



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:15 PM UTC

PDB ID : 6YR4 / pdb_00006yr4
Title : Dye-type peroxidase DtpB in the ferryl state: Spectroscopically Validated composite structure
Authors : Lucic, M.; Dworkowski, F.S.N.; Worrall, J.A.R.; Hough, M.A.
Deposited on : 2020-04-19
Resolution : 1.85 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

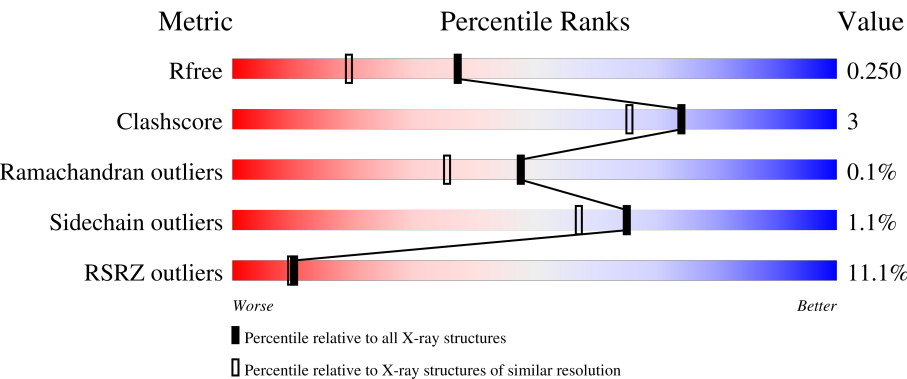
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	
1	B	316	
1	C	316	
1	D	316	
1	E	316	

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Mol	Chain	Length	Quality of chain
1	F	316	9% 92% . .

2 Entry composition [i](#)

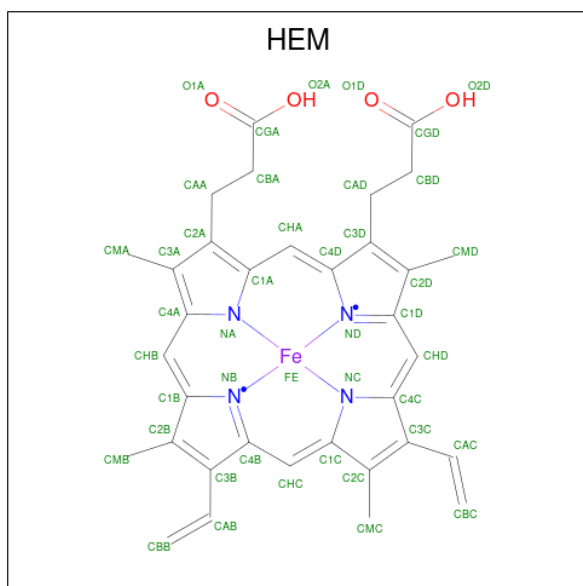
There are 6 unique types of molecules in this entry. The entry contains 15395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 iron-dependent peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	3	0
			2333	1471	398	455	9			
1	B	305	Total	C	N	O	S	0	1	0
			2317	1460	403	445	9			
1	C	306	Total	C	N	O	S	0	2	0
			2341	1474	402	455	10			
1	D	303	Total	C	N	O	S	0	0	0
			2307	1451	399	448	9			
1	E	306	Total	C	N	O	S	0	0	0
			2309	1454	396	450	9			
1	F	306	Total	C	N	O	S	0	2	0
			2314	1458	394	453	9			

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

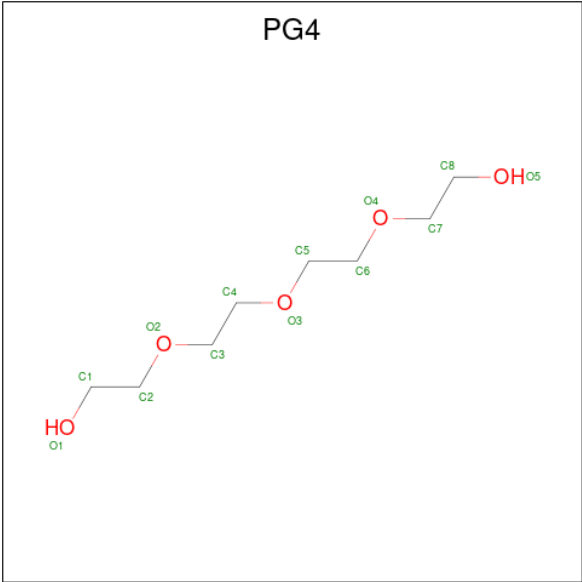
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

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



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

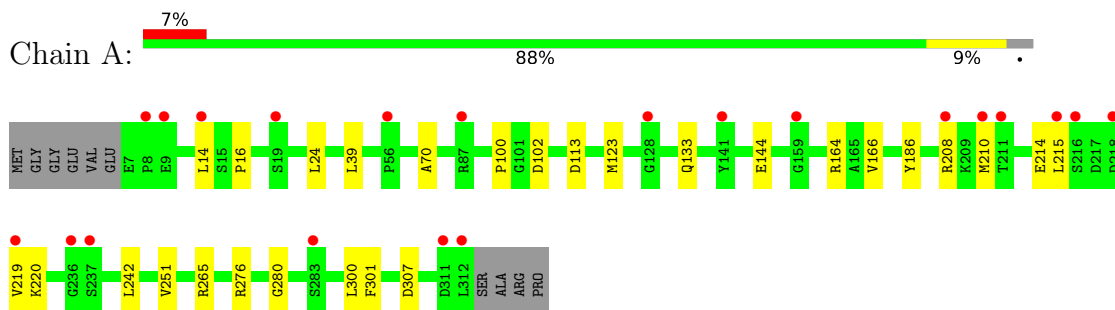
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total	O	0	0
			224	224		
6	B	140	Total	O	0	1
			140	140		
6	C	208	Total	O	0	0
			208	208		
6	D	210	Total	O	0	0
			210	210		
6	E	183	Total	O	0	0
			183	183		
6	F	230	Total	O	0	0
			230	230		

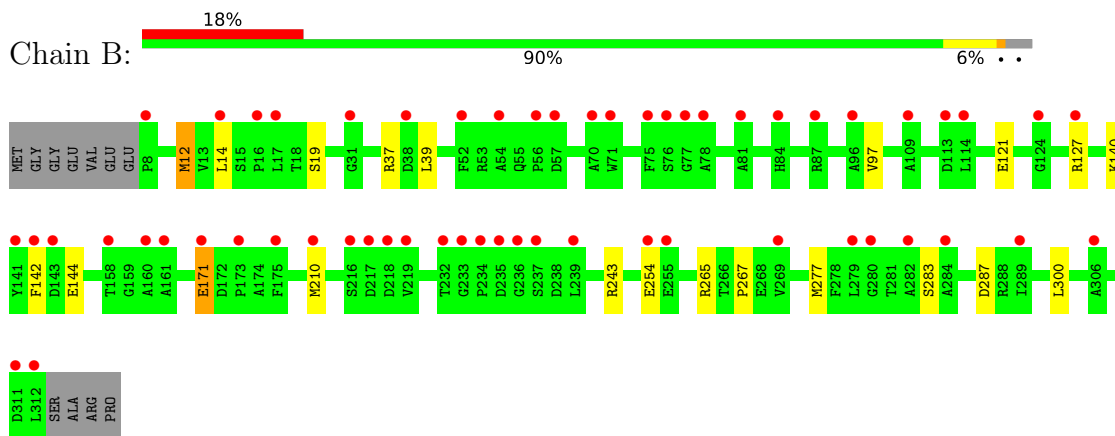
3 Residue-property plots [i](#)

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

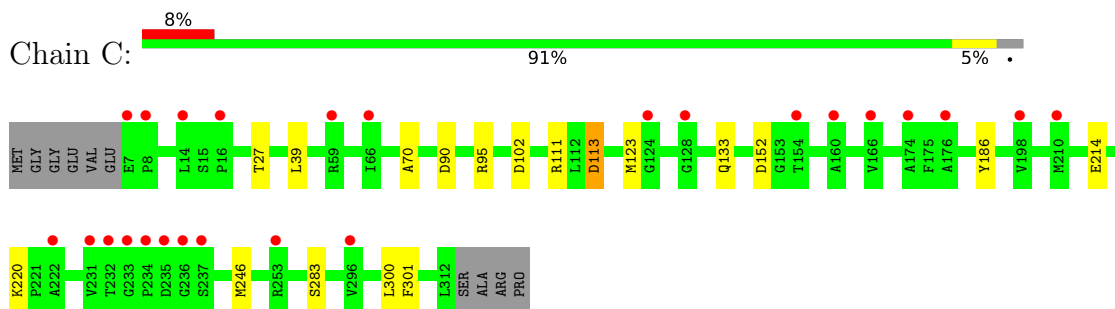
- Molecule 1: Putative iron-dependent peroxidase



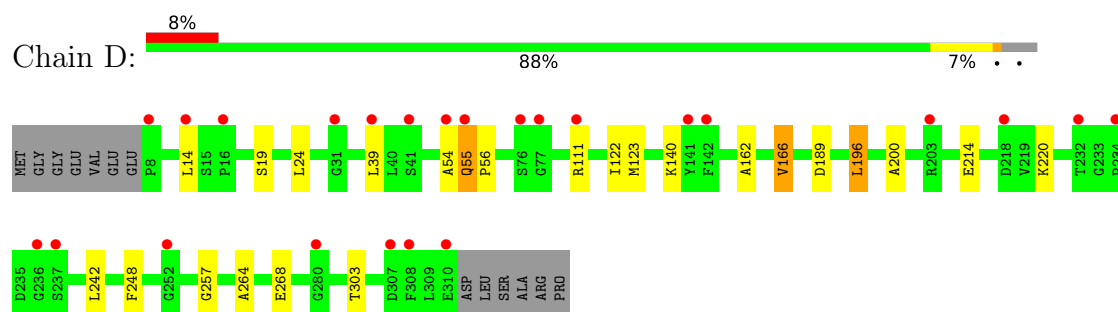
- Molecule 1: Putative iron-dependent peroxidase



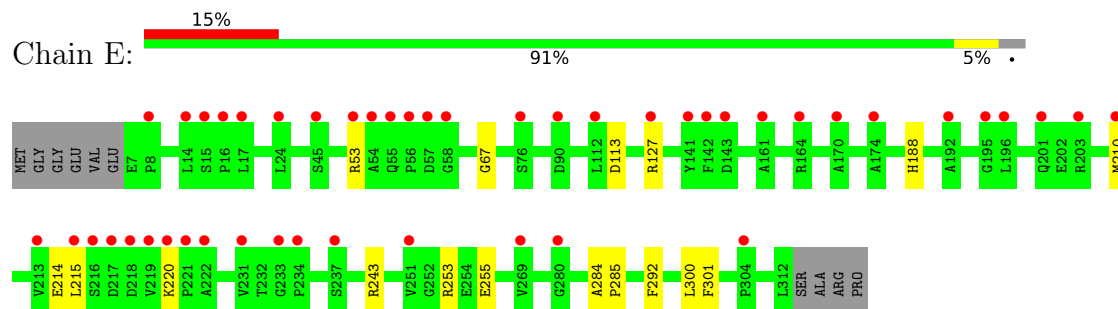
- Molecule 1: Putative iron-dependent peroxidase



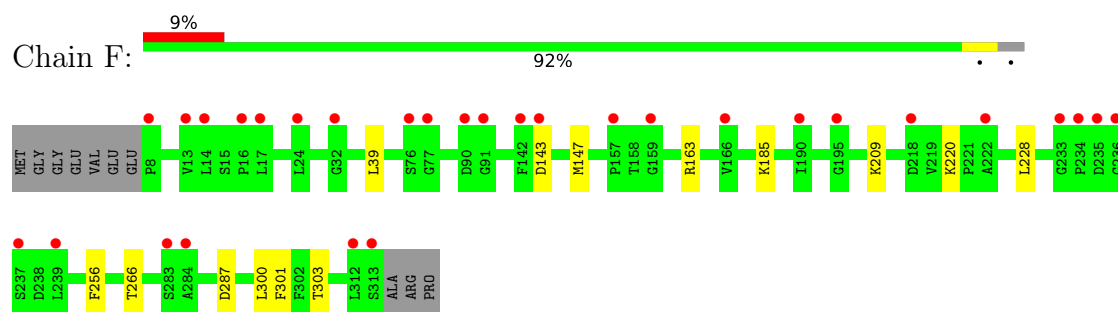
- Molecule 1: Putative iron-dependent peroxidase



- Molecule 1: Putative iron-dependent peroxidase



- Molecule 1: Putative iron-dependent peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.35Å 119.91Å 194.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 1.85 47.61 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.8 (47.61-1.85) 73.7 (47.61-1.85)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.188 , 0.232 (Not available) , 0.250	Depositor DCC
R_{free} test set	7982 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.9	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	0.92	EDS
Total number of atoms	15395	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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, O, MG, PG4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	0/2389	1.31	2/3246 (0.1%)
1	B	1.02	0/2367	1.35	1/3215 (0.0%)
1	C	1.02	0/2391	1.31	2/3248 (0.1%)
1	D	1.00	0/2357	1.33	3/3201 (0.1%)
1	E	1.03	0/2358	1.34	2/3206 (0.1%)
1	F	1.02	0/2363	1.32	1/3212 (0.0%)
All	All	1.02	0/14225	1.33	11/19328 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	PHE	CB-CA-C	6.25	121.04	109.54
1	A	113	ASP	CA-CB-CG	5.79	118.39	112.60
1	F	303	THR	CB-CA-C	5.78	115.64	110.44
1	C	113	ASP	CA-CB-CG	5.70	118.30	112.60
1	D	303	THR	CB-CA-C	5.30	115.21	110.44
1	A	16	PRO	N-CA-C	-5.26	103.81	111.33
1	E	67	GLY	CA-C-N	5.23	127.60	120.54
1	E	67	GLY	C-N-CA	5.23	127.60	120.54
1	D	264	ALA	CA-C-N	5.10	127.83	120.38
1	D	264	ALA	C-N-CA	5.10	127.83	120.38
1	C	152	ASP	CB-CA-C	5.10	117.99	110.14

There are no chirality outliers.

There are no planarity outliers.

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	2333	0	2251	16	0
1	B	2317	0	2247	21	0
1	C	2341	0	2264	12	0
1	D	2307	0	2237	14	0
1	E	2309	0	2225	10	0
1	F	2314	0	2212	12	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
2	E	43	0	30	0	0
2	F	43	0	30	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	F	1	0	0	0	0
5	D	13	0	18	0	0
6	A	224	0	0	1	0
6	B	140	0	0	2	0
6	C	208	0	0	3	0
6	D	210	0	0	2	0
6	E	183	0	0	1	0
6	F	230	0	0	2	0
All	All	15395	0	13634	86	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 (86) 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:37[B]:ARG:HH11	1:B:37[B]:ARG:HB2	1.36	0.90
1:B:12:MET:HE3	1:B:12:MET:HA	1.63	0.81
1:A:214:GLU:OE2	1:A:220:LYS:NZ	2.12	0.77
1:B:37[B]:ARG:HH11	1:B:37[B]:ARG:CB	1.99	0.75
1:A:14:LEU:HD23	1:A:242:LEU:HD22	1.72	0.72
1:A:144:GLU:OE1	6:A:501:HOH:O	2.10	0.68
1:B:37[B]:ARG:HH11	1:B:37[B]:ARG:CG	2.09	0.66
1:B:210:MET:HE1	1:F:209:LYS:HE2	1.80	0.62
2:B:401:HEM:HBC2	2:B:401:HEM:HMC2	1.83	0.60
1:A:14:LEU:HD23	1:A:242:LEU:CD2	2.31	0.60
1:C:111:ARG:HD2	1:C:113:ASP:OD1	2.02	0.59
1:A:100:PRO:O	1:A:133[B]:GLN:HG2	2.04	0.57
1:B:12:MET:HA	1:B:12:MET:CE	2.36	0.55
1:D:214:GLU:OE1	6:D:501:HOH:O	2.18	0.55
1:C:246[A]:MET:HE3	6:C:651:HOH:O	2.08	0.54
1:E:53:ARG:HD2	1:F:143:ASP:OD2	2.07	0.53
1:F:300:LEU:HD23	1:F:301:PHE:N	2.24	0.52
1:F:163:ARG:CD	1:F:163:ARG:NH1	2.72	0.52
1:D:39:LEU:O	1:D:39:LEU:HG	2.07	0.52
1:D:214:GLU:OE2	1:D:220:LYS:NZ	2.22	0.52
1:B:37[B]:ARG:CG	1:B:37[B]:ARG:NH1	2.71	0.52
2:B:401:HEM:HBC2	2:B:401:HEM:CMC	2.40	0.52
1:A:164:ARG:O	1:A:265[A]:ARG:HD2	2.10	0.51
1:B:140:LYS:HD2	1:B:144:GLU:HA	1.91	0.51
1:D:189:ASP:OD2	6:D:502:HOH:O	2.19	0.51
1:E:113:ASP:OD1	6:E:501:HOH:O	2.19	0.50
1:D:19:SER:HA	1:D:140:LYS:HB2	1.94	0.50
1:B:254:GLU:HG2	1:E:127:ARG:NH1	2.27	0.50
1:C:90:ASP:OD1	1:C:95:ARG:NH1	2.45	0.50
1:F:147:MET:CG	1:F:256:PHE:HB3	2.42	0.50
1:B:12:MET:HE2	1:B:14:LEU:O	2.12	0.49
2:A:401:HEM:HMC2	2:A:401:HEM:HBC2	1.94	0.49
1:B:39:LEU:C	1:B:39:LEU:HD13	2.38	0.48
1:D:162:ALA:O	1:D:166:VAL:HG13	2.13	0.48
1:A:251:VAL:HG12	1:C:123:MET:HG3	1.95	0.48
1:D:55:GLN:CB	1:D:56:PRO:CD	2.92	0.48
1:F:185:LYS:NZ	6:F:508:HOH:O	2.47	0.47
2:D:401:HEM:HMC2	2:D:401:HEM:HBC2	1.95	0.47
1:E:188:HIS:HA	1:E:292:PHE:O	2.14	0.47
1:D:196:LEU:HB3	1:D:200:ALA:HB3	1.96	0.47
1:C:214:GLU:OE2	1:C:220:LYS:NZ	2.40	0.47
1:A:39:LEU:C	1:A:39:LEU:HD13	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLU:OE2	1:B:265:ARG:NE	2.35	0.47
1:D:14:LEU:HD13	1:D:242:LEU:HD22	1.95	0.47
1:F:228:LEU:HD12	1:F:287:ASP:HA	1.96	0.47
1:F:147:MET:HG3	1:F:256:PHE:HB3	1.97	0.47
1:C:186:TYR:CG	2:C:401:HEM:HBB1	2.51	0.45
1:C:246[A]:MET:CE	6:C:681:HOH:O	2.64	0.45
2:F:401:HEM:HBC2	2:F:401:HEM:HMC2	1.98	0.45
1:E:243:ARG:HD2	4:E:402:O:O	2.16	0.45
1:B:267:PRO:HB3	1:B:300:LEU:HD11	1.98	0.45
1:B:97:VAL:HG13	6:B:510:HOH:O	2.17	0.45
1:E:214:GLU:OE2	1:E:220:LYS:NZ	2.37	0.44
1:D:39:LEU:HD21	1:D:122:ILE:HG23	1.99	0.44
1:D:54:ALA:C	1:D:55:GLN:HG2	2.42	0.44
1:D:55:GLN:CB	1:D:56:PRO:HD2	2.47	0.44
1:F:300:LEU:HD23	1:F:300:LEU:C	2.42	0.44
1:F:220:LYS:NZ	6:F:511:HOH:O	2.48	0.43
1:E:300:LEU:HD23	1:E:301:PHE:N	2.33	0.43
1:A:208:ARG:CZ	1:A:215:LEU:HD22	2.48	0.43
1:A:215:LEU:HB3	1:A:219:VAL:HG23	2.00	0.43
1:B:243:ARG:HD2	4:B:402:O:O	2.19	0.43
1:D:248:PHE:CZ	1:D:257:GLY:HA3	2.53	0.43
1:B:37[B]:ARG:NH1	1:B:37[B]:ARG:HG3	2.34	0.43
1:A:300:LEU:HD23	1:A:301:PHE:N	2.33	0.43
1:A:186:TYR:CD1	2:A:401:HEM:HBB1	2.54	0.43
1:C:246[A]:MET:HE2	6:C:546:HOH:O	2.18	0.43
1:A:300:LEU:HD23	1:A:300:LEU:C	2.43	0.43
1:B:210:MET:CE	1:F:209:LYS:HE2	2.47	0.42
2:C:401:HEM:HMC2	2:C:401:HEM:HBC2	2.02	0.42
1:E:253:ARG:NH1	1:E:255:GLU:OE1	2.52	0.42
1:A:276:ARG:O	1:A:280:GLY:HA2	2.20	0.41
1:C:70:ALA:HB2	1:C:102:ASP:HB3	2.02	0.41
1:F:39:LEU:C	1:F:39:LEU:HD13	2.45	0.41
1:B:254:GLU:HG2	1:E:127:ARG:CZ	2.50	0.41
1:B:121:GLU:OE2	6:B:501:HOH:O	2.21	0.41
1:C:27:THR:HG23	1:C:133:GLN:HG3	2.01	0.41
1:D:24:LEU:HD21	1:D:123:MET:CG	2.51	0.41
2:A:401:HEM:HBC2	2:A:401:HEM:CMC	2.51	0.41
1:B:300:LEU:HD23	1:B:300:LEU:C	2.46	0.41
1:C:39:LEU:HD13	1:C:39:LEU:C	2.46	0.41
1:C:300:LEU:HD12	1:C:301:PHE:N	2.36	0.41
1:B:277:MET:HA	1:B:287:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:ALA:HA	1:E:285:PRO:HD3	1.98	0.40
1:A:24:LEU:HD21	1:A:123:MET:CG	2.52	0.40
1:A:70:ALA:HB2	1:A:102:ASP:HB3	2.03	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	307/316 (97%)	301 (98%)	6 (2%)	0	100	100
1	B	304/316 (96%)	295 (97%)	9 (3%)	0	100	100
1	C	306/316 (97%)	300 (98%)	6 (2%)	0	100	100
1	D	301/316 (95%)	292 (97%)	8 (3%)	1 (0%)	36	25
1	E	304/316 (96%)	297 (98%)	7 (2%)	0	100	100
1	F	306/316 (97%)	298 (97%)	8 (3%)	0	100	100
All	All	1828/1896 (96%)	1783 (98%)	44 (2%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	55	GLN

5.3.2 Protein sidechains [i](#)

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	242/252 (96%)	239 (99%)	3 (1%)	63	55
1	B	240/252 (95%)	235 (98%)	5 (2%)	47	33
1	C	244/252 (97%)	243 (100%)	1 (0%)	84	82
1	D	242/252 (96%)	238 (98%)	4 (2%)	53	42
1	E	239/252 (95%)	237 (99%)	2 (1%)	73	67
1	F	238/252 (94%)	237 (100%)	1 (0%)	84	82
All	All	1445/1512 (96%)	1429 (99%)	16 (1%)	65	57

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	VAL
1	A	210	MET
1	A	307	ASP
1	B	12	MET
1	B	19	SER
1	B	127	ARG
1	B	171	GLU
1	B	283	SER
1	C	283	SER
1	D	111	ARG
1	D	166	VAL
1	D	196	LEU
1	D	268	GLU
1	E	210	MET
1	E	215	LEU
1	F	266	THR

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

Mol	Chain	Res	Type
1	D	55	GLN
1	F	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	401	1	50,50,50	1.58	6 (12%)	67,82,82	1.78	16 (23%)
2	HEM	F	401	1	50,50,50	1.51	8 (16%)	67,82,82	1.51	9 (13%)
2	HEM	B	401	1,4	50,50,50	1.48	10 (20%)	67,82,82	1.59	11 (16%)
2	HEM	C	401	1,4	50,50,50	1.51	8 (16%)	67,82,82	1.63	12 (17%)
2	HEM	E	401	1,4	50,50,50	1.66	12 (24%)	67,82,82	1.77	15 (22%)
2	HEM	D	401	1,4	50,50,50	1.47	9 (18%)	67,82,82	1.66	12 (17%)
5	PG4	D	402	-	12,12,12	0.25	0	11,11,11	0.16	0

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	A	401	1	-	4/14/54/54	-
2	HEM	F	401	1	-	4/14/54/54	-
2	HEM	B	401	1,4	-	4/14/54/54	-
2	HEM	C	401	1,4	-	4/14/54/54	-
2	HEM	E	401	1,4	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	401	1,4	-	4/14/54/54	-
5	PG4	D	402	-	-	2/10/10/10	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C1B-NB	-4.55	1.32	1.40
2	F	401	HEM	FE-NC	4.49	2.10	1.95
2	A	401	HEM	FE-NB	4.38	2.08	1.94
2	C	401	HEM	FE-NB	4.23	2.07	1.94
2	E	401	HEM	FE-NC	4.12	2.08	1.95
2	C	401	HEM	C1B-NB	-4.03	1.33	1.40
2	B	401	HEM	FE-NB	3.87	2.06	1.94
2	A	401	HEM	FE-NC	3.84	2.07	1.95
2	E	401	HEM	C1B-NB	-3.82	1.33	1.40
2	D	401	HEM	C1B-NB	-3.81	1.33	1.40
2	E	401	HEM	FE-NB	3.65	2.06	1.94
2	E	401	HEM	C4B-NB	-3.64	1.31	1.38
2	B	401	HEM	FE-NC	3.54	2.06	1.95
2	F	401	HEM	FE-NB	3.51	2.05	1.94
2	F	401	HEM	C4D-ND	-3.47	1.34	1.40
2	C	401	HEM	FE-NC	3.42	2.06	1.95
2	A	401	HEM	C4D-ND	-3.40	1.34	1.40
2	D	401	HEM	FE-NB	3.34	2.05	1.94
2	B	401	HEM	C4B-NB	-3.21	1.32	1.38
2	D	401	HEM	C1C-C2C	-3.08	1.39	1.45
2	D	401	HEM	C1D-ND	-3.04	1.32	1.38
2	F	401	HEM	C1B-NB	-3.03	1.35	1.40
2	C	401	HEM	C4D-ND	-3.02	1.35	1.40
2	D	401	HEM	FE-NC	2.93	2.04	1.95
2	B	401	HEM	C4D-ND	-2.84	1.35	1.40
2	E	401	HEM	C1D-ND	-2.83	1.33	1.38
2	E	401	HEM	C4C-NC	-2.78	1.34	1.39
2	B	401	HEM	C1B-NB	-2.76	1.35	1.40
2	E	401	HEM	C1C-NC	-2.74	1.34	1.39
2	E	401	HEM	C4A-NA	-2.69	1.34	1.39
2	D	401	HEM	C4B-NB	-2.66	1.33	1.38
2	B	401	HEM	C1C-NC	-2.66	1.34	1.39
2	C	401	HEM	C3C-C4C	-2.59	1.41	1.46
2	B	401	HEM	FE-ND	-2.47	1.87	1.94
2	A	401	HEM	C3B-C4B	2.47	1.49	1.44
2	F	401	HEM	C1D-ND	-2.43	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C3B-C4B	2.36	1.49	1.44
2	C	401	HEM	C1C-C2C	-2.36	1.40	1.45
2	D	401	HEM	C1C-NC	-2.28	1.35	1.39
2	D	401	HEM	C4D-C3D	2.25	1.48	1.45
2	E	401	HEM	FE-ND	-2.22	1.88	1.94
2	D	401	HEM	C4A-NA	-2.18	1.35	1.39
2	F	401	HEM	C1D-C2D	2.12	1.48	1.44
2	B	401	HEM	O2D-CGD	-2.10	1.23	1.30
2	E	401	HEM	C3D-C2D	-2.08	1.32	1.36
2	A	401	HEM	C4B-NB	-2.07	1.34	1.38
2	F	401	HEM	C1A-NA	-2.07	1.35	1.39
2	E	401	HEM	FE-NA	2.06	2.01	1.95
2	B	401	HEM	C3C-C4C	-2.06	1.42	1.46
2	F	401	HEM	C3B-C4B	2.04	1.48	1.44
2	E	401	HEM	CHB-C1B	2.03	1.42	1.38
2	B	401	HEM	C1D-ND	-2.02	1.34	1.38
2	C	401	HEM	C1D-ND	-2.01	1.34	1.38

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	CHC-C4B-NB	5.82	130.69	124.42
2	A	401	HEM	C3B-C4B-NB	-5.63	105.43	109.47
2	F	401	HEM	CHC-C4B-NB	5.46	130.30	124.42
2	D	401	HEM	CHC-C4B-NB	5.42	130.25	124.42
2	B	401	HEM	CHD-C1D-ND	5.26	130.08	124.42
2	A	401	HEM	C1B-NB-C4B	5.19	111.35	105.21
2	C	401	HEM	C3B-C4B-NB	-4.72	106.08	109.47
2	E	401	HEM	C1B-NB-C4B	4.55	110.59	105.21
2	D	401	HEM	C1B-NB-C4B	4.52	110.56	105.21
2	F	401	HEM	CHD-C1D-ND	4.22	128.97	124.42
2	A	401	HEM	CHC-C4B-NB	4.22	128.96	124.42
2	B	401	HEM	CHC-C4B-NB	3.94	128.66	124.42
2	D	401	HEM	CAD-C3D-C4D	3.61	130.99	124.70
2	C	401	HEM	CHC-C4B-NB	3.57	128.26	124.42
2	C	401	HEM	C1B-NB-C4B	3.57	109.43	105.21
2	B	401	HEM	C1B-NB-C4B	3.55	109.41	105.21
2	B	401	HEM	CHD-C1D-C2D	-3.49	119.52	125.03
2	E	401	HEM	CMD-C2D-C1D	3.47	130.45	125.03
2	F	401	HEM	C1B-NB-C4B	3.46	109.31	105.21
2	B	401	HEM	CHA-C4D-ND	3.33	128.48	124.37
2	A	401	HEM	CHD-C1D-ND	3.32	127.99	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	CHD-C4C-NC	3.30	128.05	124.45
2	E	401	HEM	CHB-C1B-NB	3.26	128.40	124.37
2	F	401	HEM	CHD-C1D-C2D	-3.18	120.01	125.03
2	D	401	HEM	CHD-C1D-C2D	-3.15	120.05	125.03
2	A	401	HEM	CHD-C1D-C2D	-3.08	120.16	125.03
2	E	401	HEM	CHA-C4D-C3D	-3.08	119.55	125.23
2	E	401	HEM	CHA-C4D-ND	3.01	128.09	124.37
2	C	401	HEM	CAB-C3B-C2B	-2.92	118.94	128.43
2	C	401	HEM	CMB-C2B-C1B	2.91	129.59	125.03
2	C	401	HEM	CHD-C1D-C2D	-2.89	120.47	125.03
2	B	401	HEM	CHA-C4D-C3D	-2.88	119.92	125.23
2	D	401	HEM	CHD-C1D-ND	2.87	127.52	124.42
2	B	401	HEM	O2A-CGA-CBA	2.81	122.88	114.00
2	A	401	HEM	CHB-C1B-NB	2.78	127.81	124.37
2	C	401	HEM	CHD-C1D-ND	2.75	127.38	124.42
2	C	401	HEM	CHD-C4C-NC	2.72	127.42	124.45
2	B	401	HEM	CHB-C1B-NB	2.71	127.72	124.37
2	E	401	HEM	CAD-C3D-C4D	2.71	129.42	124.70
2	E	401	HEM	C4C-NC-C1C	2.69	110.20	105.82
2	A	401	HEM	O2D-CGD-CBD	2.68	122.46	114.00
2	C	401	HEM	O2D-CGD-CBD	2.63	122.31	114.00
2	A	401	HEM	O2A-CGA-CBA	2.61	122.23	114.00
2	D	401	HEM	CHB-C1B-NB	2.49	127.45	124.37
2	B	401	HEM	CAD-C3D-C4D	2.46	128.99	124.70
2	A	401	HEM	CHA-C4D-C3D	-2.42	120.76	125.23
2	A	401	HEM	CHD-C4C-NC	2.42	127.09	124.45
2	A	401	HEM	O1A-CGA-CBA	-2.39	115.53	123.09
2	E	401	HEM	C2D-C1D-ND	2.38	112.65	109.90
2	A	401	HEM	CAD-C3D-C4D	2.35	128.79	124.70
2	D	401	HEM	O1D-CGD-CBD	-2.33	115.71	123.09
2	D	401	HEM	C3B-C4B-NB	-2.32	107.80	109.47
2	E	401	HEM	O2A-CGA-CBA	2.32	121.33	114.00
2	F	401	HEM	CHA-C4D-C3D	-2.31	120.98	125.23
2	C	401	HEM	CMB-C2B-C3B	-2.25	122.99	128.43
2	B	401	HEM	C3B-C4B-NB	-2.24	107.86	109.47
2	E	401	HEM	CAA-C2A-C1A	2.23	129.29	124.94
2	E	401	HEM	C3B-C4B-NB	-2.21	107.88	109.47
2	A	401	HEM	CMD-C2D-C1D	2.19	128.46	125.03
2	D	401	HEM	O2D-CGD-CBD	2.16	120.82	114.00
2	F	401	HEM	C3D-C4D-ND	2.15	112.53	110.17
2	A	401	HEM	CMB-C2B-C1B	2.15	128.39	125.03
2	B	401	HEM	C4C-CHD-C1D	-2.14	121.46	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	O2A-CGA-CBA	2.13	120.74	114.00
2	A	401	HEM	CAB-C3B-C2B	-2.12	121.53	128.43
2	D	401	HEM	CHD-C4C-NC	2.10	126.74	124.45
2	A	401	HEM	CHA-C4D-ND	2.10	126.96	124.37
2	D	401	HEM	C2D-C1D-ND	2.08	112.30	109.90
2	F	401	HEM	CMA-C3A-C2A	2.07	130.02	125.62
2	C	401	HEM	CAB-C3B-C4B	2.07	133.54	124.39
2	E	401	HEM	CHD-C1D-C2D	-2.07	121.77	125.03
2	F	401	HEM	C3B-C4B-NB	-2.06	107.99	109.47
2	C	401	HEM	CHA-C4D-C3D	-2.05	121.45	125.23
2	E	401	HEM	C1A-CHA-C4D	-2.05	121.44	126.25
2	D	401	HEM	CHA-C1A-NA	2.02	127.52	123.86

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	402	PG4	C8-C7-O4-C6
5	D	402	PG4	C5-C6-O4-C7
2	A	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAA-CBA-CGA-O2A
2	E	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAA-CBA-CGA-O1A
2	D	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	A	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	E	401	HEM	CAA-CBA-CGA-O2A
2	E	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	F	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAD-CBD-CGD-O2D

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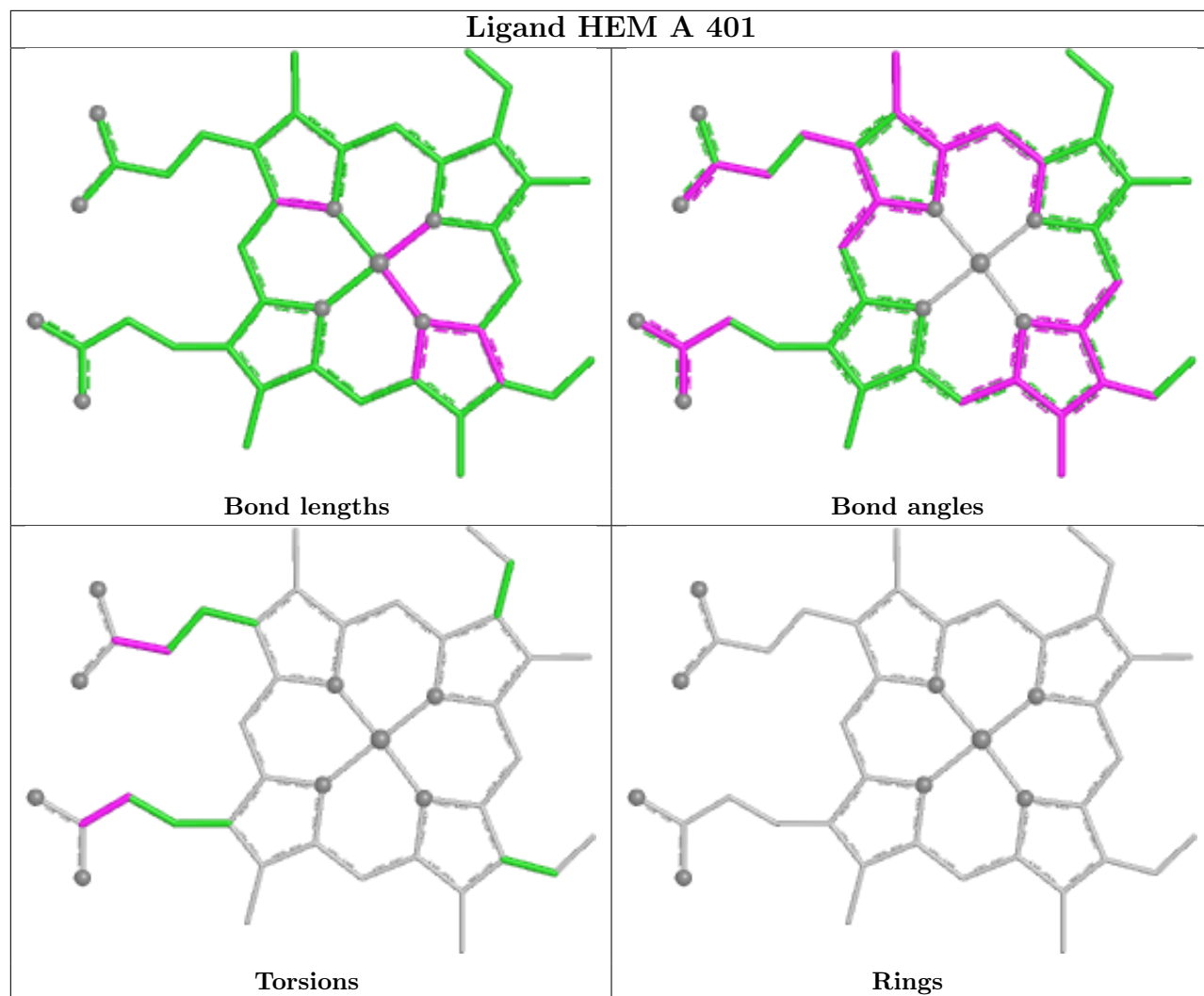
Mol	Chain	Res	Type	Atoms
2	C	401	HEM	CAA-CBA-CGA-O1A

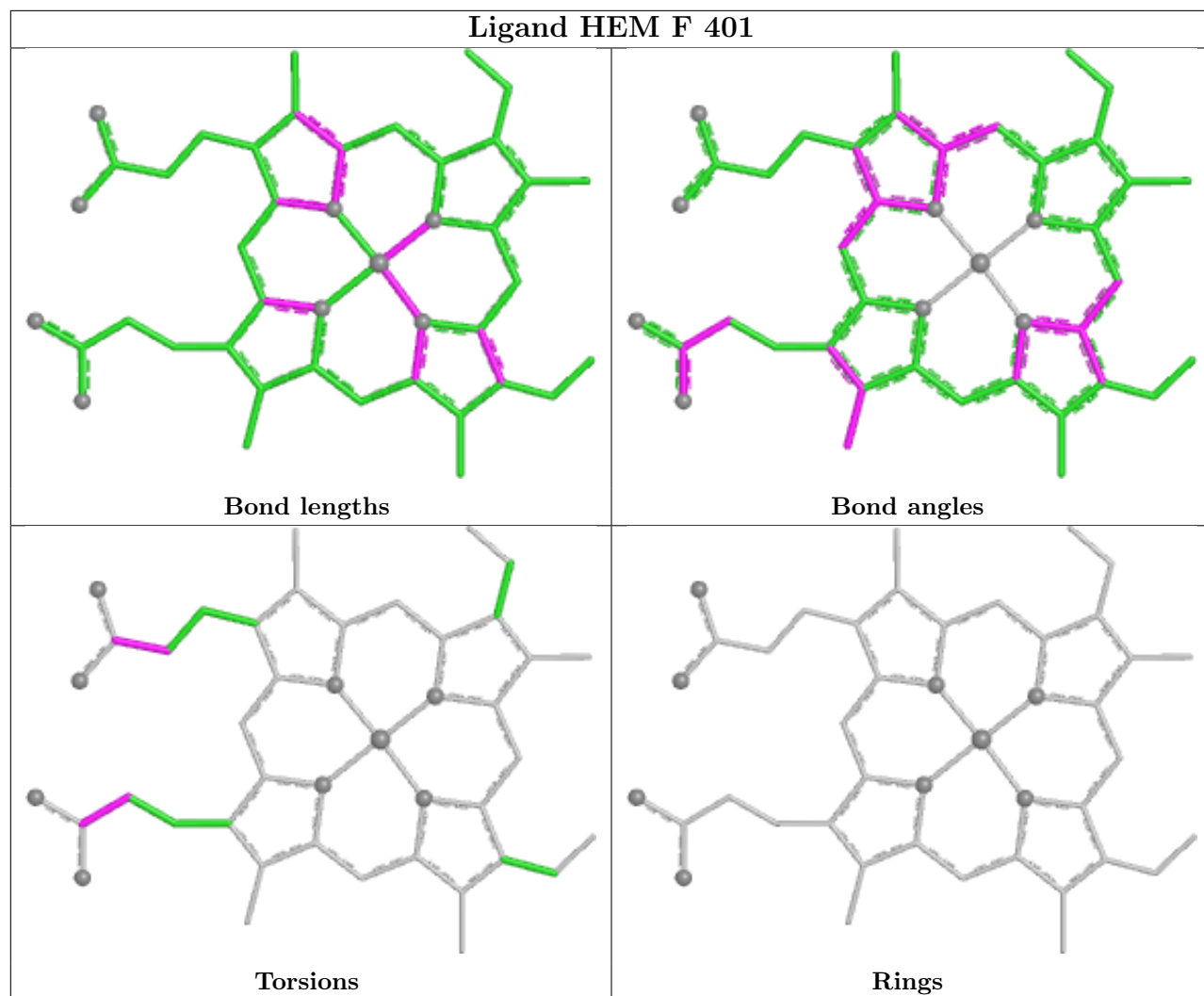
There are no ring outliers.

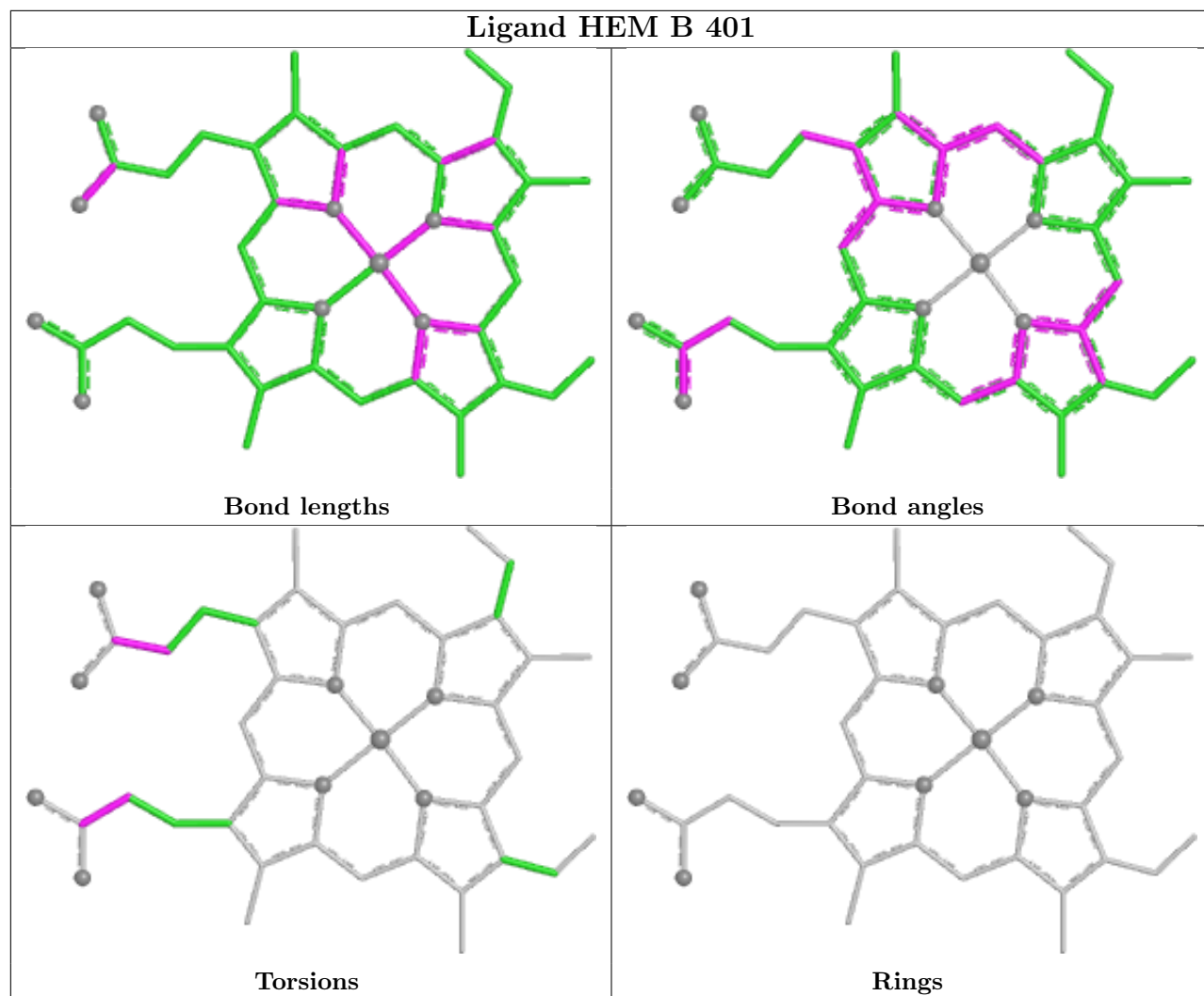
5 monomers are involved in 9 short contacts:

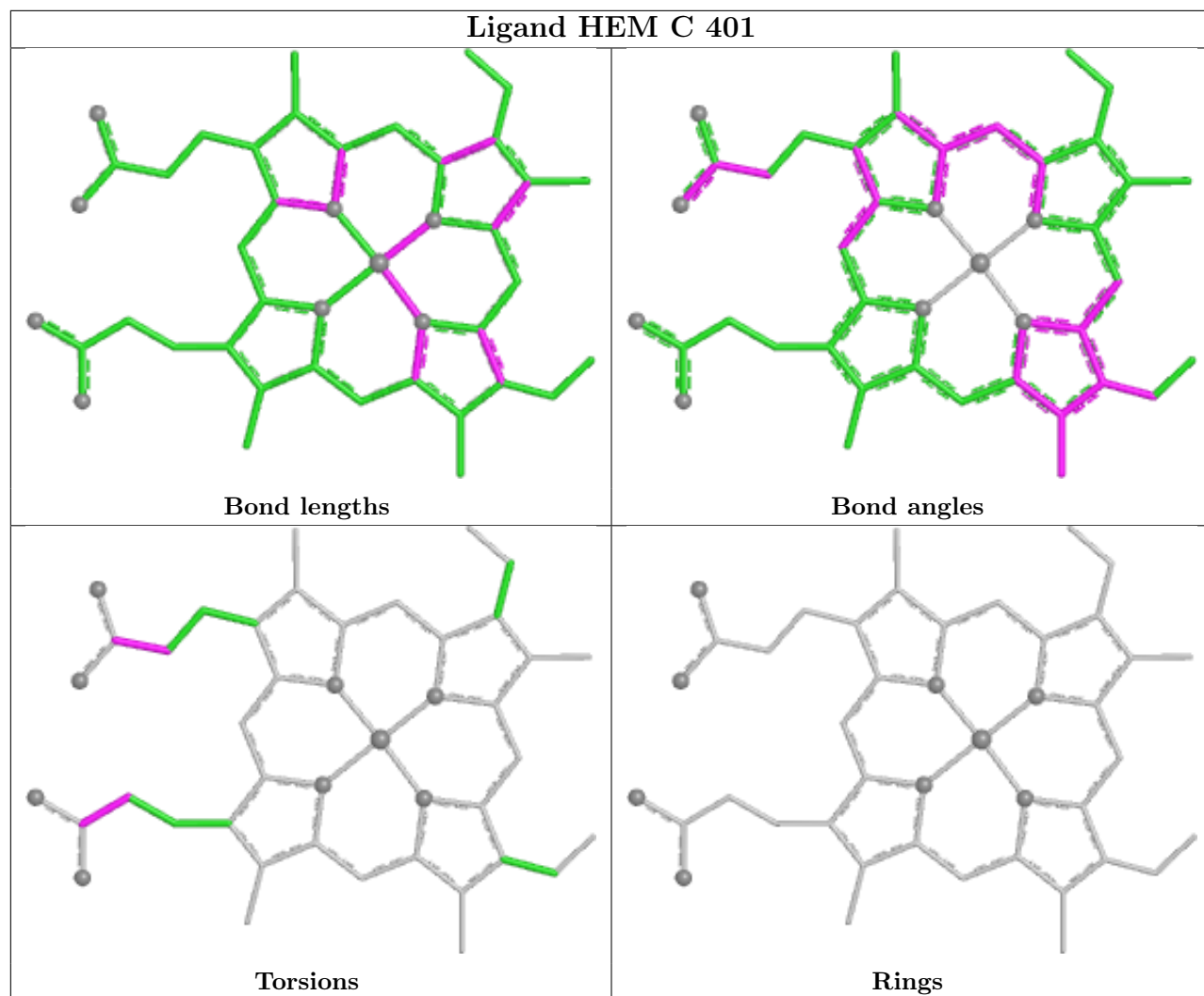
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	3	0
2	F	401	HEM	1	0
2	B	401	HEM	2	0
2	C	401	HEM	2	0
2	D	401	HEM	1	0

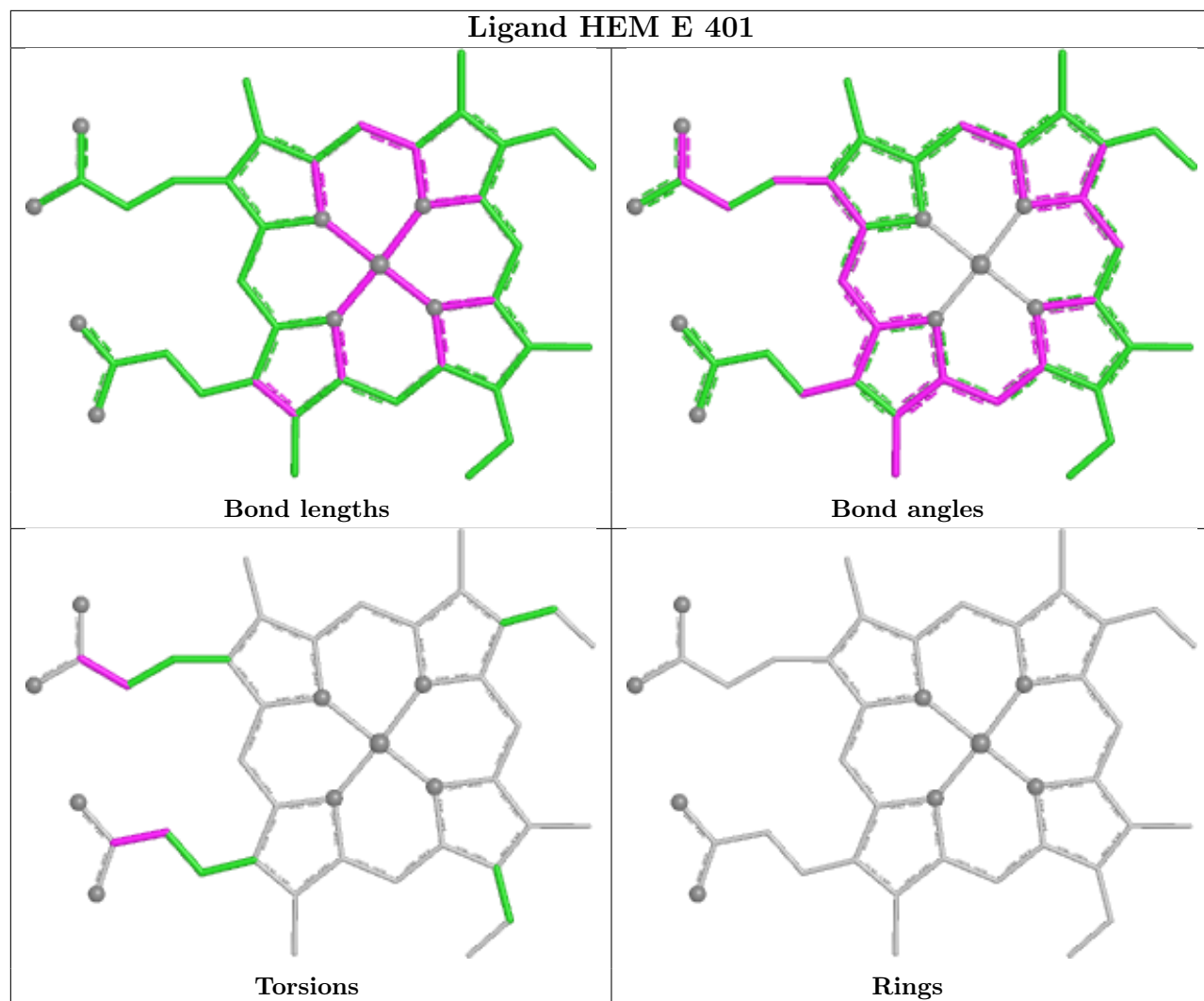
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

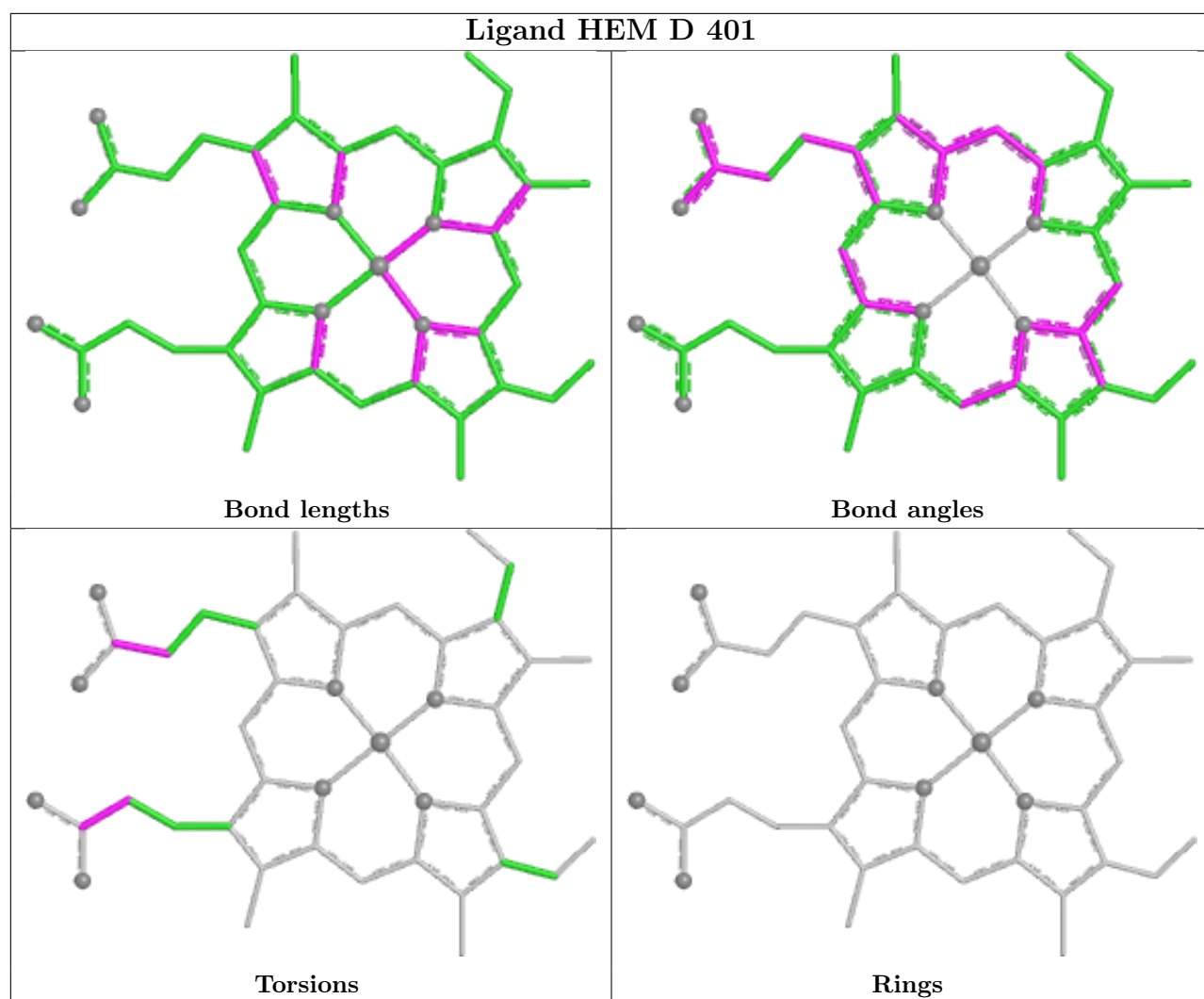












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.60	21 (6%)	23 25	12, 23, 39, 56	3 (0%)
1	B	305/316 (96%)	1.11	57 (18%)	3 3	17, 27, 47, 70	1 (0%)
1	C	306/316 (96%)	0.79	25 (8%)	17 18	11, 24, 41, 67	2 (0%)
1	D	303/316 (95%)	0.76	24 (7%)	18 19	16, 24, 42, 58	0
1	E	306/316 (96%)	0.93	47 (15%)	5 5	19, 26, 45, 67	0
1	F	306/316 (96%)	0.84	30 (9%)	13 13	11, 24, 40, 68	2 (0%)
All	All	1832/1896 (96%)	0.84	204 (11%)	10 10	11, 25, 43, 70	8 (0%)

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	GLY	7.5
1	A	218	ASP	6.4
1	E	142	PHE	6.0
1	D	77	GLY	5.8
1	F	234	PRO	5.7
1	B	142	PHE	5.6
1	F	233	GLY	5.4
1	E	219	VAL	4.9
1	F	142	PHE	4.9
1	D	55	GLN	4.7
1	B	284	ALA	4.5
1	B	312	LEU	4.4
1	C	234	PRO	4.4
1	D	234	PRO	4.4
1	F	235	ASP	4.3
1	B	8	PRO	4.3
1	E	17	LEU	4.2
1	B	70	ALA	4.2
1	B	16	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	237	SER	4.1
1	F	313	SER	4.0
1	C	16	PRO	3.9
1	E	56	PRO	3.9
1	F	312	LEU	3.9
1	B	219	VAL	3.9
1	F	32	GLY	3.8
1	B	56	PRO	3.8
1	C	231	VAL	3.8
1	E	234	PRO	3.7
1	A	141	TYR	3.7
1	D	141	TYR	3.7
1	E	143	ASP	3.7
1	F	8	PRO	3.7
1	B	76	SER	3.6
1	B	233	GLY	3.5
1	D	236	GLY	3.5
1	F	90	ASP	3.5
1	E	55	GLN	3.4
1	B	87	ARG	3.4
1	E	54	ALA	3.3
1	B	17	LEU	3.3
1	B	239	LEU	3.3
1	B	210	MET	3.2
1	C	124	GLY	3.2
1	C	166	VAL	3.1
1	B	71	TRP	3.1
1	A	311	ASP	3.1
1	A	128	GLY	3.1
1	B	218	ASP	3.1
1	B	127	ARG	3.1
1	E	76	SER	3.1
1	B	171	GLU	3.1
1	B	234	PRO	3.1
1	C	236	GLY	3.1
1	B	143	ASP	3.0
1	F	195	GLY	3.0
1	B	311	ASP	3.0
1	E	195	GLY	3.0
1	C	174	ALA	3.0
1	E	57	ASP	2.9
1	B	173	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	81	ALA	2.9
1	A	14	LEU	2.9
1	E	141	TYR	2.9
1	B	175	PHE	2.9
1	B	217	ASP	2.9
1	F	17	LEU	2.9
1	B	52	PHE	2.9
1	C	8	PRO	2.8
1	B	306	ALA	2.8
1	A	236	GLY	2.8
1	B	77	GLY	2.8
1	F	91	GLY	2.8
1	E	251	VAL	2.8
1	B	279	LEU	2.8
1	E	201	GLN	2.8
1	B	158	THR	2.8
1	B	54	ALA	2.7
1	D	54	ALA	2.7
1	E	192	ALA	2.7
1	F	222	ALA	2.7
1	E	280	GLY	2.7
1	F	236	GLY	2.7
1	A	8	PRO	2.7
1	D	142	PHE	2.7
1	B	113	ASP	2.7
1	C	59	ARG	2.7
1	A	237	SER	2.7
1	F	16	PRO	2.7
1	B	78	ALA	2.6
1	B	96	ALA	2.6
1	D	310	GLU	2.6
1	E	164	ARG	2.6
1	D	31	GLY	2.6
1	D	8	PRO	2.6
1	B	14	LEU	2.6
1	E	14	LEU	2.6
1	E	90	ASP	2.6
1	D	252	GLY	2.6
1	F	77	GLY	2.6
1	E	231	VAL	2.6
1	B	235	ASP	2.5
1	F	218	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	15	SER	2.5
1	B	232	THR	2.5
1	A	312	LEU	2.5
1	A	87	ARG	2.5
1	B	282	ALA	2.5
1	E	161	ALA	2.5
1	D	111	ARG	2.4
1	E	45	SER	2.4
1	B	289	ILE	2.4
1	C	176	ALA	2.4
1	D	218	ASP	2.4
1	C	198	VAL	2.4
1	D	16	PRO	2.4
1	E	220	LYS	2.4
1	B	109	ALA	2.4
1	E	127	ARG	2.4
1	E	269	VAL	2.4
1	E	210	MET	2.4
1	D	14	LEU	2.4
1	E	24	LEU	2.4
1	F	239	LEU	2.4
1	B	141	TYR	2.4
1	E	218	ASP	2.4
1	B	255	GLU	2.4
1	C	128	GLY	2.4
1	E	58	GLY	2.4
1	D	308	PHE	2.3
1	A	9	GLU	2.3
1	C	232	THR	2.3
1	A	56	PRO	2.3
1	B	216	SER	2.3
1	B	38	ASP	2.3
1	E	8	PRO	2.3
1	E	16	PRO	2.3
1	D	280	GLY	2.3
1	E	233	GLY	2.3
1	A	216	SER	2.3
1	D	41	SER	2.3
1	A	219	VAL	2.3
1	E	196	LEU	2.3
1	D	232	THR	2.3
1	C	222	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	GLY	2.3
1	D	307	ASP	2.3
1	E	217	ASP	2.3
1	B	269	VAL	2.3
1	C	14	LEU	2.3
1	D	39	LEU	2.3
1	E	215	LEU	2.3
1	C	160	ALA	2.2
1	E	304	PRO	2.2
1	D	76	SER	2.2
1	F	190	ILE	2.2
1	C	296	VAL	2.2
1	A	211	THR	2.2
1	B	31	GLY	2.2
1	C	237	SER	2.2
1	E	221	PRO	2.2
1	F	76	SER	2.2
1	B	75	PHE	2.2
1	F	14	LEU	2.2
1	E	174	ALA	2.2
1	D	203	ARG	2.2
1	C	7	GLU	2.2
1	F	13	VAL	2.2
1	B	237	SER	2.2
1	F	237	SER	2.2
1	B	124	GLY	2.2
1	B	84	HIS	2.1
1	B	57	ASP	2.1
1	E	213	VAL	2.1
1	F	159	GLY	2.1
1	A	208	ARG	2.1
1	A	215	LEU	2.1
1	B	114	LEU	2.1
1	C	253	ARG	2.1
1	E	53	ARG	2.1
1	B	254	GLU	2.1
1	B	160	ALA	2.1
1	A	19	SER	2.1
1	A	283	SER	2.1
1	C	154	THR	2.1
1	E	216	SER	2.1
1	B	280	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	210	MET	2.1
1	F	24	LEU	2.1
1	E	170	ALA	2.1
1	F	284	ALA	2.1
1	E	222	ALA	2.1
1	F	283	SER	2.0
1	A	159	GLY	2.0
1	E	112	LEU	2.0
1	B	161	ALA	2.0
1	C	235	ASP	2.0
1	F	143	ASP	2.0
1	D	237	SER	2.0
1	C	210	MET	2.0
1	C	66	ILE	2.0
1	F	157	PRO	2.0
1	E	203	ARG	2.0
1	F	166	VAL	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
5	PG4	D	402	13/13	0.82	0.17	41,49,52,53	0
2	HEM	F	401	43/43	0.95	0.09	17,19,21,22	0
2	HEM	A	401	43/43	0.96	0.08	17,19,22,27	0
4	O	B	402	1/1	0.96	0.11	24,24,24,24	0
2	HEM	C	401	43/43	0.96	0.08	17,20,22,28	0
2	HEM	B	401	43/43	0.97	0.07	18,19,22,25	0

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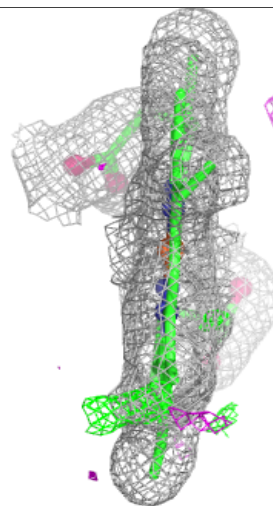
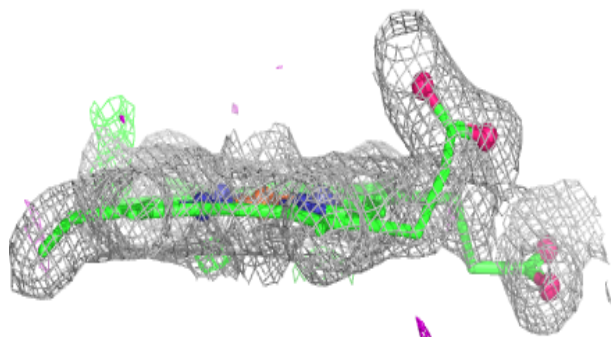
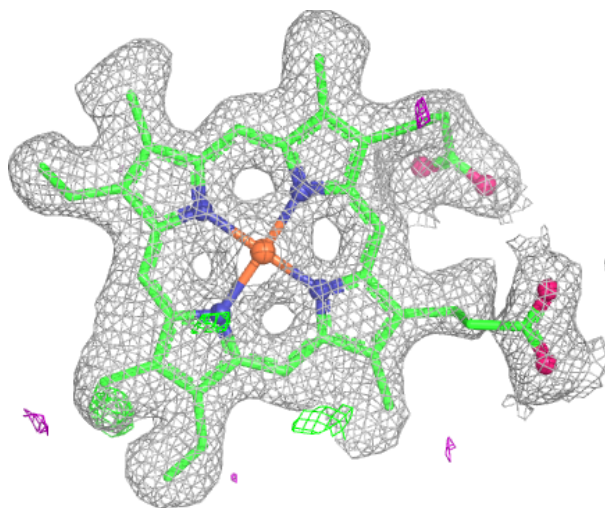
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	D	401	43/43	0.97	0.08	15,17,20,21	0
4	O	E	402	1/1	0.97	0.08	21,21,21,21	0
4	O	F	402	1/1	0.97	0.11	20,20,20,20	0
2	HEM	E	401	43/43	0.97	0.07	18,21,23,24	0
4	O	D	403	1/1	0.98	0.08	18,18,18,18	0
3	MG	A	402	1/1	0.98	0.02	21,21,21,21	0
3	MG	C	402	1/1	0.99	0.02	24,24,24,24	0
4	O	C	403	1/1	0.99	0.04	20,20,20,20	0
4	O	A	403	1/1	0.99	0.04	17,17,17,17	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.

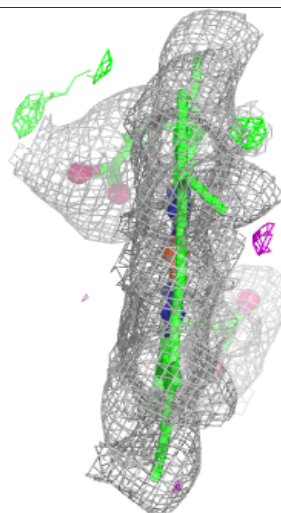
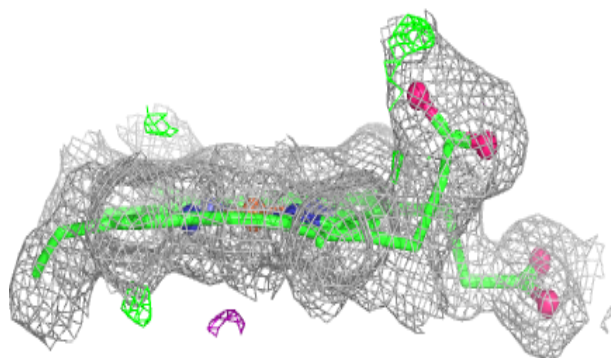
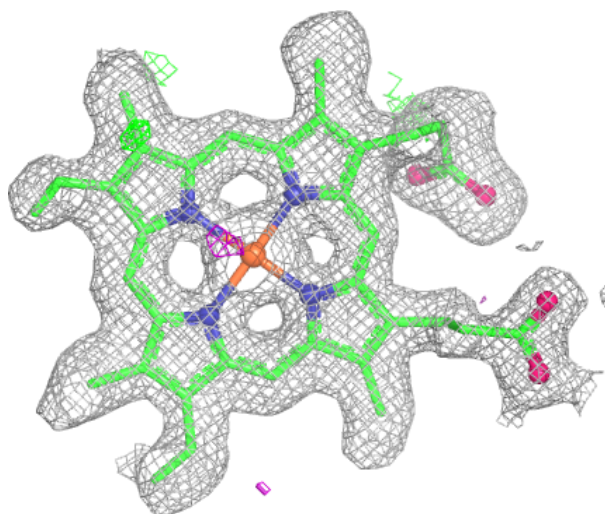
Electron density around HEM F 401:

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



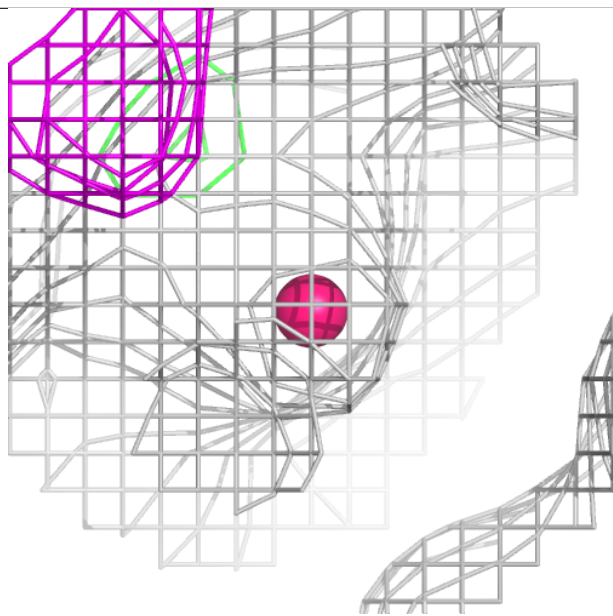
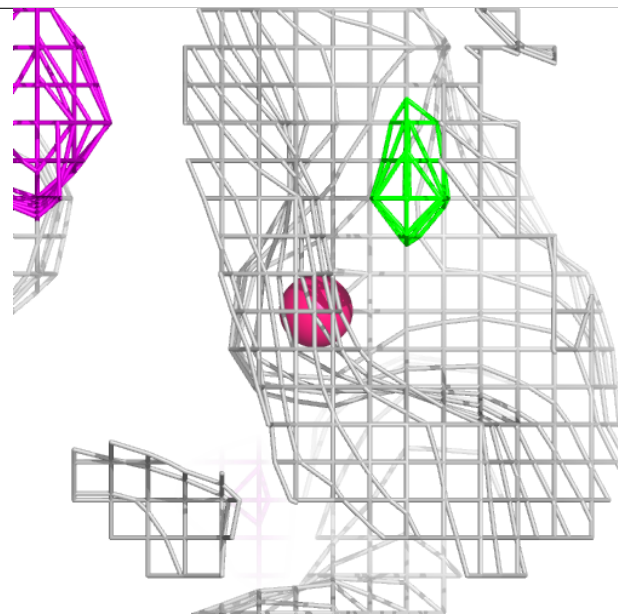
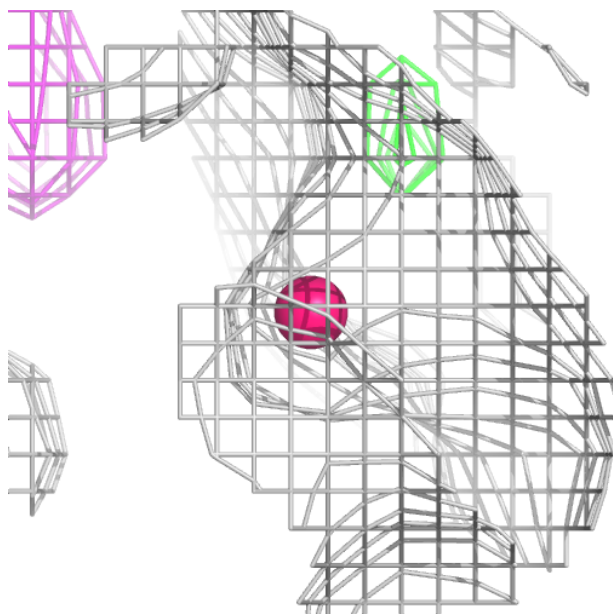
Electron density around HEM A 401:

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



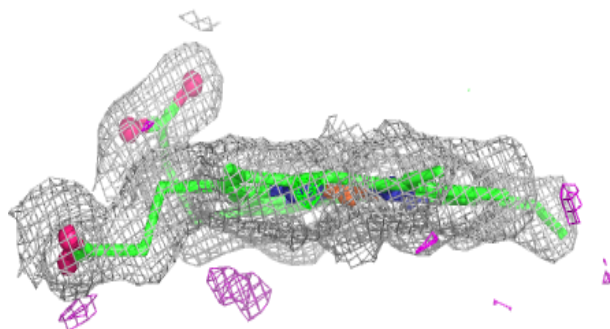
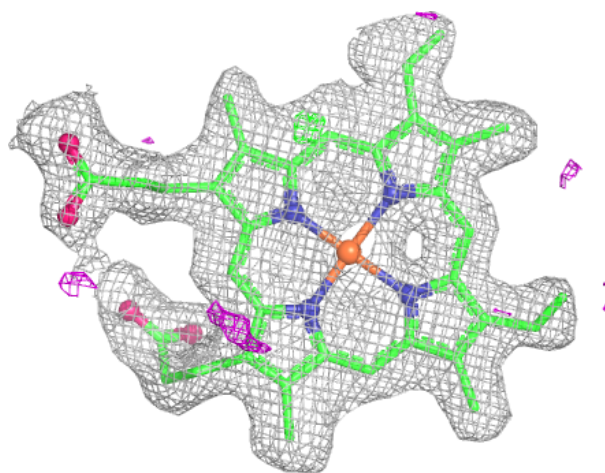
Electron density around O B 402:

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and green (positive)



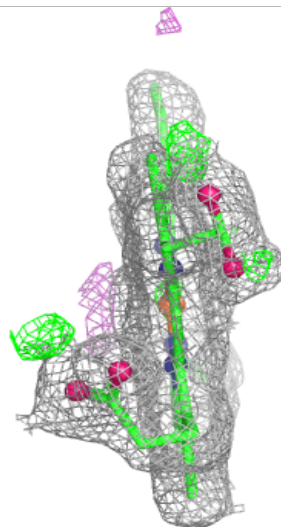
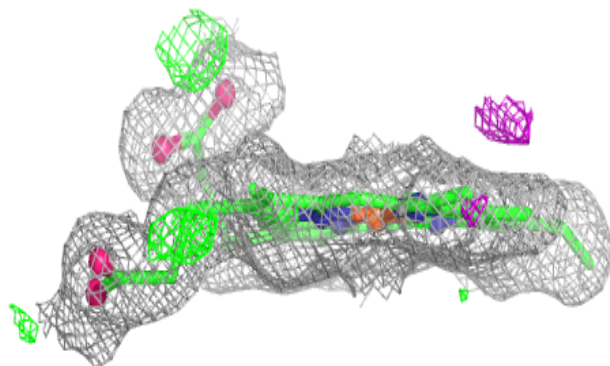
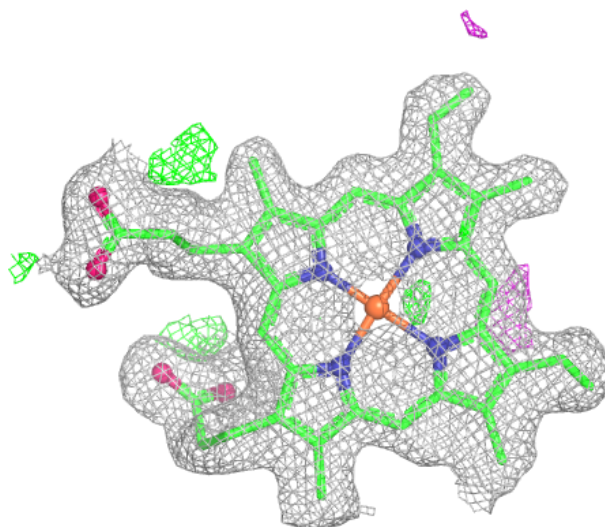
Electron density around HEM C 401:

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



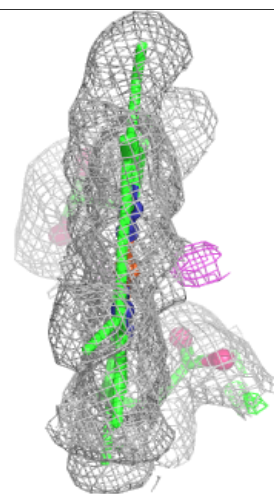
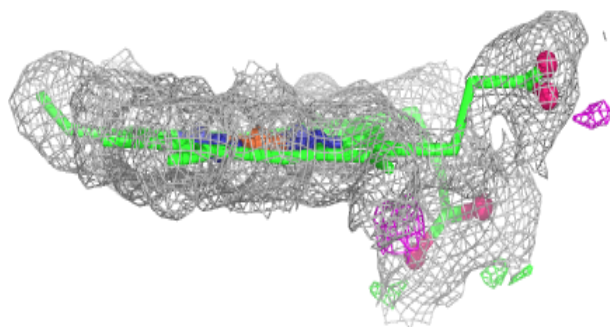
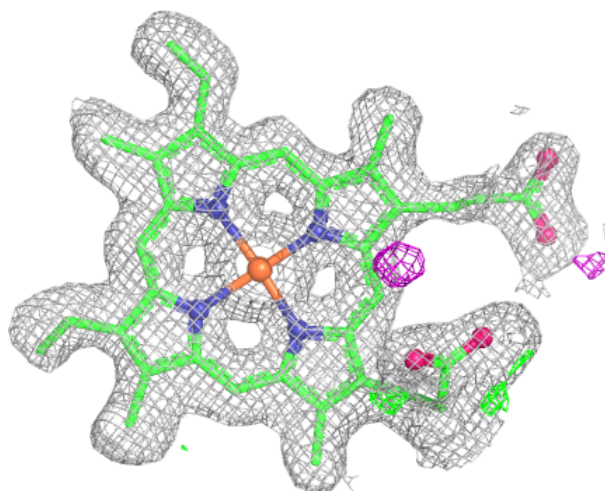
Electron density around HEM B 401:

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



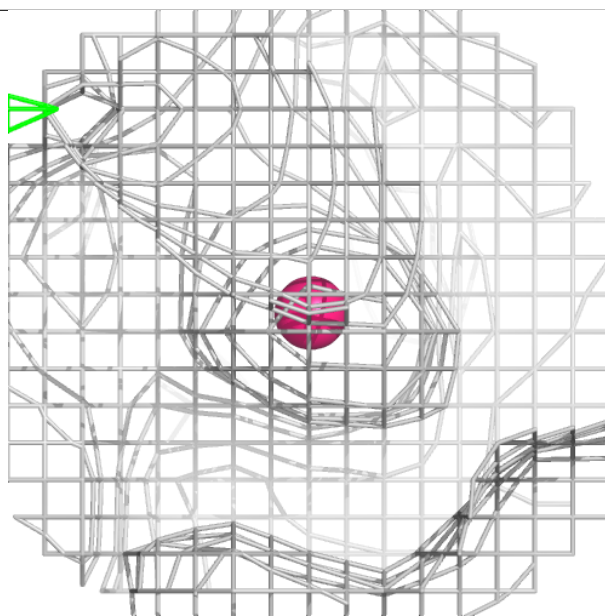
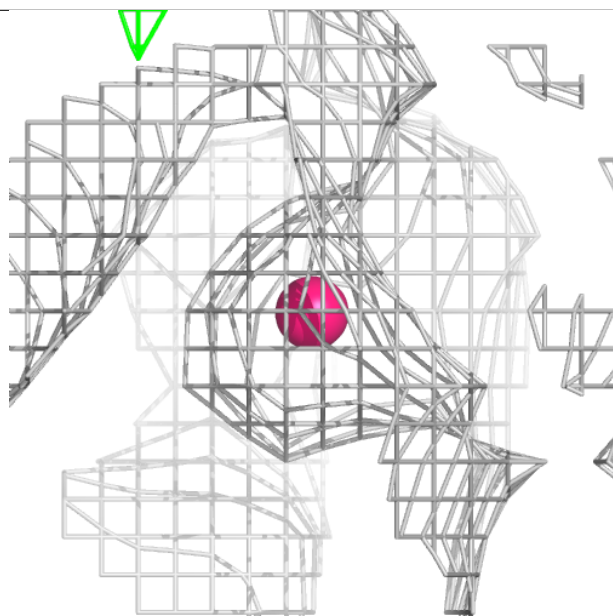
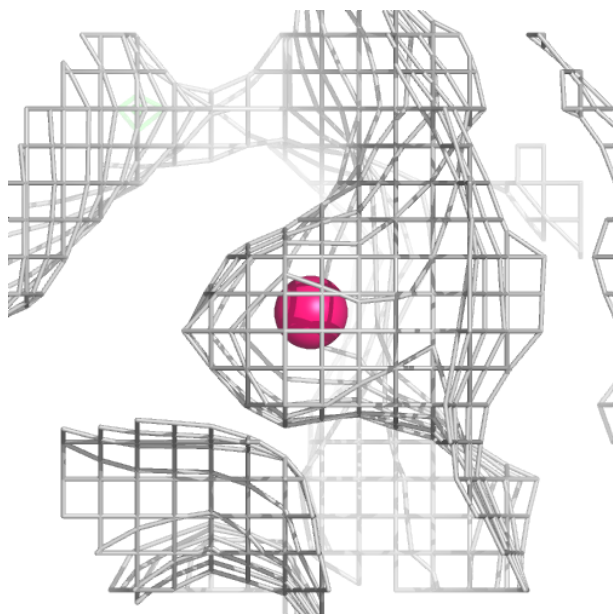
Electron density around HEM D 401:

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



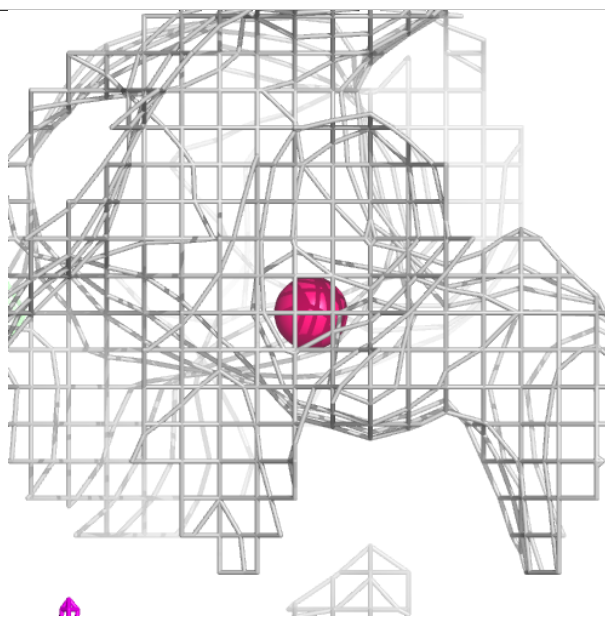
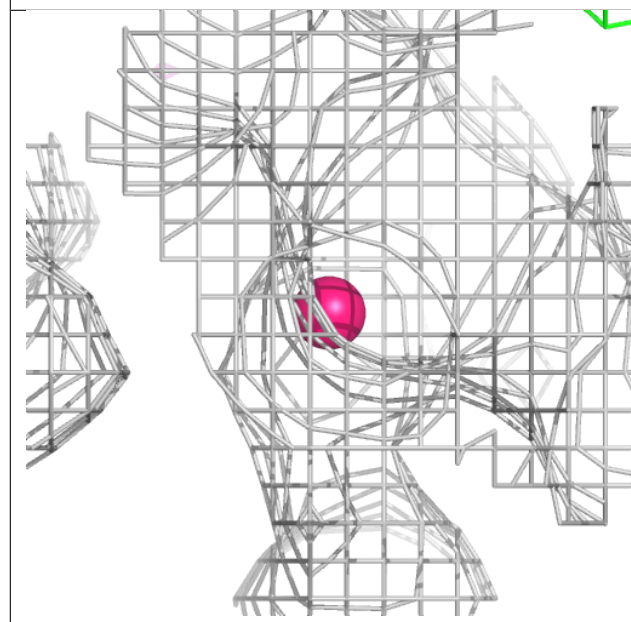
Electron density around O E 402:

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



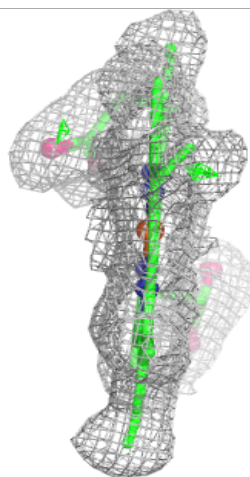
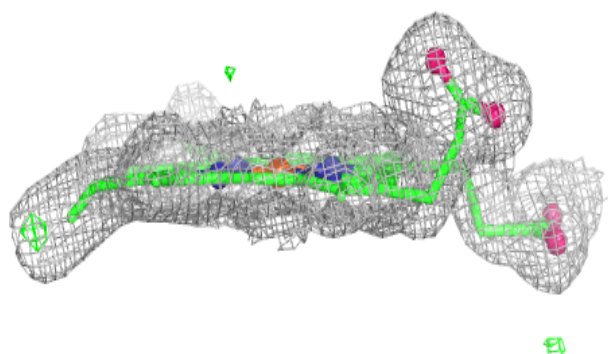
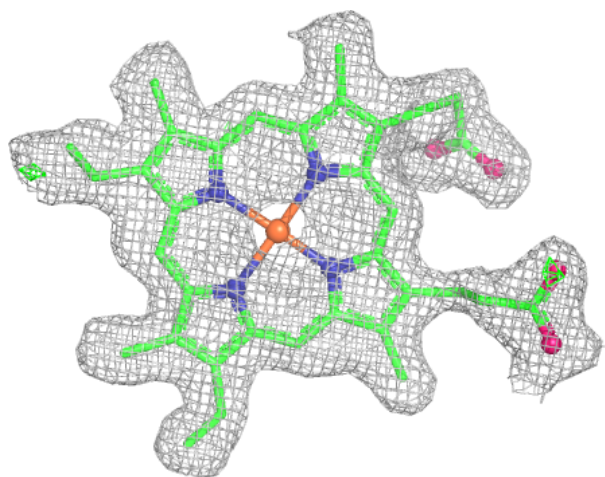
Electron density around O F 402:

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and green (positive)



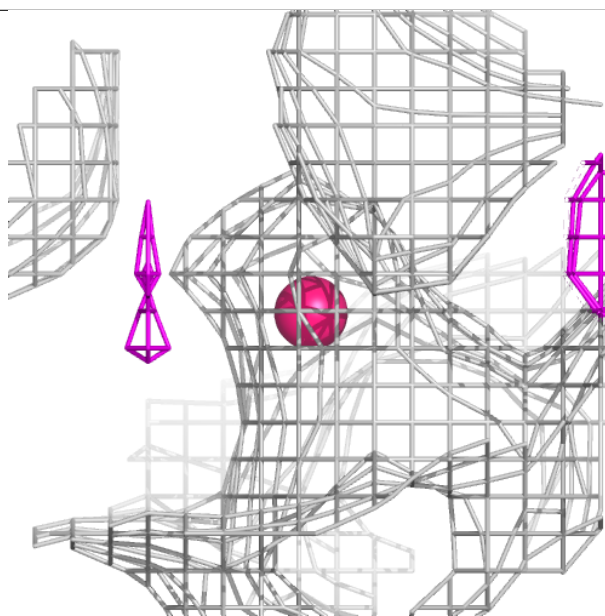
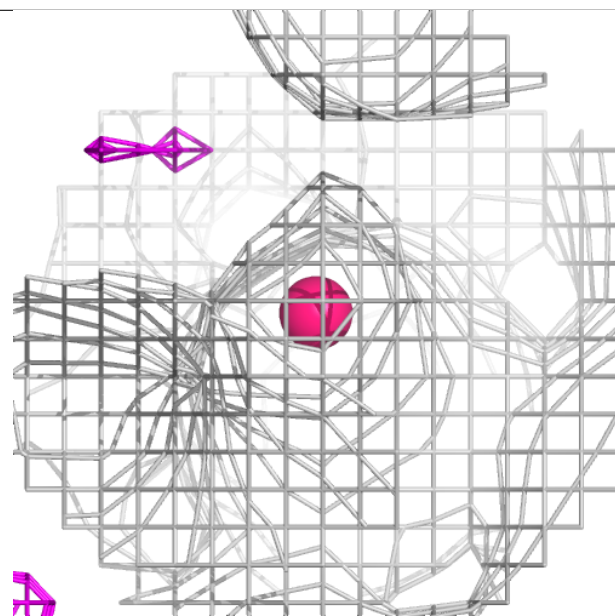
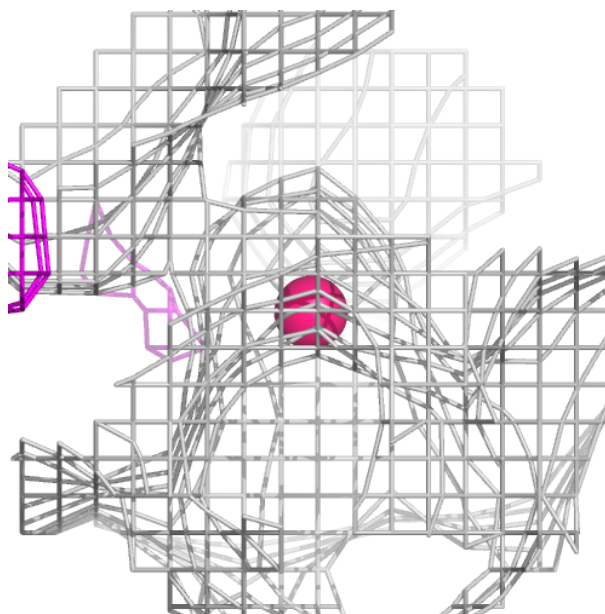
Electron density around HEM E 401:

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



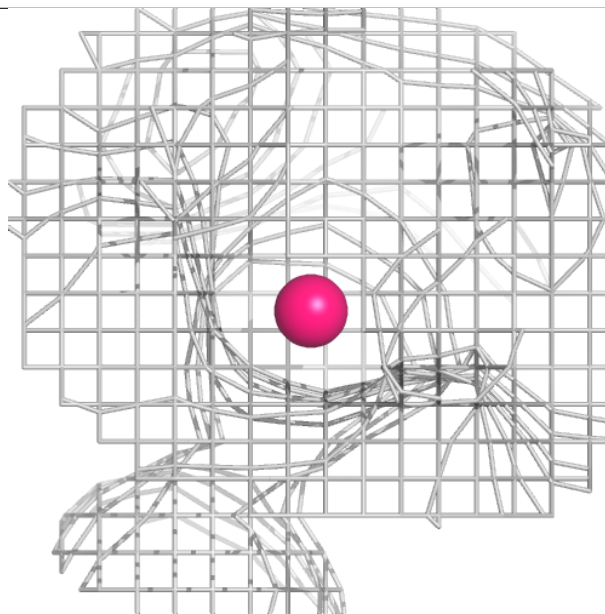
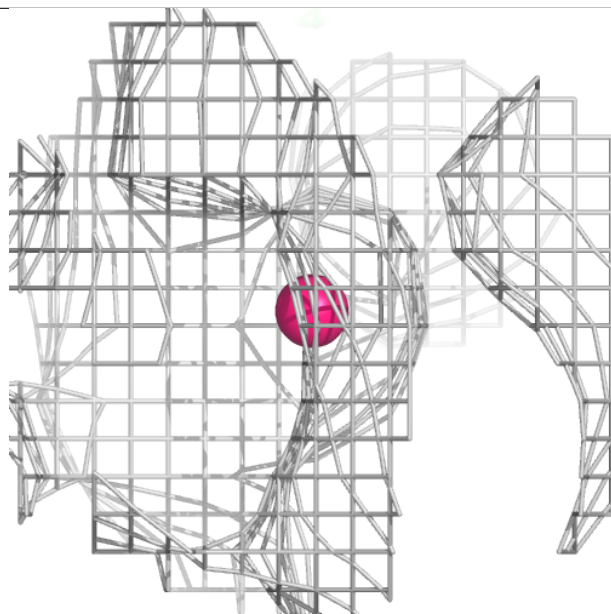
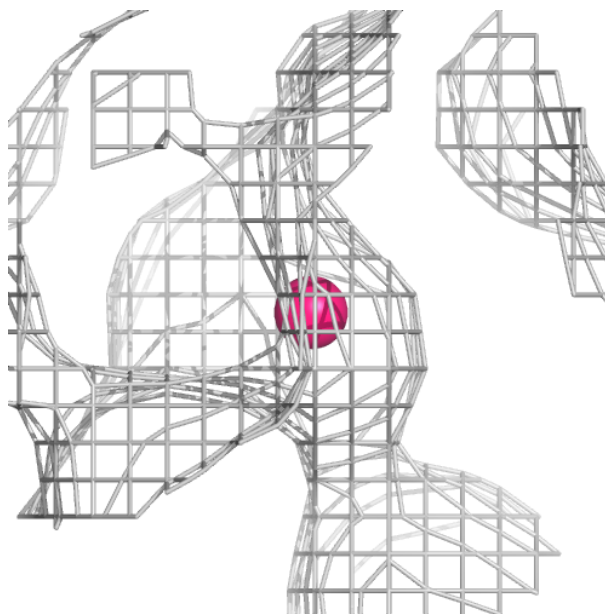
Electron density around O D 403:

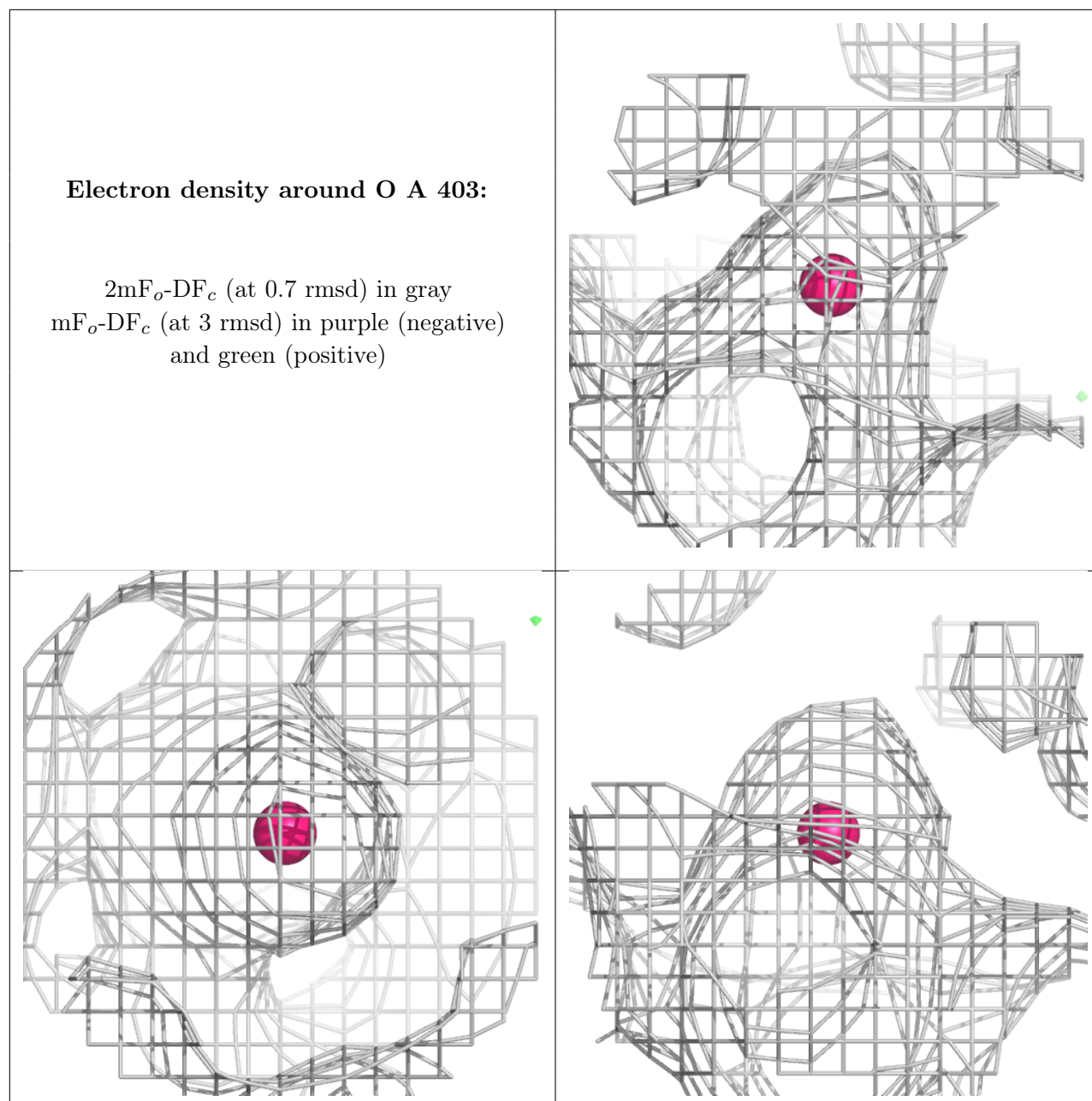
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around O C 403:

$2mF_o-DF_c$ (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.