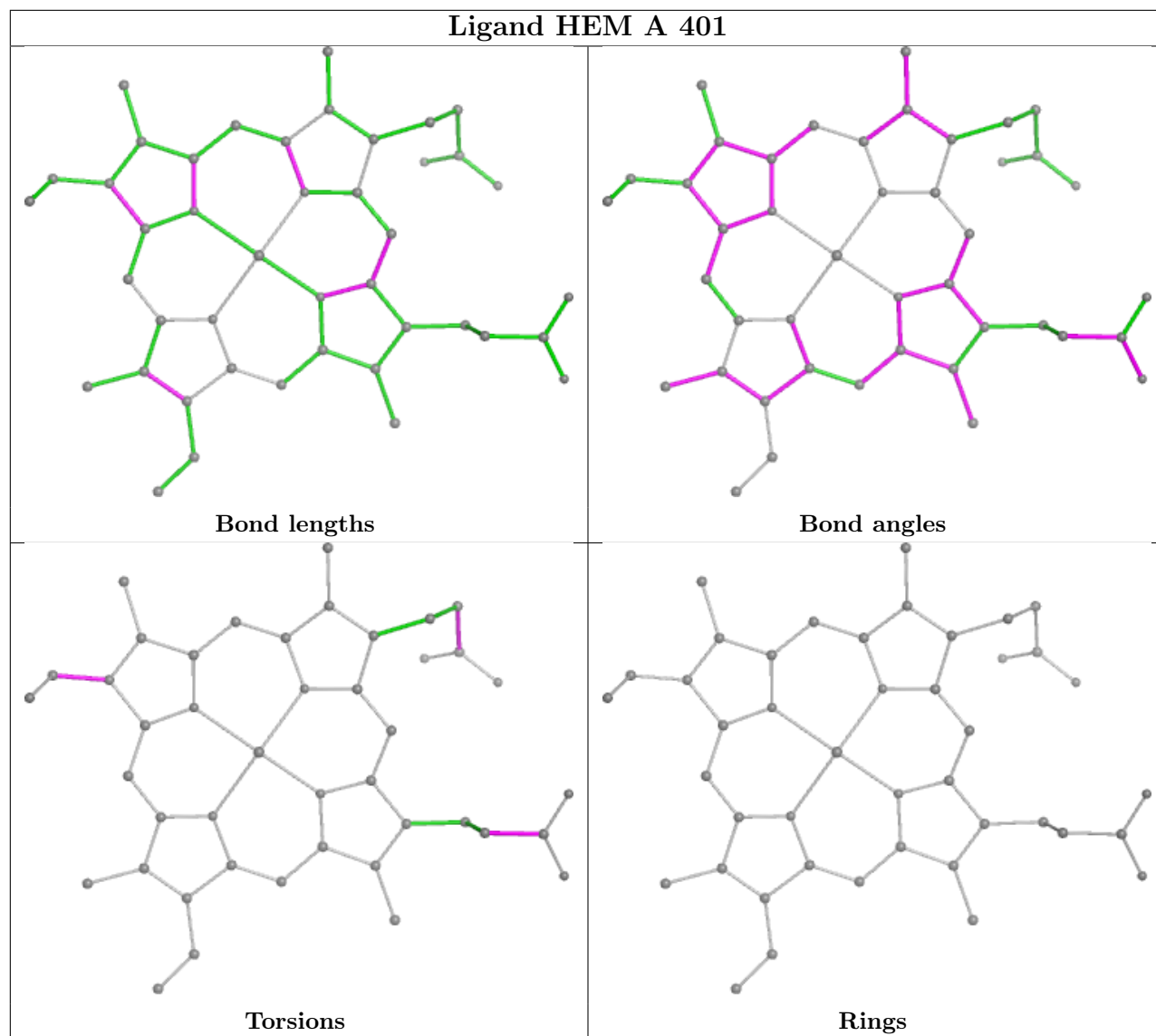
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	2	0
2	A	401	HEM	1	0
3	B	402	NO	2	0
2	E	401	HEM	1	0
3	F	402	NO	4	0
3	D	402	NO	2	0
2	B	401	HEM	1	0

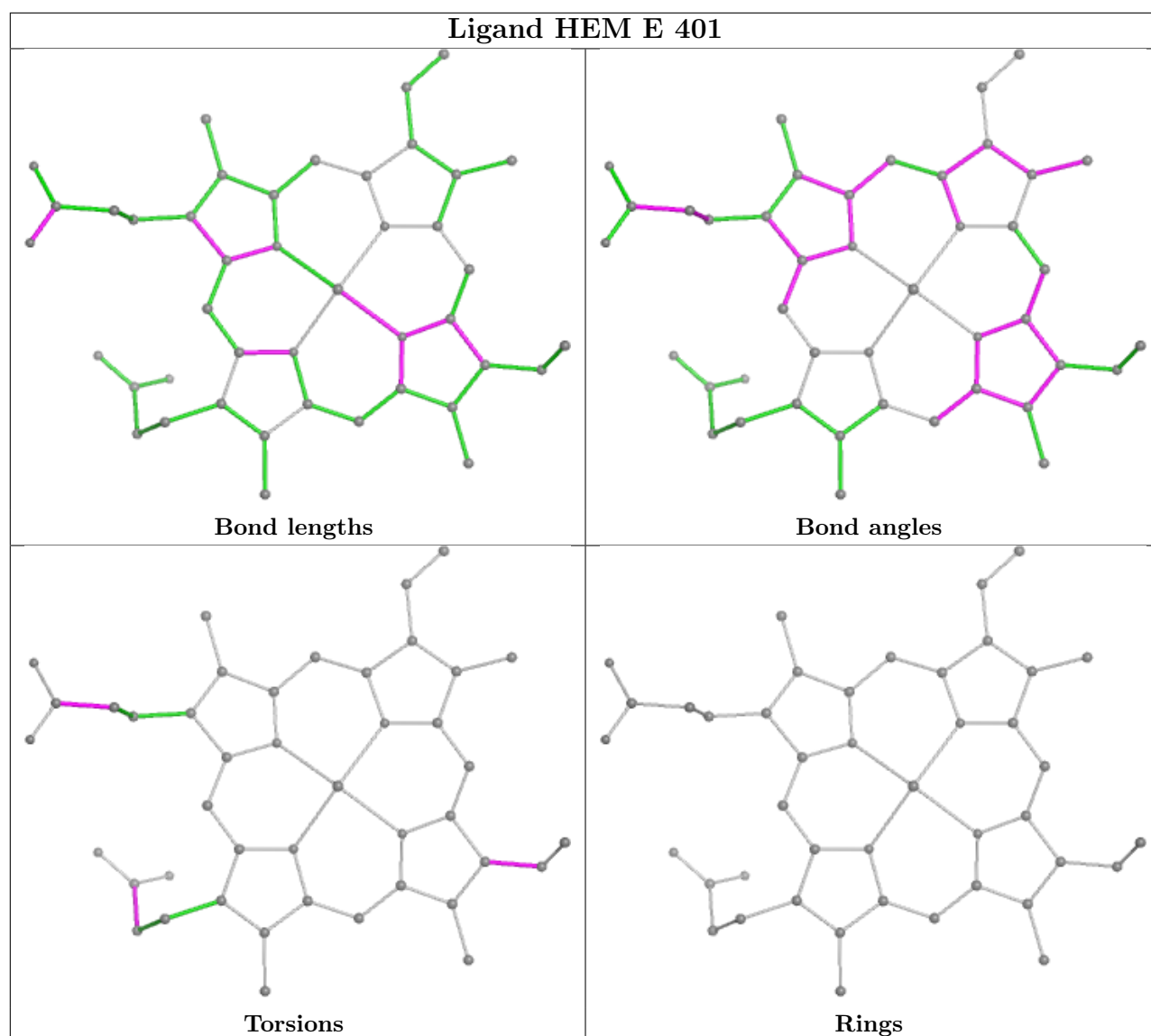
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

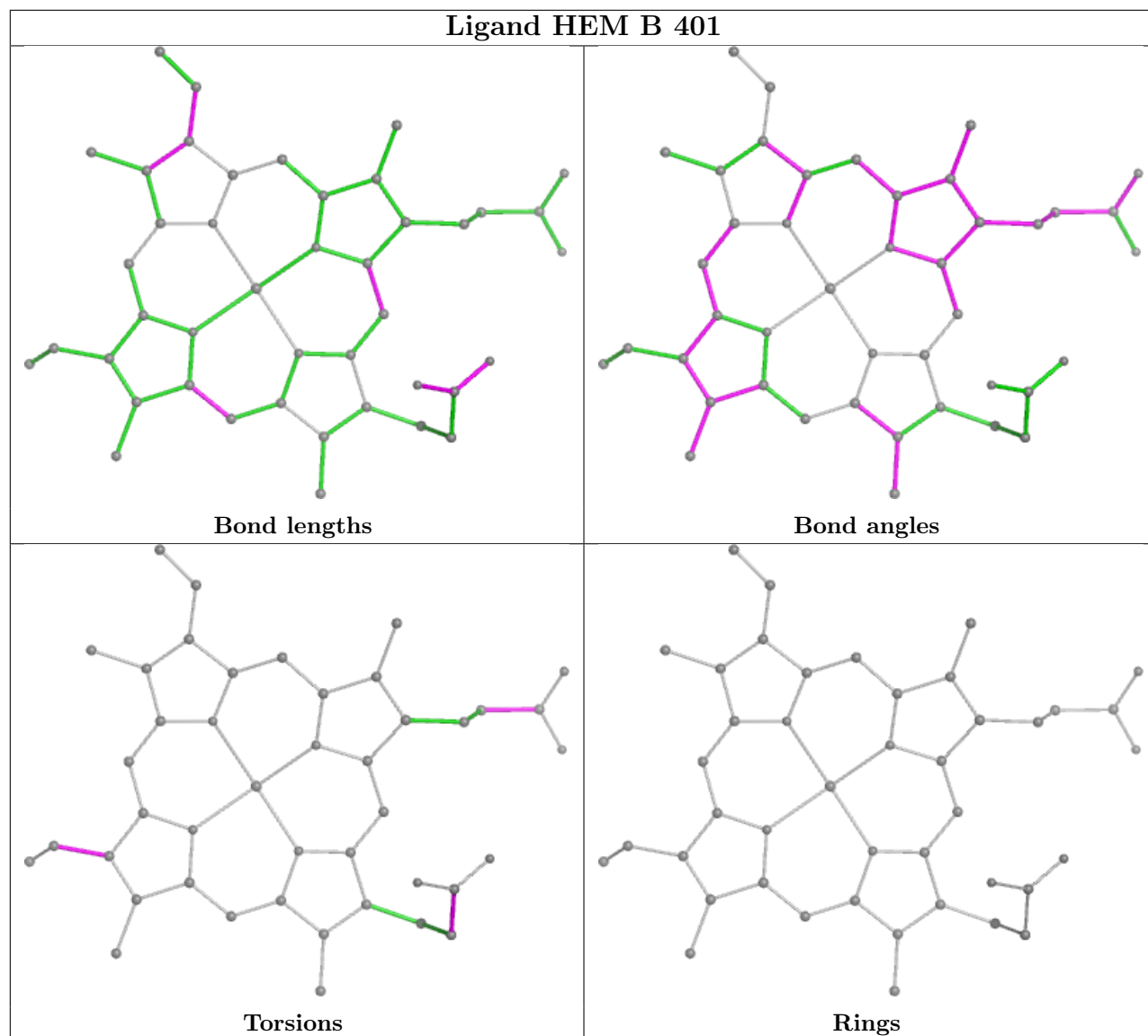












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	311:ASP	C	313:LEU	N	2.10

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%)	0.38	22 (7%)	23	25	10, 20, 43, 78	2 (0%)
1	B	306/316 (96%)	0.18	23 (7%)	22	24	7, 16, 42, 75	9 (2%)
1	C	306/316 (96%)	0.97	50 (16%)	5	5	12, 25, 55, 82	2 (0%)
1	D	306/316 (96%)	0.28	27 (8%)	17	18	6, 18, 44, 87	5 (1%)
1	E	305/316 (96%)	0.32	27 (8%)	17	18	9, 19, 45, 79	2 (0%)
1	F	305/316 (96%)	0.25	24 (7%)	20	22	7, 18, 44, 84	6 (1%)
All	All	1834/1896 (96%)	0.40	173 (9%)	15	17	6, 19, 47, 87	26 (1%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	313	LEU	7.7
1	C	219	VAL	6.4
1	B	312	LEU	6.3
1	C	312	LEU	6.2
1	C	234	PRO	5.8
1	E	8	PRO	5.3
1	D	234	PRO	5.2
1	F	8	PRO	4.8
1	C	8	PRO	4.5
1	C	93	VAL	4.5
1	C	222	ALA	4.4
1	B	234	PRO	4.3
1	D	236	GLY	4.2
1	F	234	PRO	4.1
1	E	234	PRO	4.0
1	C	218	ASP	4.0
1	E	235	ASP	4.0
1	C	170	ALA	3.9
1	D	237	SER	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	VAL	3.9
1	B	238	ASP	3.9
1	B	237	SER	3.8
1	E	237	SER	3.8
1	B	93	VAL	3.8
1	E	218	ASP	3.7
1	D	239	LEU	3.7
1	E	312	LEU	3.7
1	E	236	GLY	3.6
1	C	239	LEU	3.6
1	D	311	ASP	3.6
1	D	235	ASP	3.6
1	D	219	VAL	3.5
1	C	92	PRO	3.4
1	E	231	VAL	3.3
1	D	310	GLU	3.3
1	C	282	ALA	3.2
1	A	222	ALA	3.2
1	E	238	ASP	3.2
1	D	217	ASP	3.2
1	C	7	GLU	3.1
1	C	238	ASP	3.1
1	B	235	ASP	3.1
1	B	236	GLY	3.1
1	C	231	VAL	3.1
1	E	170	ALA	3.1
1	F	76	SER	3.1
1	C	75	PHE	3.1
1	E	233	GLY	3.1
1	C	235	ASP	3.0
1	D	232	THR	3.0
1	D	8	PRO	3.0
1	D	7	GLU	3.0
1	F	239	LEU	3.0
1	C	30	SER	3.0
1	B	127	ARG	2.9
1	F	312	LEU	2.9
1	C	233	GLY	2.9
1	A	282	ALA	2.9
1	E	219	VAL	2.9
1	C	127	ARG	2.9
1	C	76	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	173	PRO	2.9
1	E	239	LEU	2.9
1	A	128	GLY	2.8
1	C	195	GLY	2.8
1	D	233	GLY	2.8
1	F	30	SER	2.8
1	E	311	ASP	2.8
1	B	8	PRO	2.8
1	C	37	ARG	2.8
1	C	77	GLY	2.7
1	D	282	ALA	2.7
1	A	234	PRO	2.7
1	C	56	PRO	2.7
1	F	235	ASP	2.7
1	A	232	THR	2.7
1	E	282	ALA	2.7
1	A	218	ASP	2.6
1	D	76	SER	2.6
1	C	221	PRO	2.6
1	C	128	GLY	2.6
1	E	222	ALA	2.6
1	D	238	ASP	2.6
1	A	127	ARG	2.6
1	A	8	PRO	2.6
1	A	310	GLU	2.6
1	D	231	VAL	2.5
1	C	278	PHE	2.5
1	F	283	SER	2.5
1	A	7	GLU	2.5
1	B	92	PRO	2.5
1	B	87	ARG	2.5
1	C	279	LEU	2.5
1	F	236	GLY	2.5
1	F	231	VAL	2.5
1	C	308	PHE	2.5
1	C	236	GLY	2.5
1	B	232	THR	2.5
1	D	268	GLU	2.5
1	F	237	SER	2.5
1	C	95	ARG	2.4
1	F	127	ARG	2.4
1	B	283	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	55	GLN	2.4
1	B	311	ASP	2.4
1	C	216	SER	2.4
1	F	282	ALA	2.4
1	C	232	THR	2.4
1	C	55	GLN	2.4
1	D	253	ARG	2.4
1	B	7	GLU	2.4
1	B	282	ALA	2.4
1	E	78	ALA	2.4
1	E	232	THR	2.4
1	D	92	PRO	2.4
1	B	217	ASP	2.4
1	A	163	ARG	2.3
1	F	310	GLU	2.3
1	C	78	ALA	2.3
1	C	98	ALA	2.3
1	A	311	ASP	2.3
1	B	218	ASP	2.3
1	B	219	VAL	2.3
1	C	97	VAL	2.3
1	E	57	ASP	2.3
1	F	232	THR	2.3
1	E	93	VAL	2.3
1	E	76	SER	2.3
1	C	311	ASP	2.3
1	C	39	LEU	2.3
1	C	74	LEU	2.3
1	A	92	PRO	2.3
1	A	216	SER	2.3
1	D	56	PRO	2.3
1	C	71	TRP	2.3
1	C	223	ASP	2.3
1	F	238	ASP	2.3
1	E	163	ARG	2.2
1	B	239	LEU	2.2
1	D	279	LEU	2.2
1	D	77	GLY	2.2
1	B	271	GLU	2.2
1	C	174	ALA	2.2
1	F	233	GLY	2.2
1	B	310	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	85	PRO	2.2
1	A	55	GLN	2.2
1	B	55	GLN	2.2
1	C	283	SER	2.2
1	E	284	ALA	2.1
1	F	216	SER	2.1
1	E	310	GLU	2.1
1	A	93	VAL	2.1
1	A	195	GLY	2.1
1	E	92	PRO	2.1
1	E	174	ALA	2.1
1	C	163	ARG	2.1
1	D	163	ARG	2.1
1	A	279	LEU	2.1
1	A	312	LEU	2.1
1	E	56	PRO	2.1
1	F	93	VAL	2.1
1	C	310	GLU	2.1
1	F	160	ALA	2.1
1	C	90	ASP	2.1
1	F	218	ASP	2.1
1	A	239	LEU	2.1
1	A	236	GLY	2.1
1	F	307	ASP	2.0
1	D	93	VAL	2.0
1	F	219	VAL	2.0
1	C	217	ASP	2.0
1	D	218	ASP	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,

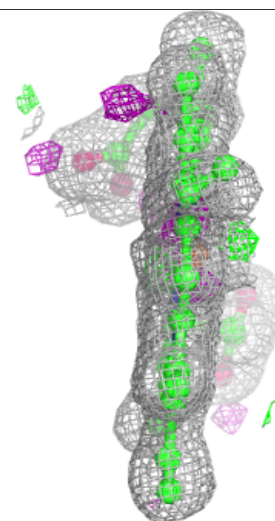
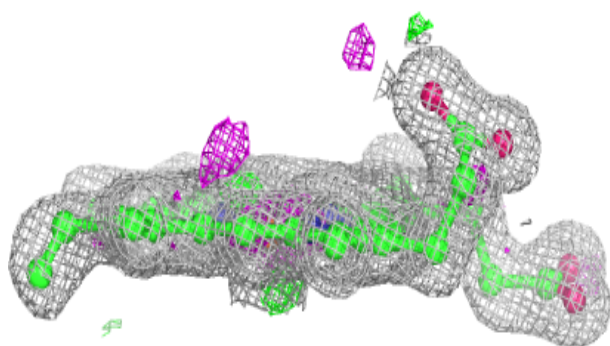
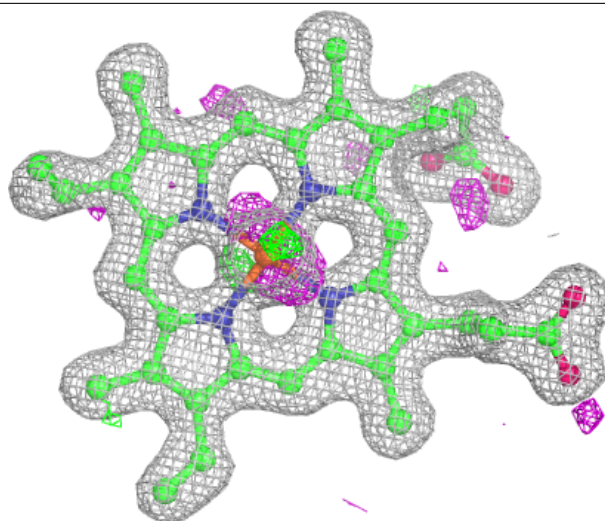
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NO	F	402	2/2	0.88	0.24	30,30,30,58	0
3	NO	C	402	2/2	0.91	0.16	38,38,38,52	0
3	NO	D	402	2/2	0.94	0.20	35,35,35,37	0
3	NO	A	402	2/2	0.94	0.16	30,30,30,49	0
3	NO	E	402	2/2	0.96	0.22	32,32,32,45	0
2	HEM	C	401	43/43	0.97	0.07	15,20,27,36	0
3	NO	B	402	2/2	0.97	0.21	31,31,31,44	0
2	HEM	A	401	43/43	0.98	0.06	13,16,20,27	0
2	HEM	E	401	43/43	0.99	0.05	12,14,21,26	0
2	HEM	F	401	43/43	0.99	0.06	11,13,18,23	0
2	HEM	B	401	43/43	0.99	0.04	9,11,17,20	0
2	HEM	D	401	43/43	0.99	0.05	12,14,20,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

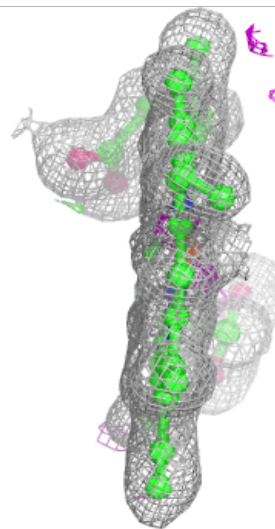
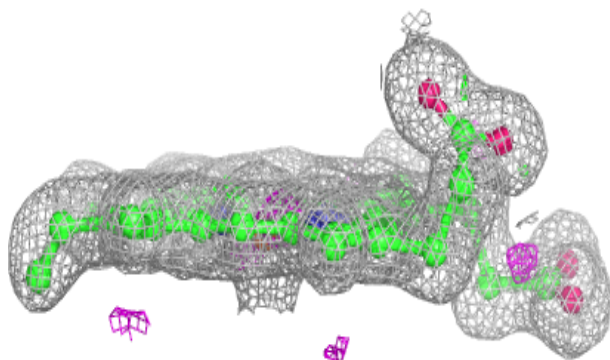
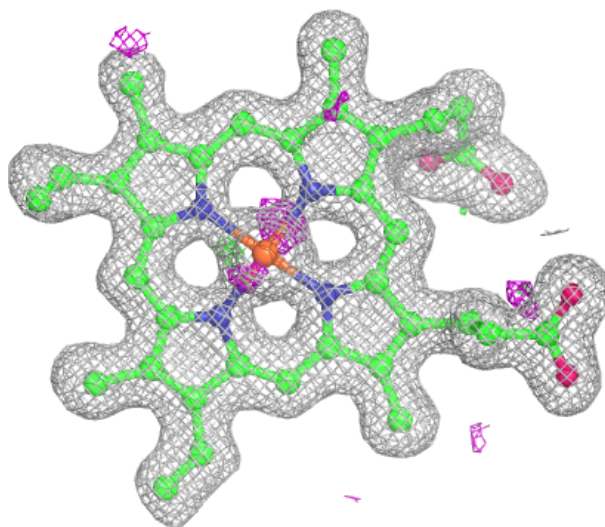
Electron density around HEM C 401:

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



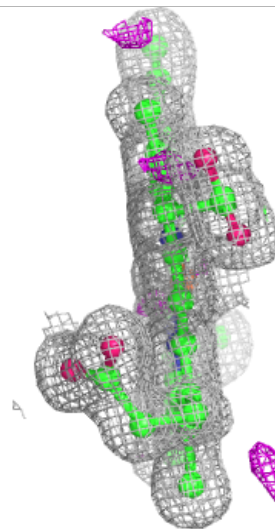
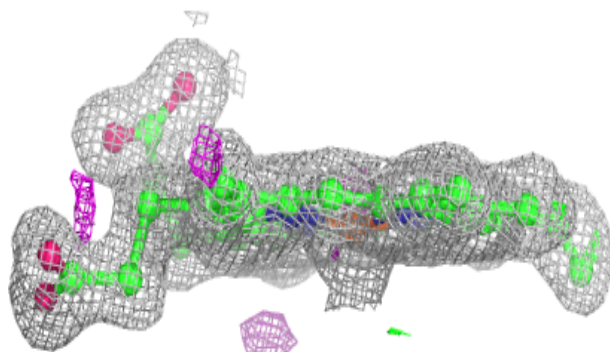
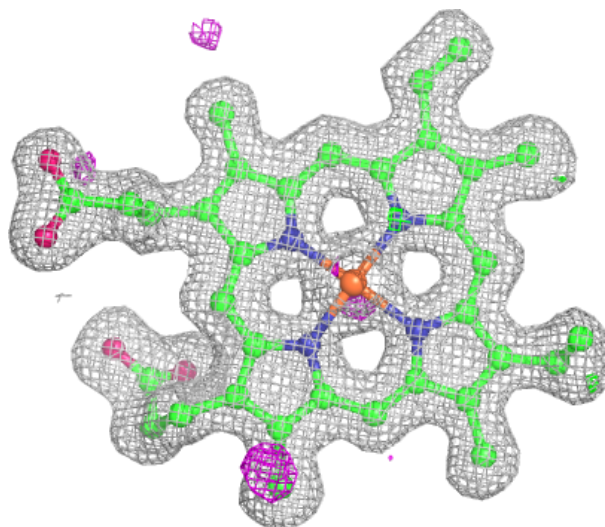
Electron density around HEM A 401:

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



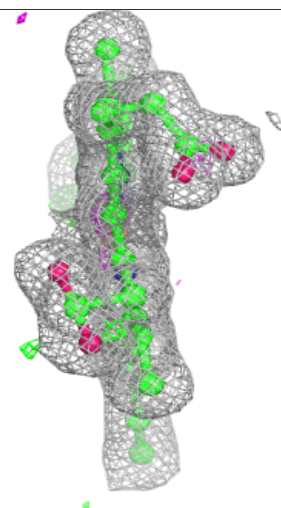
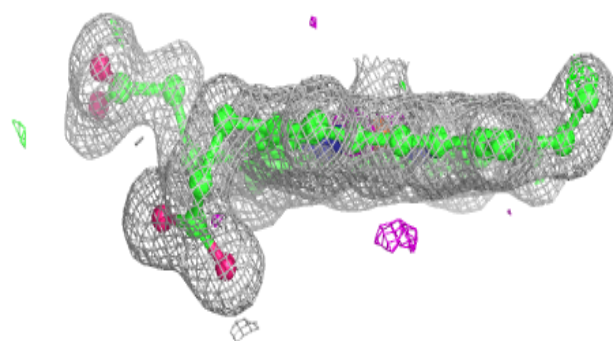
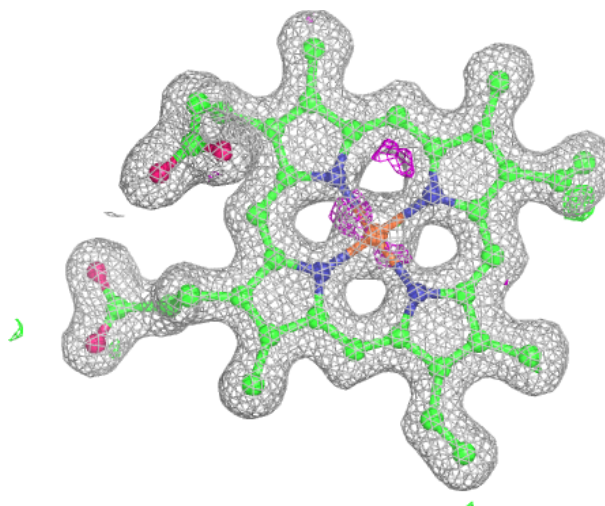
Electron density around HEM E 401:

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



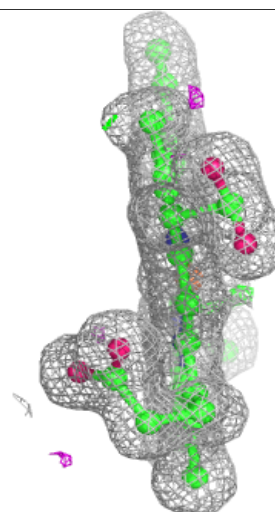
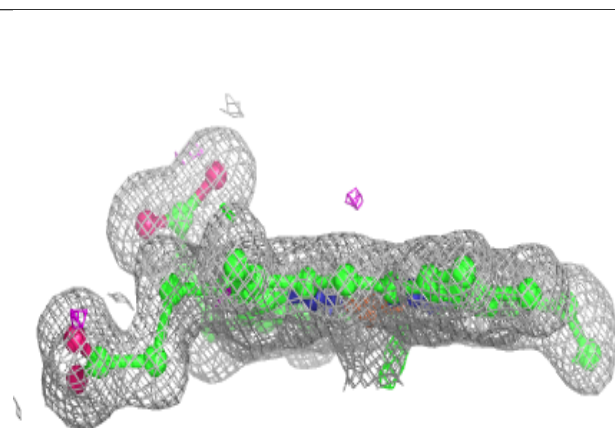
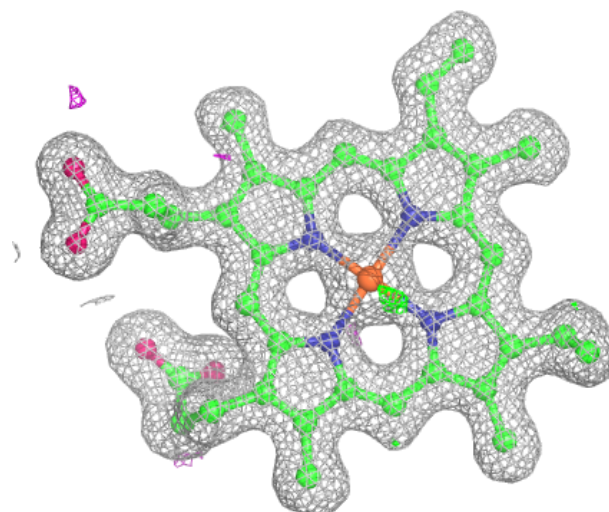
Electron density around HEM F 401:

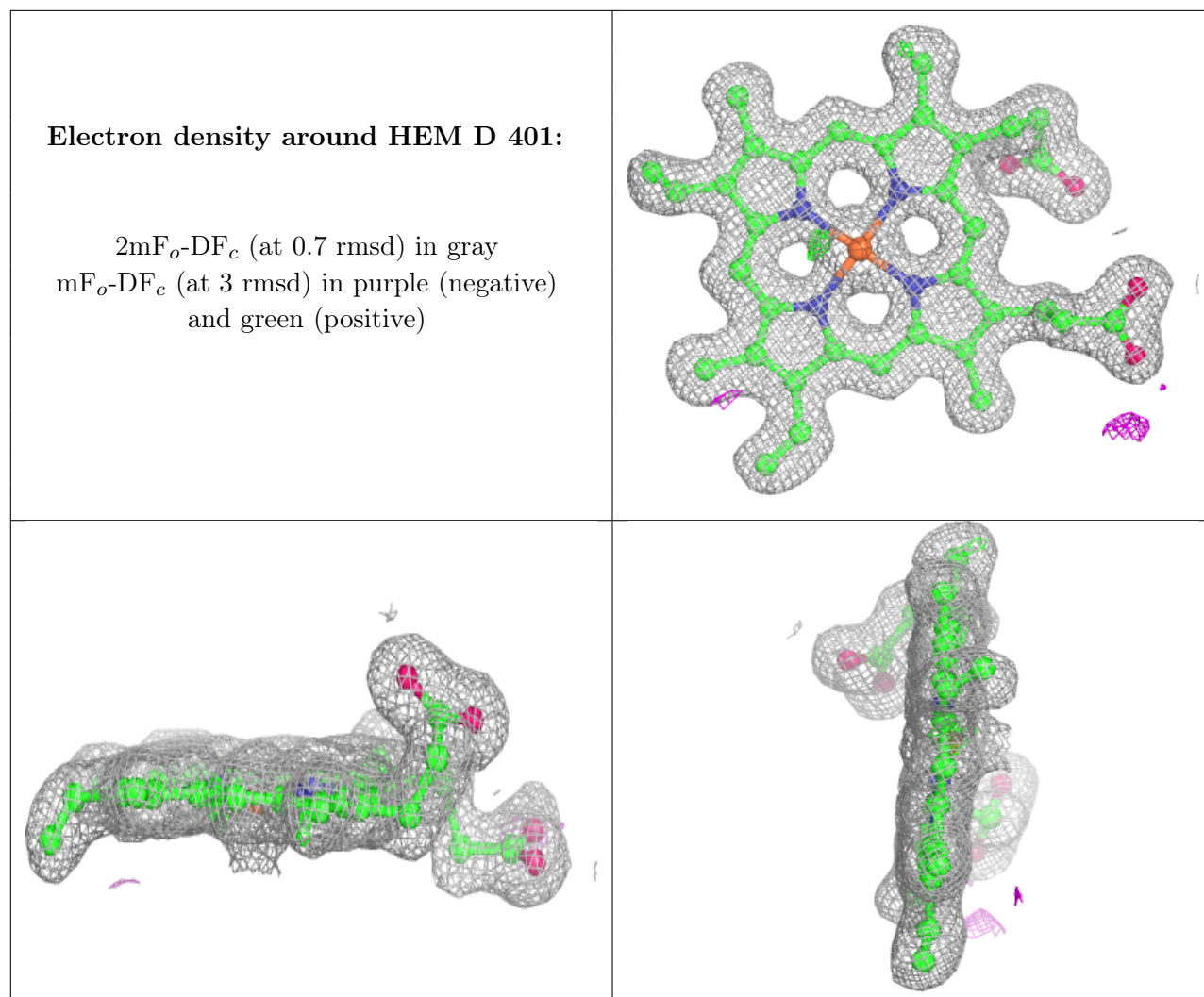
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.