



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:24 AM UTC

PDB ID : 7P6L / pdb_00007p6l
Title : Heme domain of CYP505A30, a fungal hydroxylase from *Myceliophthora thermophila*, bound to dodecanoic acid
Authors : Opperman, D.J.; Aschenbrenner, J.C.; Tolmie, C.; Ebrecht, A.C.
Deposited on : 2021-07-16
Resolution : 2.33 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

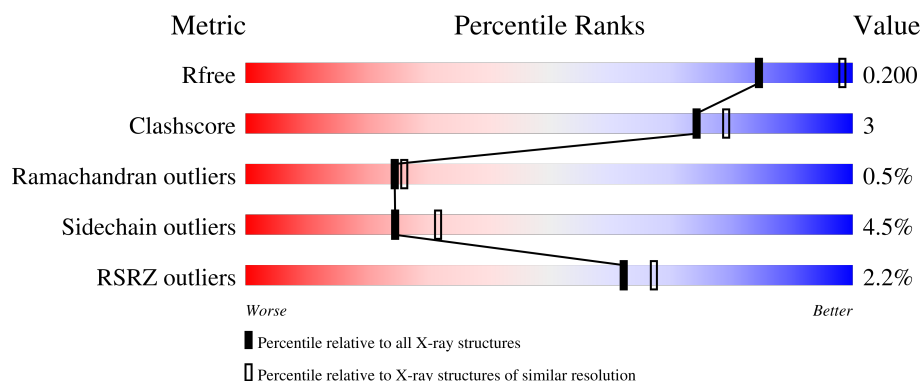
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	464	% 86% 12% ..
1	B	464	 88% 11% ..
1	C	464	2% 85% 12% ..
1	D	464	5% 88% 11% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14979 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			
1	A	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			
1	C	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			
1	D	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			

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



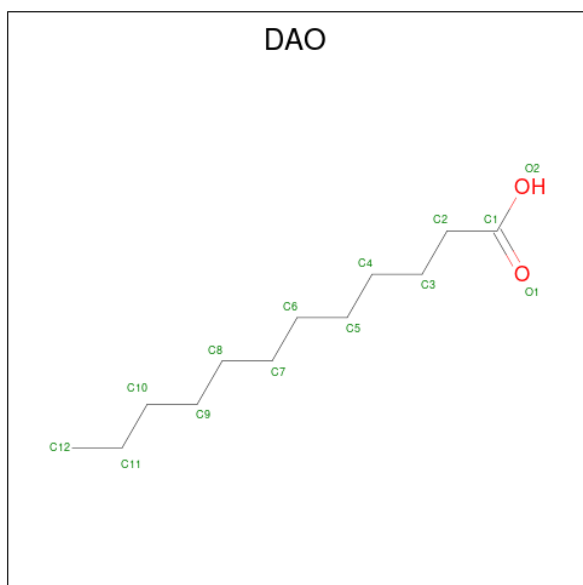
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	

- Molecule 3 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O		
			14	12	2	0	0
3	A	1	Total	C	O		
			14	12	2	0	0
3	C	1	Total	C	O		
			14	12	2	0	0
3	D	1	Total	C	O		
			14	12	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	32	Total	O		
			32	32	0	0
4	A	38	Total	O		
			38	38	0	0
4	C	32	Total	O		
			32	32	0	0

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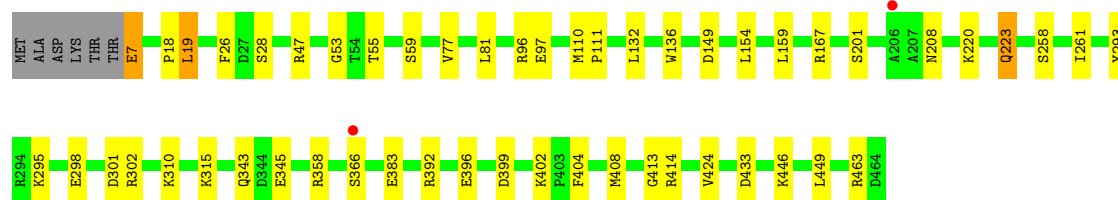
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	25	Total	O	0	0
			25	25		

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.

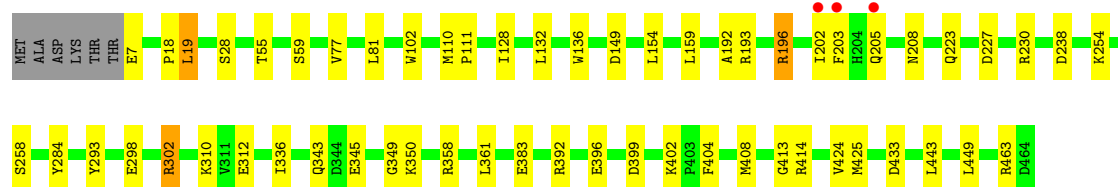
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

Chain B: 



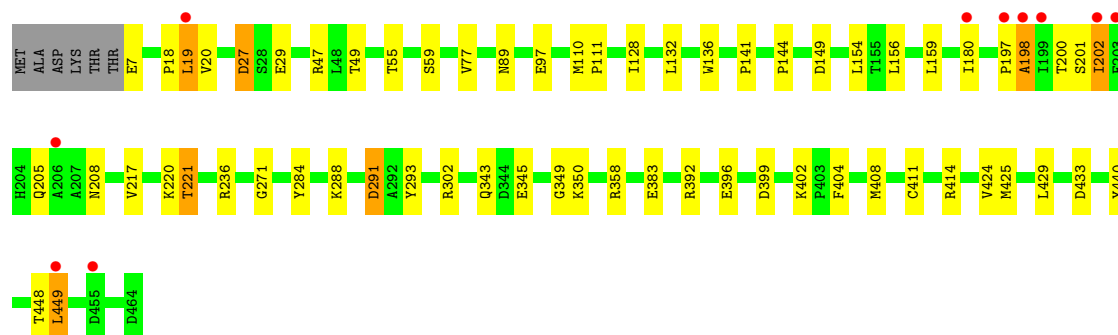
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

Chain A: 

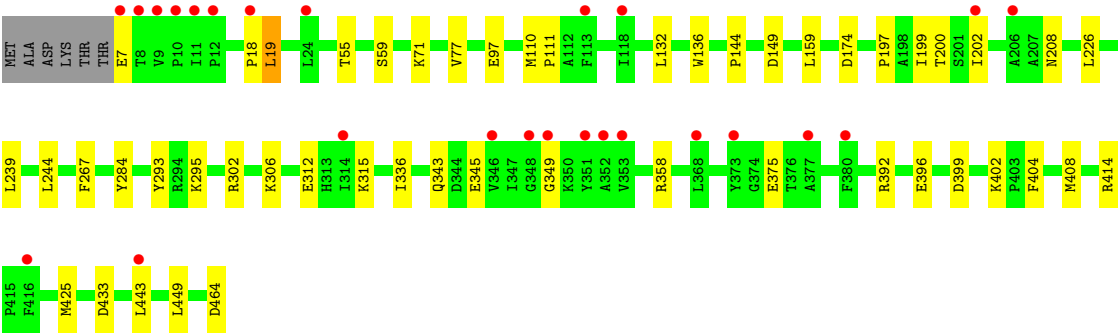
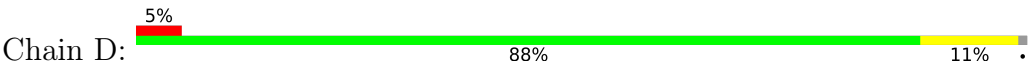


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

Chain C: 



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.49Å 171.49Å 175.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.43 – 2.33 61.43 – 2.33	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.43-2.33) 100.0 (61.43-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.234 (Not available) , 0.200	Depositor DCC
R_{free} test set	5477 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14979	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, DAO

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	1.06	1/3745 (0.0%)	1.42	7/5080 (0.1%)
1	B	1.07	2/3745 (0.1%)	1.43	6/5080 (0.1%)
1	C	1.08	2/3745 (0.1%)	1.44	4/5080 (0.1%)
1	D	1.07	1/3745 (0.0%)	1.43	2/5080 (0.0%)
All	All	1.07	6/14980 (0.0%)	1.43	19/20320 (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	C	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	366	SER	C-O	7.21	1.33	1.24
1	C	144	PRO	C-O	-7.03	1.15	1.23
1	C	141	PRO	C-O	-5.84	1.17	1.24
1	B	53	GLY	C-O	5.32	1.28	1.23
1	A	28	SER	C-O	5.25	1.30	1.24
1	D	144	PRO	C-O	-5.24	1.17	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	ASP	CA-CB-CG	8.66	121.26	112.60
1	B	298	GLU	CB-CG-CD	6.72	124.02	112.60
1	B	26	PHE	CB-CA-C	5.68	119.09	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	89	ASN	CB-CA-C	-5.49	110.23	116.54
1	A	227	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	383	GLU	CA-C-N	5.22	127.53	120.38
1	B	383	GLU	C-N-CA	5.22	127.53	120.38
1	C	383	GLU	CA-C-N	5.21	127.52	120.38
1	C	383	GLU	C-N-CA	5.21	127.52	120.38
1	A	383	GLU	CA-C-N	5.20	127.50	120.38
1	A	383	GLU	C-N-CA	5.20	127.50	120.38
1	A	203	PHE	CA-CB-CG	5.14	118.94	113.80
1	B	96	ARG	CG-CD-NE	-5.13	100.72	112.00
1	A	463	ARG	CA-C-N	5.08	130.84	121.70
1	A	463	ARG	C-N-CA	5.08	130.84	121.70
1	D	174	ASP	O-C-N	5.08	127.30	122.07
1	B	383	GLU	CB-CG-CD	5.06	121.20	112.60
1	D	199	ILE	CA-C-O	-5.02	115.83	121.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	201	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3656	0	3653	25	0
1	B	3656	0	3653	17	0
1	C	3656	0	3653	27	0
1	D	3656	0	3653	18	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	5	0
2	D	43	0	30	1	0
3	A	14	0	23	1	0
3	B	14	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	14	0	23	0	0
3	D	14	0	23	1	0
4	A	38	0	0	0	0
4	B	32	0	0	1	0
4	C	32	0	0	0	0
4	D	25	0	0	0	0
All	All	14979	0	14824	92	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 (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD21	1:A:424:VAL:HG11	1.69	0.74
1:A:298:GLU:OE2	1:A:302:ARG:NH2	2.25	0.69
1:B:55:THR:HG23	1:B:358:ARG:HD3	1.76	0.67
1:C:217:VAL:O	1:C:221:THR:HG23	1.96	0.65
1:C:154:LEU:HD21	1:C:424:VAL:HG21	1.79	0.64
1:B:7:GLU:N	1:B:7:GLU:OE2	2.34	0.61
1:A:55:THR:HG23	1:A:358:ARG:HD3	1.81	0.61
1:B:154:LEU:HD21	1:B:424:VAL:HG21	1.84	0.59
1:C:197:PRO:C	1:C:198:ALA:O	2.44	0.59
1:D:55:THR:HG23	1:D:358:ARG:HD3	1.85	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.87	0.57
1:A:413:GLY:HA3	2:A:501:HEM:C3C	2.40	0.56
1:C:19:LEU:HD23	1:C:20:VAL:HG13	1.87	0.56
1:A:102:TRP:CZ3	1:A:408:MET:HE3	2.41	0.55
1:C:55:THR:HG23	1:C:358:ARG:HD3	1.90	0.54
1:A:298:GLU:CD	1:A:302:ARG:HH21	2.15	0.54
1:C:159:LEU:C	1:C:159:LEU:HD13	2.33	0.53
1:C:156:LEU:HD22	1:C:180:ILE:HD11	1.92	0.52
1:C:200:THR:O	1:C:200:THR:HG22	2.09	0.52
1:B:343:GLN:O	1:B:345:GLU:HG2	2.11	0.51
1:C:343:GLN:O	1:C:345:GLU:HG2	2.11	0.50
1:A:343:GLN:O	1:A:345:GLU:HG2	2.12	0.50
1:D:343:GLN:O	1:D:345:GLU:HG2	2.13	0.49
1:D:306:LYS:HE3	1:D:464:ASP:OD1	2.13	0.48
1:B:293:TYR:OH	1:B:433:ASP:HA	2.13	0.48
1:A:159:LEU:C	1:A:159:LEU:HD13	2.39	0.47
1:A:336:ILE:HB	3:A:502:DAO:H21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.98	0.46
1:C:271:GLY:HA2	2:C:501:HEM:C3C	2.51	0.46
1:C:399:ASP:HA	1:C:402:LYS:HD3	1.98	0.46
1:C:197:PRO:O	1:C:198:ALA:O	2.33	0.46
1:D:284:TYR:CE2	1:D:443:LEU:HB2	2.51	0.45
1:D:392:ARG:NH2	1:D:396:GLU:OE1	2.49	0.45
1:C:284:TYR:CZ	1:C:288:LYS:HG3	2.52	0.45
1:D:159:LEU:C	1:D:159:LEU:HD13	2.42	0.45
1:B:392:ARG:NH2	1:B:396:GLU:OE1	2.49	0.44
1:A:18:PRO:O	1:A:19:LEU:HB2	2.16	0.44
1:C:271:GLY:HA2	2:C:501:HEM:C2C	2.52	0.44
1:B:159:LEU:C	1:B:159:LEU:HD13	2.42	0.44
1:A:193:ARG:NH1	1:C:27:ASP:OD2	2.50	0.44
1:D:404:PHE:CG	1:D:414:ARG:HG3	2.53	0.44
1:D:399:ASP:HA	1:D:402:LYS:HD3	2.00	0.44
1:A:110:MET:N	1:A:111:PRO:CD	2.81	0.43
1:C:293:TYR:OH	1:C:433:ASP:HA	2.17	0.43
1:D:239:LEU:HD21	1:D:267:PHE:CD2	2.54	0.43
1:B:404:PHE:CG	1:B:414:ARG:HG3	2.53	0.43
1:C:404:PHE:CG	1:C:414:ARG:HG3	2.53	0.43
1:A:293:TYR:OH	1:A:433:ASP:HA	2.19	0.43
1:A:404:PHE:CG	1:A:414:ARG:HG3	2.54	0.43
1:D:110:MET:N	1:D:111:PRO:CD	2.82	0.42
1:B:110:MET:N	1:B:111:PRO:CD	2.82	0.42
1:A:128:ILE:HG22	1:A:154:LEU:HD12	2.02	0.42
1:D:425:MET:HE3	1:D:425:MET:HB2	1.93	0.42
1:A:284:TYR:CE2	1:A:443:LEU:HB2	2.55	0.42
1:A:392:ARG:NH2	1:A:396:GLU:OE1	2.53	0.42
1:C:425:MET:HE3	1:C:425:MET:HB2	1.93	0.42
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	2.01	0.42
1:B:18:PRO:O	1:B:19:LEU:HB2	2.19	0.42
1:C:411:CYS:HB2	2:C:501:HEM:NA	2.33	0.42
1:A:102:TRP:CH2	1:A:408:MET:HE3	2.55	0.42
1:A:230:ARG:HG2	1:C:440:TYR:CZ	2.55	0.42
1:D:132:LEU:HD11	1:D:136:TRP:CE2	2.55	0.41
1:B:223:GLN:OE1	1:B:261:ILE:HD11	2.19	0.41
1:A:425:MET:HE3	1:A:425:MET:HB2	1.91	0.41
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.50	0.41
1:C:128:ILE:HG22	1:C:154:LEU:HD12	2.02	0.41
1:A:399:ASP:HA	1:A:402:LYS:HD3	2.03	0.41
1:C:18:PRO:O	1:C:19:LEU:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ILE:HB	3:D:502:DAO:H21	2.01	0.41
1:C:110:MET:N	1:C:111:PRO:CD	2.84	0.41
1:C:448:THR:O	1:C:449:LEU:HB2	2.21	0.41
1:B:413:GLY:HA3	2:B:501:HEM:C3C	2.56	0.41
1:D:197:PRO:HG2	1:D:200:THR:HG23	2.03	0.41
1:B:399:ASP:HA	1:B:402:LYS:HD3	2.01	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.51	0.41
1:C:132:LEU:HD11	1:C:136:TRP:CE2	2.56	0.41
1:B:132:LEU:HD11	1:B:136:TRP:CE2	2.56	0.41
1:B:167:ARG:HA	4:B:623:HOH:O	2.21	0.41
1:A:132:LEU:HD11	1:A:136:TRP:CE2	2.55	0.41
1:D:18:PRO:O	1:D:19:LEU:HB2	2.21	0.41
1:D:239:LEU:HD21	1:D:267:PHE:CG	2.56	0.41
1:A:192:ALA:O	1:A:196:ARG:HB2	2.21	0.40
1:D:293:TYR:OH	1:D:433:ASP:HA	2.21	0.40
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.77	0.40
1:B:301:ASP:OD1	1:B:463:ARG:NH2	2.52	0.40
1:C:392:ARG:NH2	1:C:396:GLU:OE1	2.55	0.40
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.98	0.40
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.81	0.40
1:A:361:LEU:N	1:A:361:LEU:HD12	2.36	0.40
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.51	0.40
1:D:226:LEU:HD11	1:D:244:LEU:HD21	2.04	0.40
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.51	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	456/464 (98%)	436 (96%)	18 (4%)	2 (0%)	30 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	456/464 (98%)	440 (96%)	15 (3%)	1 (0%)	43	50
1	C	456/464 (98%)	437 (96%)	15 (3%)	4 (1%)	14	13
1	D	456/464 (98%)	439 (96%)	15 (3%)	2 (0%)	30	32
All	All	1824/1856 (98%)	1752 (96%)	63 (4%)	9 (0%)	24	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	ALA
1	C	202	ILE
1	A	349	GLY
1	D	77	VAL
1	A	77	VAL
1	C	77	VAL
1	B	77	VAL
1	D	349	GLY
1	C	349	GLY

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	376/393 (96%)	360 (96%)	16 (4%)	26	33
1	B	388/393 (99%)	369 (95%)	19 (5%)	22	28
1	C	388/393 (99%)	368 (95%)	20 (5%)	21	25
1	D	388/393 (99%)	373 (96%)	15 (4%)	28	37
All	All	1540/1572 (98%)	1470 (96%)	70 (4%)	24	32

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	GLU
1	B	19	LEU

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Mol	Chain	Res	Type
1	B	28	SER
1	B	47	ARG
1	B	59	SER
1	B	97	GLU
1	B	149	ASP
1	B	201	SER
1	B	208	ASN
1	B	220	LYS
1	B	223	GLN
1	B	258	SER
1	B	295	LYS
1	B	302	ARG
1	B	310	LYS
1	B	315	LYS
1	B	408	MET
1	B	446	LYS
1	B	449	LEU
1	A	7	GLU
1	A	19	LEU
1	A	59	SER
1	A	149	ASP
1	A	196	ARG
1	A	202	ILE
1	A	205	GLN
1	A	208	ASN
1	A	223	GLN
1	A	254	LYS
1	A	258	SER
1	A	302	ARG
1	A	310	LYS
1	A	312	GLU
1	A	350	LYS
1	A	449	LEU
1	C	7	GLU
1	C	19	LEU
1	C	27	ASP
1	C	29	GLU
1	C	47	ARG
1	C	49	THR
1	C	59	SER
1	C	97	GLU
1	C	149	ASP

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Mol	Chain	Res	Type
1	C	202	ILE
1	C	205	GLN
1	C	208	ASN
1	C	220	LYS
1	C	221	THR
1	C	236	ARG
1	C	291	ASP
1	C	302	ARG
1	C	350	LYS
1	C	408	MET
1	C	449	LEU
1	D	7	GLU
1	D	19	LEU
1	D	59	SER
1	D	71	LYS
1	D	97	GLU
1	D	149	ASP
1	D	202	ILE
1	D	208	ASN
1	D	295	LYS
1	D	302	ARG
1	D	312	GLU
1	D	315	LYS
1	D	375	GLU
1	D	408	MET
1	D	449	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	437	HIS
1	C	232	HIS
1	D	365	GLN
1	D	437	HIS

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](#)

8 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	$\# Z > 2$
3	DAO	B	502	-	13,13,13	1.04	0	13,13,13	0.70	0
2	HEM	C	501	1	50,50,50	1.56	7 (14%)	67,82,82	1.52	9 (13%)
3	DAO	C	502	-	13,13,13	0.75	0	13,13,13	0.84	0
2	HEM	B	501	1	50,50,50	1.76	9 (18%)	67,82,82	1.93	20 (29%)
3	DAO	D	502	-	13,13,13	0.86	1 (7%)	13,13,13	0.79	0
2	HEM	A	501	1	50,50,50	1.76	10 (20%)	67,82,82	1.58	9 (13%)
3	DAO	A	502	-	13,13,13	0.97	1 (7%)	13,13,13	0.73	1 (7%)
2	HEM	D	501	1	50,50,50	1.73	11 (22%)	67,82,82	1.59	13 (19%)

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
3	DAO	B	502	-	-	5/11/11/11	-
2	HEM	C	501	1	-	2/14/54/54	-
3	DAO	C	502	-	-	4/11/11/11	-
2	HEM	B	501	1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAO	D	502	-	-	7/11/11/11	-
2	HEM	A	501	1	-	2/14/54/54	-
3	DAO	A	502	-	-	5/11/11/11	-
2	HEM	D	501	1	-	4/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NC	6.01	2.15	1.95
2	C	501	HEM	FE-NC	5.52	2.13	1.95
2	D	501	HEM	FE-NC	5.43	2.13	1.95
2	B	501	HEM	FE-NB	4.95	2.10	1.94
2	D	501	HEM	FE-NB	4.72	2.09	1.94
2	B	501	HEM	FE-NC	4.65	2.10	1.95
2	C	501	HEM	FE-NB	4.39	2.08	1.94
2	B	501	HEM	C1B-NB	-3.52	1.34	1.40
2	A	501	HEM	FE-NA	3.41	2.06	1.95
2	A	501	HEM	FE-NB	3.35	2.05	1.94
2	C	501	HEM	C4B-NB	-3.31	1.32	1.38
2	D	501	HEM	C4B-NB	-3.28	1.32	1.38
2	A	501	HEM	C1C-NC	-3.14	1.33	1.39
2	B	501	HEM	CHB-C1B	3.14	1.44	1.38
2	A	501	HEM	C3B-C4B	3.05	1.50	1.44
2	A	501	HEM	C4B-NB	-2.95	1.33	1.38
2	D	501	HEM	C4D-ND	-2.93	1.35	1.40
3	A	502	DAO	O1-C1	2.91	1.31	1.22
2	D	501	HEM	C1B-NB	-2.89	1.35	1.40
2	D	501	HEM	FE-NA	2.87	2.04	1.95
2	D	501	HEM	C4D-C3D	2.75	1.49	1.45
2	A	501	HEM	C1B-NB	-2.67	1.35	1.40
2	A	501	HEM	CHA-C4D	2.65	1.43	1.38
2	A	501	HEM	C4A-NA	-2.61	1.34	1.39
2	B	501	HEM	C4D-ND	-2.61	1.35	1.40
2	B	501	HEM	C2A-C3A	-2.56	1.32	1.38
2	C	501	HEM	O2A-CGA	-2.55	1.22	1.30
2	A	501	HEM	C3C-C4C	-2.47	1.41	1.46
2	D	501	HEM	C2A-C3A	-2.47	1.32	1.38
2	B	501	HEM	C1D-ND	-2.44	1.34	1.38
2	C	501	HEM	C1C-C2C	-2.42	1.40	1.45
2	B	501	HEM	C4A-NA	-2.37	1.35	1.39
2	C	501	HEM	C1C-NC	-2.35	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C1C-C2C	-2.23	1.40	1.45
2	B	501	HEM	O1D-CGD	2.13	1.29	1.22
3	D	502	DAO	O1-C1	2.12	1.29	1.22
2	D	501	HEM	C3B-C4B	2.09	1.49	1.44
2	C	501	HEM	C1B-NB	-2.06	1.36	1.40
2	D	501	HEM	C1C-NC	-2.02	1.35	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C1B-NB-C4B	5.74	112.00	105.21
2	A	501	HEM	C1B-NB-C4B	5.30	111.48	105.21
2	C	501	HEM	CHC-C4B-NB	5.28	130.10	124.42
2	A	501	HEM	CHD-C1D-ND	4.87	129.66	124.42
2	B	501	HEM	CHC-C4B-NB	4.64	129.42	124.42
2	D	501	HEM	CAD-C3D-C4D	4.33	132.24	124.70
2	A	501	HEM	CHC-C4B-NB	4.23	128.97	124.42
2	B	501	HEM	CMD-C2D-C1D	4.22	131.63	125.03
2	C	501	HEM	CHD-C1D-ND	4.20	128.94	124.42
2	A	501	HEM	CHB-C1B-NB	4.16	129.51	124.37
2	D	501	HEM	CHB-C1B-NB	4.14	129.49	124.37
2	C	501	HEM	C1B-NB-C4B	4.02	109.96	105.21
2	D	501	HEM	CHC-C4B-NB	3.87	128.59	124.42
2	B	501	HEM	C3B-C4B-NB	-3.69	106.82	109.47
2	D	501	HEM	C1B-NB-C4B	3.66	109.55	105.21
2	B	501	HEM	CAD-C3D-C4D	3.59	130.96	124.70
2	B	501	HEM	CMA-C3A-C4A	3.56	130.84	125.42
2	A	501	HEM	CHA-C4D-ND	3.54	128.74	124.37
2	A	501	HEM	C3B-C4B-NB	-3.34	107.07	109.47
2	B	501	HEM	CHD-C1D-ND	3.31	127.99	124.42
2	C	501	HEM	CHA-C4D-ND	3.25	128.39	124.37
2	D	501	HEM	CMA-C3A-C4A	3.18	130.26	125.42
2	B	501	HEM	CAD-C3D-C2D	-3.17	121.93	127.87
2	B	501	HEM	CAA-C2A-C1A	3.16	131.11	124.94
2	C	501	HEM	CHD-C1D-C2D	-3.13	120.09	125.03
2	B	501	HEM	CHD-C1D-C2D	-3.11	120.12	125.03
2	B	501	HEM	C3B-C2B-C1B	3.08	108.73	106.41
2	B	501	HEM	CMA-C3A-C2A	-2.69	119.91	125.62
2	A	501	HEM	CHD-C1D-C2D	-2.65	120.85	125.03
2	C	501	HEM	C3B-C4B-NB	-2.64	107.57	109.47
2	B	501	HEM	CHB-C1B-NB	2.60	127.58	124.37
2	B	501	HEM	O2A-CGA-CBA	2.49	121.87	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CAD-C3D-C2D	-2.43	123.32	127.87
2	D	501	HEM	C3B-C4B-NB	-2.43	107.72	109.47
2	B	501	HEM	C2B-C1B-NB	-2.39	107.09	109.84
2	C	501	HEM	CHB-C1B-NB	2.34	127.26	124.37
2	D	501	HEM	O1A-CGA-CBA	-2.29	115.82	123.09
2	B	501	HEM	CHA-C4D-ND	2.27	127.17	124.37
2	A	501	HEM	CHB-C1B-C2B	-2.21	120.67	126.95
2	D	501	HEM	C4B-C3B-C2B	-2.21	105.25	107.28
2	D	501	HEM	CHD-C1D-ND	2.16	126.74	124.42
2	C	501	HEM	CMD-C2D-C1D	2.13	128.37	125.03
2	A	501	HEM	C4C-CHD-C1D	-2.13	121.48	126.02
2	B	501	HEM	C4A-C3A-C2A	2.12	109.25	106.82
2	B	501	HEM	C4B-C3B-C2B	-2.12	105.33	107.28
2	B	501	HEM	C4C-C3C-C2C	-2.10	104.99	106.81
2	D	501	HEM	CHB-C1B-C2B	-2.07	121.06	126.95
2	B	501	HEM	C3C-C2C-C1C	2.07	109.00	107.05
3	A	502	DAO	C3-C2-C1	2.03	119.81	114.51
2	D	501	HEM	C3B-C2B-C1B	2.03	107.93	106.41
2	C	501	HEM	C1A-CHA-C4D	-2.01	121.53	126.25
2	D	501	HEM	CAA-C2A-C1A	2.00	128.85	124.94

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	DAO	C1-C2-C3-C4
3	D	502	DAO	C3-C4-C5-C6
3	A	502	DAO	C3-C4-C5-C6
3	C	502	DAO	C11-C10-C9-C8
3	B	502	DAO	C1-C2-C3-C4
3	B	502	DAO	C4-C5-C6-C7
3	B	502	DAO	C3-C4-C5-C6
3	C	502	DAO	C2-C3-C4-C5
3	D	502	DAO	C5-C6-C7-C8
3	D	502	DAO	C7-C8-C9-C10
3	A	502	DAO	C11-C10-C9-C8
3	B	502	DAO	C11-C10-C9-C8
3	C	502	DAO	C9-C10-C11-C12
3	A	502	DAO	C1-C2-C3-C4
3	B	502	DAO	C7-C8-C9-C10
3	D	502	DAO	C11-C10-C9-C8
3	A	502	DAO	O2-C1-C2-C3

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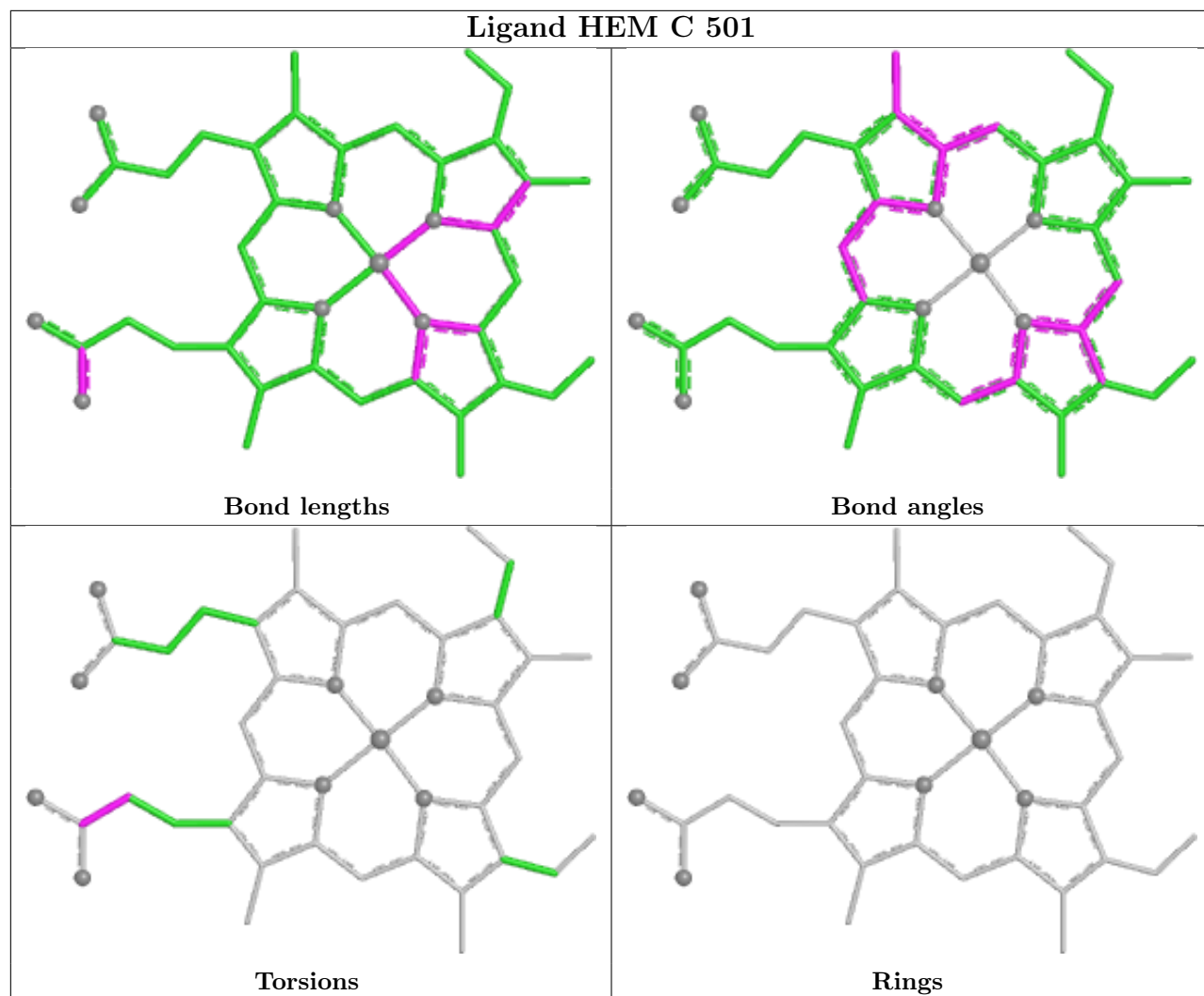
Mol	Chain	Res	Type	Atoms
2	A	501	HEM	CAA-CBA-CGA-O2A
3	C	502	DAO	C3-C4-C5-C6
2	B	501	HEM	CAD-CBD-CGD-O2D
3	A	502	DAO	O1-C1-C2-C3
2	A	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
3	D	502	DAO	O1-C1-C2-C3
2	C	501	HEM	CAA-CBA-CGA-O1A
3	D	502	DAO	O2-C1-C2-C3

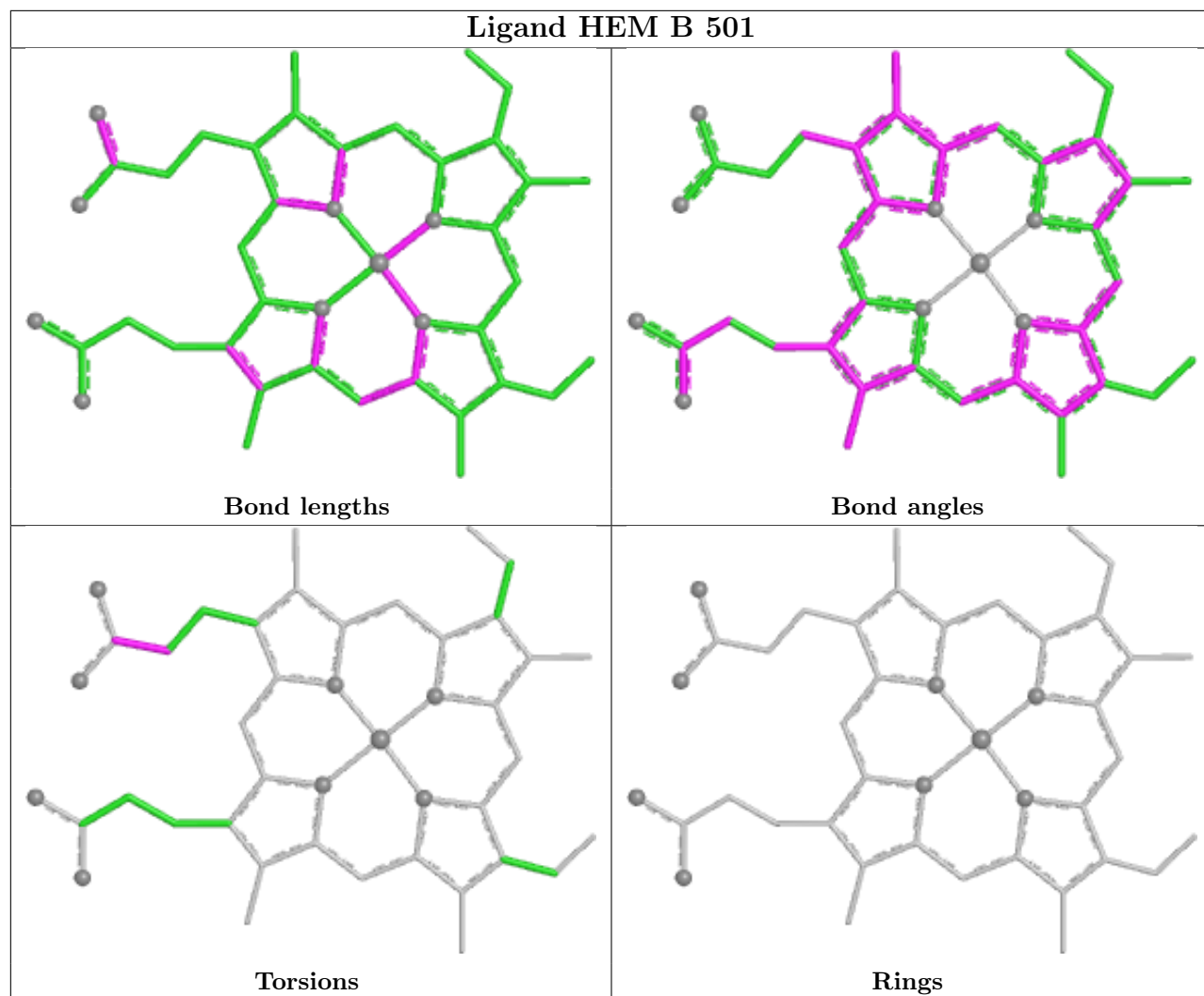
There are no ring outliers.

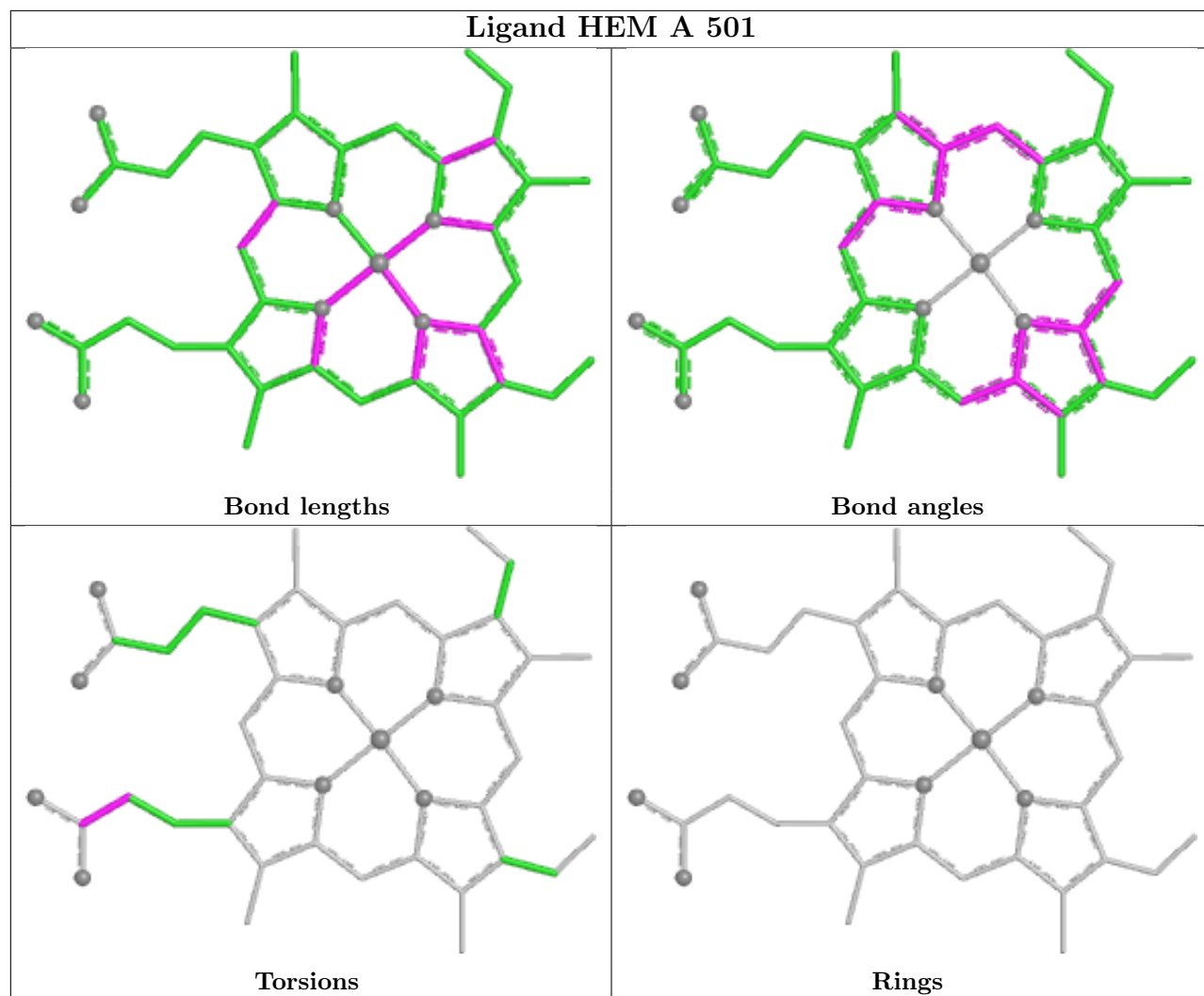
6 monomers are involved in 14 short contacts:

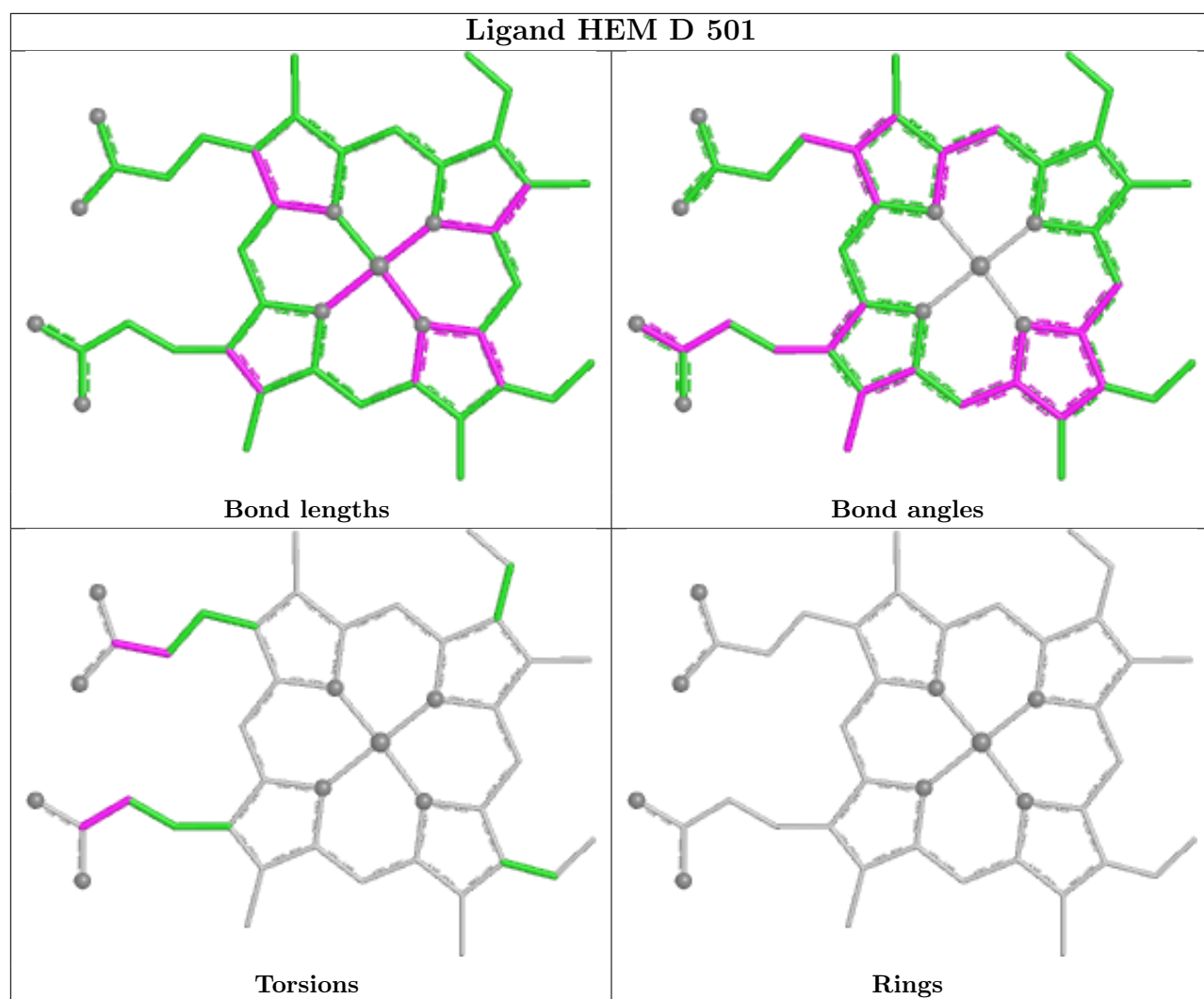
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	5	0
2	B	501	HEM	2	0
3	D	502	DAO	1	0
2	A	501	HEM	4	0
3	A	502	DAO	1	0
2	D	501	HEM	1	0

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









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	458/464 (98%)	-0.00	3 (0%) 84 87	60, 80, 109, 145	0
1	B	458/464 (98%)	0.02	2 (0%) 88 90	60, 82, 107, 149	0
1	C	458/464 (98%)	0.23	10 (2%) 62 67	58, 88, 131, 193	0
1	D	458/464 (98%)	0.44	25 (5%) 30 36	60, 93, 132, 163	0
All	All	1832/1856 (98%)	0.17	40 (2%) 62 67	58, 84, 125, 193	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	377	ALA	4.6
1	D	9	VAL	4.5
1	C	203	PHE	4.4
1	C	199	ILE	4.1
1	C	19	LEU	3.7
1	D	10	PRO	3.6
1	C	449	LEU	3.6
1	D	7	GLU	3.3
1	C	202	ILE	3.3
1	D	368	LEU	3.2
1	C	198	ALA	3.1
1	D	11	ILE	3.1
1	D	346	VAL	3.0
1	A	202	ILE	2.9
1	D	380	PHE	2.8
1	D	348	GLY	2.7
1	C	180	ILE	2.6
1	B	366	SER	2.5
1	D	443	LEU	2.5
1	C	206	ALA	2.4
1	D	206	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	352	ALA	2.4
1	D	202	ILE	2.4
1	D	353	VAL	2.4
1	D	416	PHE	2.4
1	D	8	THR	2.4
1	D	373	TYR	2.3
1	D	314	ILE	2.3
1	D	12	PRO	2.3
1	D	349	GLY	2.3
1	B	206	ALA	2.3
1	A	203	PHE	2.2
1	D	351	TYR	2.1
1	C	197	PRO	2.1
1	D	18	PRO	2.1
1	D	24	LEU	2.1
1	A	205	GLN	2.1
1	D	113	PHE	2.1
1	C	455	ASP	2.1
1	D	118	ILE	2.1

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($\text{\AA}^2$)	Q<0.9
3	DAO	C	502	14/14	0.94	0.19	89,96,110,113	0
3	DAO	D	502	14/14	0.94	0.17	79,91,115,116	0
3	DAO	A	502	14/14	0.95	0.14	67,70,98,99	0
3	DAO	B	502	14/14	0.96	0.14	79,84,98,100	0

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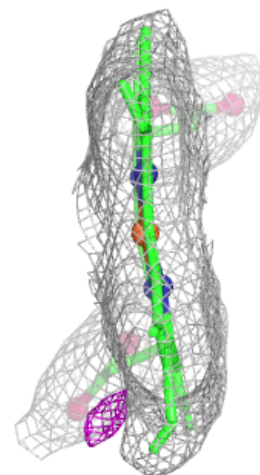
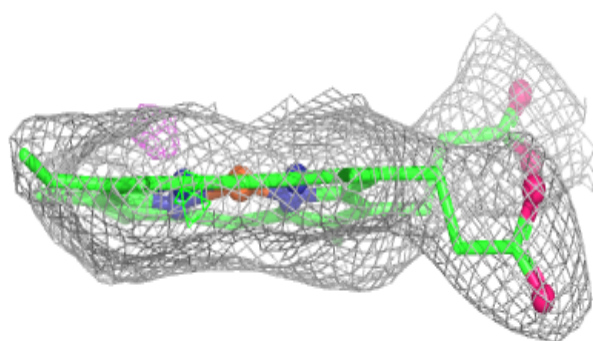
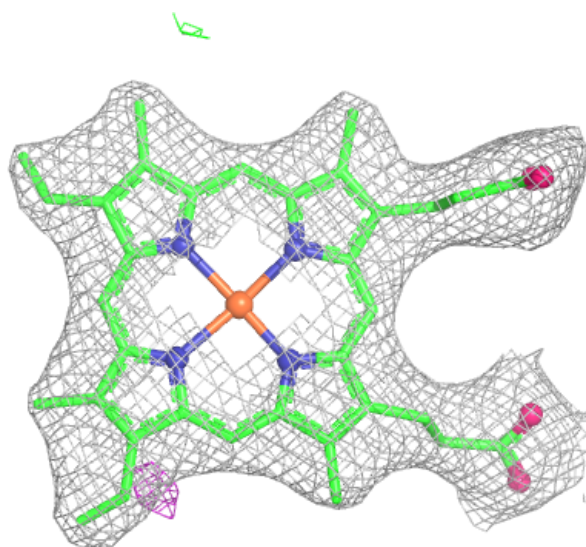
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	C	501	43/43	0.98	0.06	66,70,74,79	0
2	HEM	D	501	43/43	0.98	0.07	73,81,86,87	0
2	HEM	B	501	43/43	0.99	0.05	66,79,84,87	0
2	HEM	A	501	43/43	0.99	0.06	62,66,72,75	0

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.

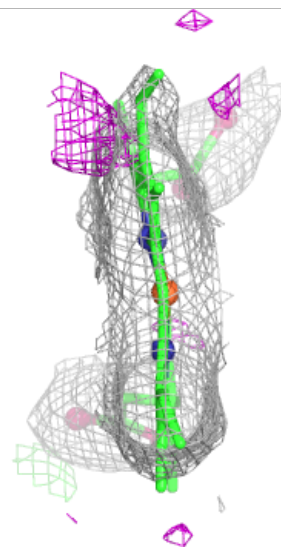
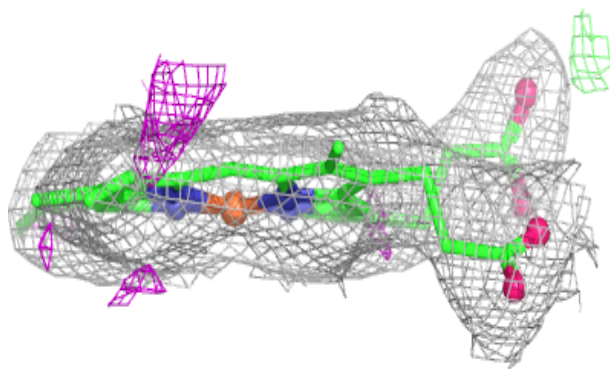
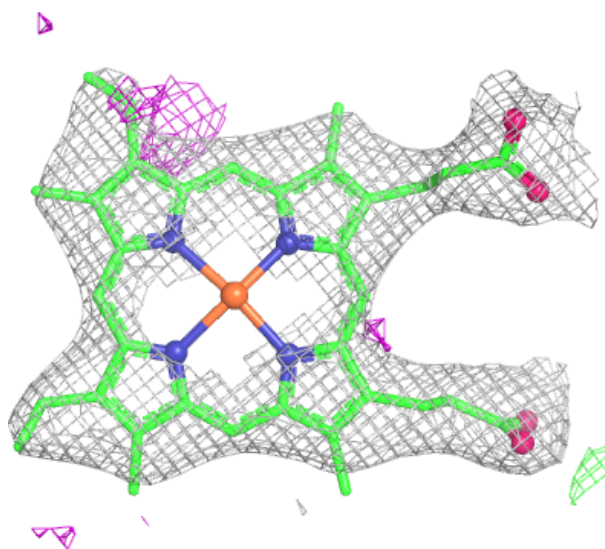
Electron density around HEM C 501:

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



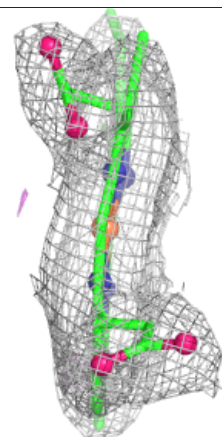
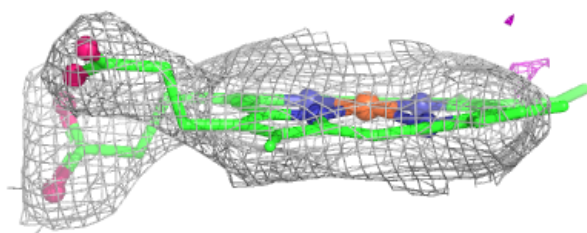
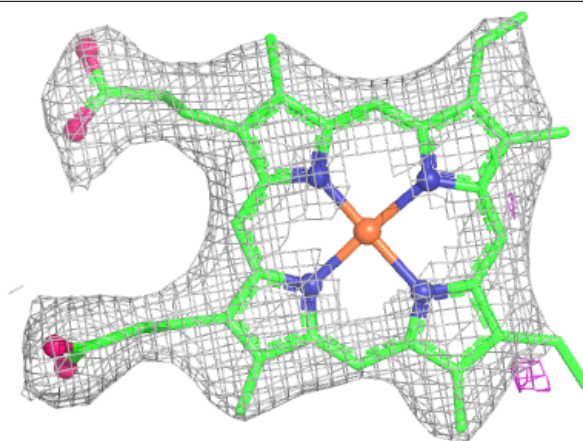
Electron density around HEM D 501:

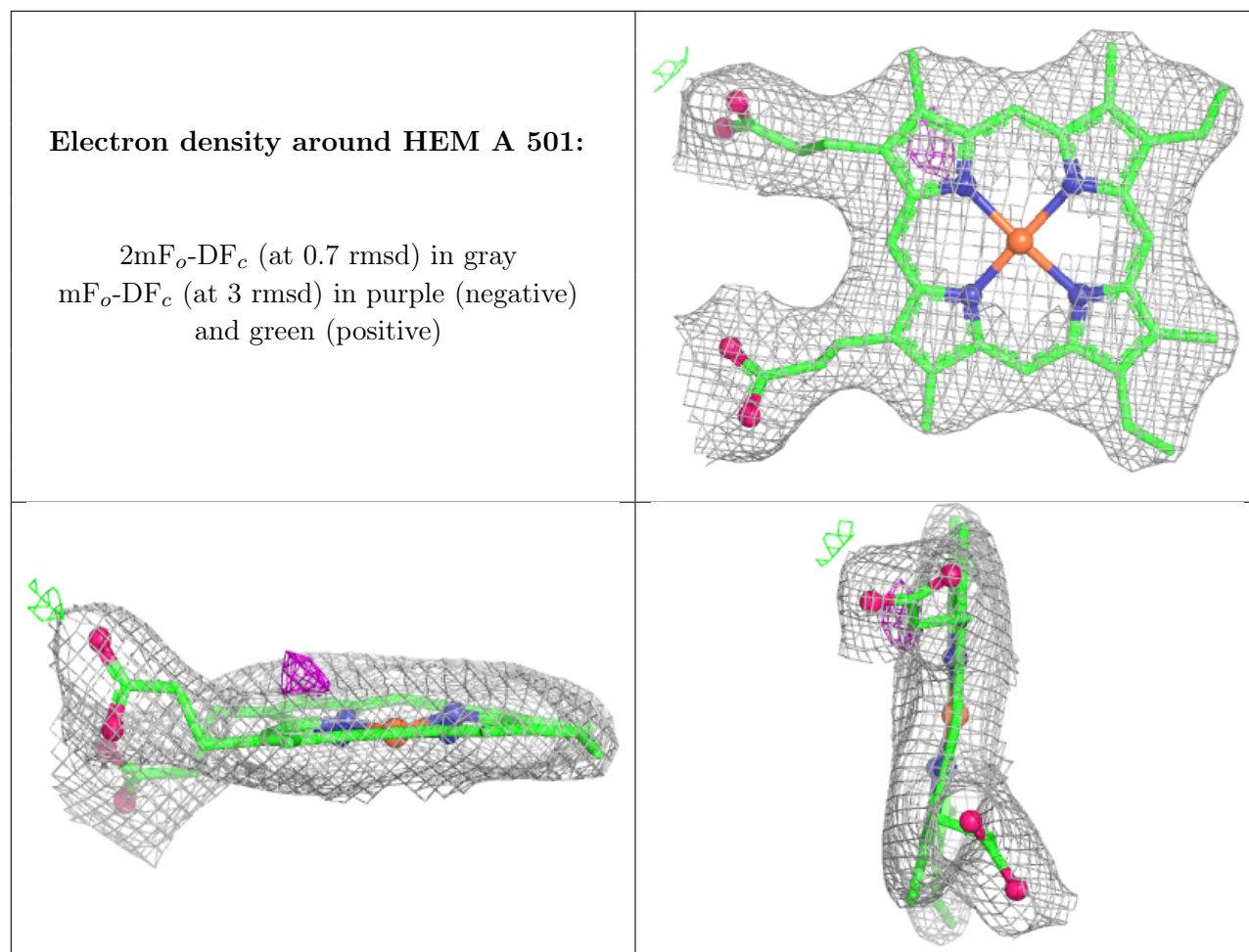
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.