WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 07:01 AM EDT

PDB ID	:	7LES
Title	:	Acanthamoeba castellanii CYP51 (AcCYP51)-Imidazole complex
Authors	:	Sharma, V.; Podust, L.M.
Deposited on	:	2021-01-15
Resolution	:	2.65 Å(reported)

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

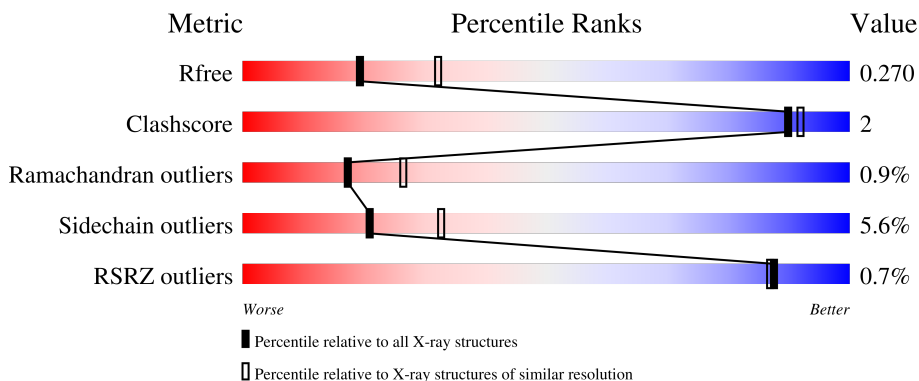|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.65 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		2
Ramachandran outliers		0.9%
Sidechain outliers		5.6%
RSRZ outliers		0.7%

Worse *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	460	89% 8% •
1	B	460	88% 9% •
1	C	460	88% 9% •
1	D	460	87% 10% •

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	PEG	B	501	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 14572 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 Obtusifoliol 14alphademethylase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total 3594	C 2322	N 599	O 655	S 18	0	2	0
1	B	448	Total 3571	C 2312	N 596	O 645	S 18	0	1	0
1	C	449	Total 3577	C 2313	N 598	O 648	S 18	0	1	0
1	D	447	Total 3550	C 2298	N 590	O 644	S 18	0	1	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	initiating methionine	UNP L8GJB3
A	34	ALA	-	expression tag	UNP L8GJB3
A	35	LYS	-	expression tag	UNP L8GJB3
A	36	LYS	-	expression tag	UNP L8GJB3
A	37	THR	-	expression tag	UNP L8GJB3
A	38	SER	-	expression tag	UNP L8GJB3
A	39	SER	-	expression tag	UNP L8GJB3
A	40	LYS	-	expression tag	UNP L8GJB3
A	41	GLY	-	expression tag	UNP L8GJB3
A	42	LYS	-	expression tag	UNP L8GJB3
A	487	HIS	-	expression tag	UNP L8GJB3
A	488	HIS	-	expression tag	UNP L8GJB3
A	489	HIS	-	expression tag	UNP L8GJB3
A	490	HIS	-	expression tag	UNP L8GJB3
A	491	HIS	-	expression tag	UNP L8GJB3
A	492	HIS	-	expression tag	UNP L8GJB3
B	33	MET	-	initiating methionine	UNP L8GJB3
B	34	ALA	-	expression tag	UNP L8GJB3
B	35	LYS	-	expression tag	UNP L8GJB3
B	36	LYS	-	expression tag	UNP L8GJB3
B	37	THR	-	expression tag	UNP L8GJB3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	SER	-	expression tag	UNP L8GJB3
B	39	SER	-	expression tag	UNP L8GJB3
B	40	LYS	-	expression tag	UNP L8GJB3
B	41	GLY	-	expression tag	UNP L8GJB3
B	42	LYS	-	expression tag	UNP L8GJB3
B	487	HIS	-	expression tag	UNP L8GJB3
B	488	HIS	-	expression tag	UNP L8GJB3
B	489	HIS	-	expression tag	UNP L8GJB3
B	490	HIS	-	expression tag	UNP L8GJB3
B	491	HIS	-	expression tag	UNP L8GJB3
B	492	HIS	-	expression tag	UNP L8GJB3
C	33	MET	-	initiating methionine	UNP L8GJB3
C	34	ALA	-	expression tag	UNP L8GJB3
C	35	LYS	-	expression tag	UNP L8GJB3
C	36	LYS	-	expression tag	UNP L8GJB3
C	37	THR	-	expression tag	UNP L8GJB3
C	38	SER	-	expression tag	UNP L8GJB3
C	39	SER	-	expression tag	UNP L8GJB3
C	40	LYS	-	expression tag	UNP L8GJB3
C	41	GLY	-	expression tag	UNP L8GJB3
C	42	LYS	-	expression tag	UNP L8GJB3
C	487	HIS	-	expression tag	UNP L8GJB3
C	488	HIS	-	expression tag	UNP L8GJB3
C	489	HIS	-	expression tag	UNP L8GJB3
C	490	HIS	-	expression tag	UNP L8GJB3
C	491	HIS	-	expression tag	UNP L8GJB3
C	492	HIS	-	expression tag	UNP L8GJB3
D	33	MET	-	initiating methionine	UNP L8GJB3
D	34	ALA	-	expression tag	UNP L8GJB3
D	35	LYS	-	expression tag	UNP L8GJB3
D	36	LYS	-	expression tag	UNP L8GJB3
D	37	THR	-	expression tag	UNP L8GJB3
D	38	SER	-	expression tag	UNP L8GJB3
D	39	SER	-	expression tag	UNP L8GJB3
D	40	LYS	-	expression tag	UNP L8GJB3
D	41	GLY	-	expression tag	UNP L8GJB3
D	42	LYS	-	expression tag	UNP L8GJB3
D	487	HIS	-	expression tag	UNP L8GJB3
D	488	HIS	-	expression tag	UNP L8GJB3
D	489	HIS	-	expression tag	UNP L8GJB3
D	490	HIS	-	expression tag	UNP L8GJB3
D	491	HIS	-	expression tag	UNP L8GJB3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	492	HIS	-	expression tag	UNP L8GJB3

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	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		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

C4
OH O4
O2
O
C3
C1
C2
HO
O1

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	C 4	O 3	0	0
3	B	1	Total 7	C 4	O 3	0	0
3	B	1	Total 7	C 4	O 3	0	0
3	D	1	Total 7	C 4	O 3	0	0
3	D	1	Total 7	C 4	O 3	0	0
3	D	1	Total 7	C 4	O 3	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$) (labeled as "Ligand of Interest" by depositor).

IMD

N3

C4   C2

C5   N1
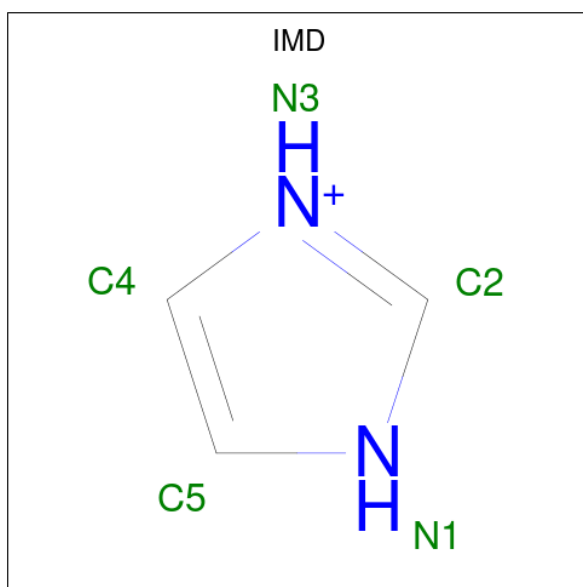
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	C 3	N 2	0	0
4	B	1	Total 5	C 3	N 2	0	0
4	C	1	Total 5	C 3	N 2	0	0
4	D	1	Total 5	C 3	N 2	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

FMT

C

OH O2

O

O1
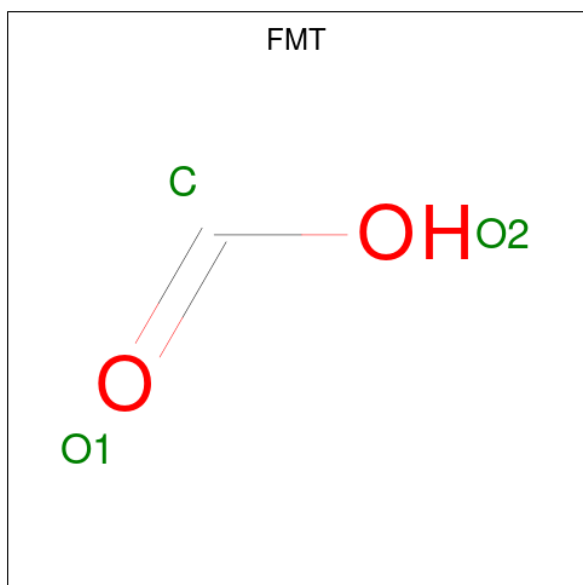
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 3	C 1	O 2	0	0
5	B	1	Total 3	C 1	O 2	0	0
5	C	1	Total 3	C 1	O 2	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total 16	O 16	0	0
6	B	8	Total 8	O 8	0	0
6	C	9	Total 9	O 9	0	0
6	D	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Obtusifoliol 14alphademethylase, putative
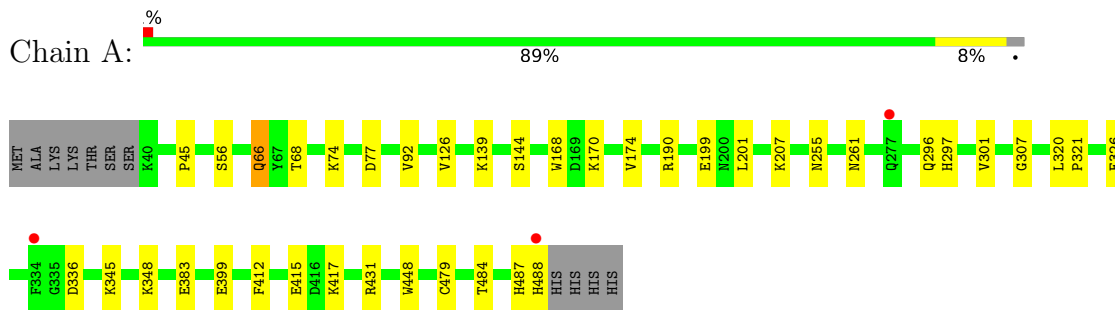
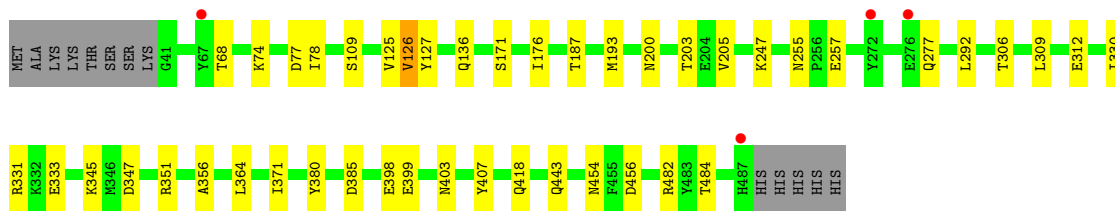• Molecule 1: Obtusifoliol 14alphademethylase, putative
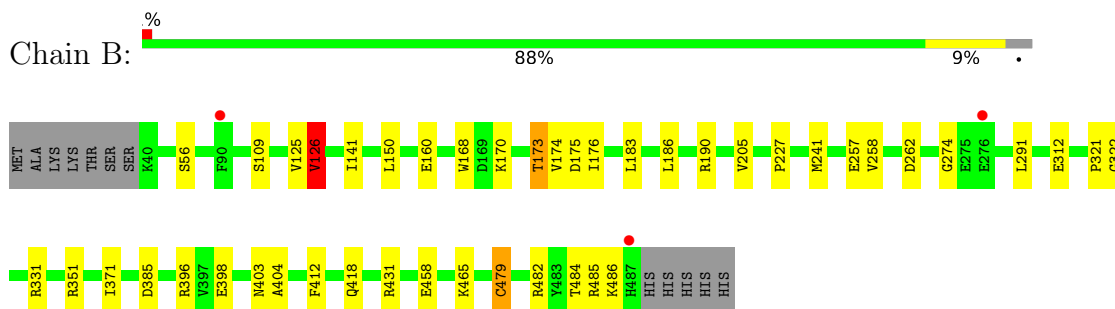
• Molecule 1: Obtusifoliol 14alphademethylase, putative
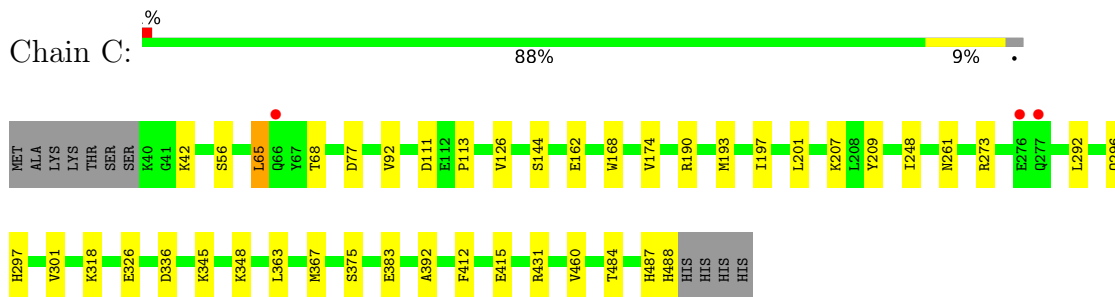
• Molecule 1: Obtusifoliol 14alphademethylase, putative
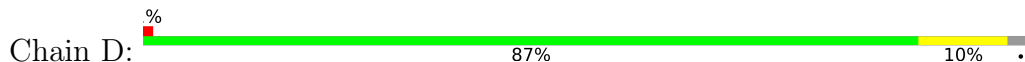
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.56Å 125.58Å 100.51Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	100.71 – 2.65 100.51 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (100.71-2.65) 99.8 (100.51-2.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.275 0.196 , 0.270	Depositor DCC
R_{free} test set	3178 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.3	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.459 for h,-k,-l 0.001 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14572	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, PEG, FMT, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.56	0/3684	0.74	0/4988
1	B	0.55	0/3660	0.74	0/4953
1	C	0.56	0/3667	0.73	0/4965
1	D	0.56	0/3638	0.74	0/4928
All	All	0.56	0/14649	0.74	0/19834

There are no bond length outliers.

There are no bond angle outliers.

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	3594	0	3551	9	0
1	B	3571	0	3546	13	0
1	C	3577	0	3541	13	0
1	D	3550	0	3501	11	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	20	0	0
3	D	21	0	30	0	0
4	A	5	0	5	0	0
4	B	5	0	5	0	0
4	C	5	0	5	1	0
4	D	5	0	5	0	0
5	A	3	0	1	0	0
5	B	3	0	1	0	0
5	C	3	0	1	0	0
6	A	16	0	0	0	0
6	B	8	0	0	0	0
6	C	9	0	0	0	0
6	D	4	0	0	0	0
All	All	14572	0	14342	52	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 2.

All (52) 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:125:VAL:HG12	1:D:126:VAL:HG12	1.84	0.60
1:B:109:SER:HB2	1:B:371:ILE:HD11	1.86	0.57
2:B:502:HEM:HBC2	2:B:502:HEM:HMC2	1.87	0.57
2:D:502:HEM:HMC2	2:D:502:HEM:HBC2	1.86	0.56
1:C:412:PHE:HA	1:C:415:GLU:HB3	1.88	0.55
1:B:398:GLU:OE1	1:B:403:ASN:N	2.38	0.55
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.89	0.53
1:A:412:PHE:HA	1:A:415:GLU:HB3	1.89	0.53
1:B:173:THR:HG22	1:B:482:ARG:HG2	1.92	0.52
1:C:65:LEU:HD21	1:C:392:ALA:HB1	1.92	0.52
1:A:297:HIS:O	1:A:301:VAL:HG13	2.10	0.51
1:D:398:GLU:OE1	1:D:403:ASN:N	2.44	0.51
1:C:197:ILE:HG13	1:C:248:ILE:HD13	1.93	0.50
1:C:193:MET:CE	1:C:292:LEU:HD11	2.42	0.50
1:C:168:TRP:CH2	1:C:174:VAL:HG11	2.48	0.49
1:C:77:ASP:HB2	1:C:92:VAL:O	2.13	0.48
1:C:193:MET:HE1	1:C:292:LEU:HD11	1.96	0.48
1:A:66:GLN:HG2	1:B:227:PRO:HB2	1.94	0.48
1:C:326:GLU:OE2	1:C:348:LYS:N	2.46	0.48
1:C:209:TYR:HH	1:C:297:HIS:CD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:MET:HE1	1:D:292:LEU:HD11	1.95	0.47
1:A:77:ASP:HB2	1:A:92:VAL:O	2.15	0.47
1:D:187:THR:HG21	1:D:443:GLN:HE22	1.80	0.47
1:C:363:LEU:HD11	4:C:502:IMD:C5	2.44	0.47
1:A:320:LEU:N	1:A:321:PRO:HD2	2.29	0.47
1:B:125:VAL:HG12	1:B:126:VAL:HG22	1.97	0.46
1:D:193:MET:CE	1:D:292:LEU:HD11	2.45	0.46
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.96	0.46
1:C:297:HIS:O	1:C:301:VAL:HG13	2.16	0.45
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.97	0.45
1:A:307:GLY:HA3	1:A:448:TRP:CH2	2.51	0.44
1:B:175:ASP:HA	1:B:479:CYS:O	2.18	0.44
1:B:168:TRP:CH2	1:B:174:VAL:HG11	2.53	0.44
1:B:396:ARG:HA	1:B:404:ALA:HB1	1.98	0.44
2:B:502:HEM:CMB	2:B:502:HEM:HBB2	2.48	0.44
1:D:306:THR:HA	1:D:356:ALA:HB2	2.00	0.43
2:D:502:HEM:CMB	2:D:502:HEM:HBB2	2.49	0.43
1:B:141:ILE:HG23	1:B:291:LEU:HD21	2.01	0.43
1:B:160:GLU:OE1	1:B:190:ARG:NH2	2.52	0.43
1:C:42:LYS:O	1:D:380:TYR:N	2.50	0.42
1:A:307:GLY:HA3	1:A:448:TRP:CZ2	2.54	0.42
1:A:326:GLU:OE2	1:A:348:LYS:N	2.48	0.42
1:B:351:ARG:HD2	1:B:412:PHE:HB2	2.02	0.41
1:D:347:ASP:O	1:D:351:ARG:HG3	2.21	0.41
1:B:183:LEU:O	1:B:186:LEU:HB2	2.21	0.41
1:B:321:PRO:O	1:B:322:GLY:C	2.60	0.41
1:D:126:VAL:HG22	1:D:127:TYR:N	2.36	0.40
1:D:309:LEU:HB3	1:D:407:TYR:CE1	2.56	0.40
1:C:113:PRO:HB3	1:C:367:MET:CG	2.51	0.40
1:D:109:SER:HB2	1:D:371:ILE:HD11	2.03	0.40
2:B:502:HEM:HBB2	2:B:502:HEM:HMB2	2.03	0.40
1:A:168:TRP:CH2	1:A:174:VAL:HG11	2.56	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	449/460 (98%)	427 (95%)	19 (4%)	3 (1%)	22	33
1	B	447/460 (97%)	422 (94%)	22 (5%)	3 (1%)	22	33
1	C	448/460 (97%)	415 (93%)	29 (6%)	4 (1%)	17	26
1	D	446/460 (97%)	416 (93%)	24 (5%)	6 (1%)	12	18
All	All	1790/1840 (97%)	1680 (94%)	94 (5%)	16 (1%)	17	26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	VAL
1	D	78	ILE
1	D	257	GLU
1	D	277	GLN
1	A	296	GLN
1	B	257	GLU
1	C	65	LEU
1	C	273	ARG
1	D	74	LYS
1	D	126	VAL
1	A	126	VAL
1	B	274	GLY
1	C	126	VAL
1	D	77	ASP
1	C	296	GLN
1	A	45	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	382/397 (96%)	359 (94%)	23 (6%)	19	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	378/397 (95%)	357 (94%)	21 (6%)	21	33
1	C	380/397 (96%)	361 (95%)	19 (5%)	24	38
1	D	373/397 (94%)	351 (94%)	22 (6%)	19	30
All	All	1513/1588 (95%)	1428 (94%)	85 (6%)	21	33

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	66	GLN
1	A	68	THR
1	A	74	LYS
1	A	139	LYS
1	A	144	SER
1	A	170	LYS
1	A	190	ARG
1	A	199	GLU
1	A	201	LEU
1	A	207	LYS
1	A	255	ASN
1	A	261	ASN
1	A	336	ASP
1	A	345	LYS
1	A	383	GLU
1	A	399	GLU
1	A	417	LYS
1	A	431	ARG
1	A	479	CYS
1	A	484	THR
1	A	487	HIS
1	A	488	HIS
1	B	56	SER
1	B	126	VAL
1	B	150	LEU
1	B	170	LYS
1	B	173	THR
1	B	176	ILE
1	B	205	VAL
1	B	241	MET
1	B	258	VAL
1	B	262	ASP

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Mol	Chain	Res	Type
1	B	312	GLU
1	B	331	ARG
1	B	385	ASP
1	B	418	GLN
1	B	431	ARG
1	B	458	GLU
1	B	465	LYS
1	B	479	CYS
1	B	484	THR
1	B	485	ARG
1	B	486	LYS
1	C	56	SER
1	C	68	THR
1	C	111	ASP
1	C	144	SER
1	C	162	GLU
1	C	190	ARG
1	C	201	LEU
1	C	207	LYS
1	C	261	ASN
1	C	318	LYS
1	C	336	ASP
1	C	345	LYS
1	C	375	SER
1	C	383	GLU
1	C	431	ARG
1	C	460	VAL
1	C	484	THR
1	C	487	HIS
1	C	488	HIS
1	D	68	THR
1	D	136	GLN
1	D	171	SER
1	D	176	ILE
1	D	200	ASN
1	D	203	THR
1	D	205	VAL
1	D	247	LYS
1	D	255	ASN
1	D	312	GLU
1	D	330	ILE
1	D	331	ARG

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Mol	Chain	Res	Type
1	D	333	GLU
1	D	345	LYS
1	D	364	LEU
1	D	385	ASP
1	D	399	GLU
1	D	418	GLN
1	D	454	ASN
1	D	456	ASP
1	D	482	ARG
1	D	484	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	297	HIS
1	A	454	ASN
1	B	443	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	D	502	1,4	41,50,50	1.42	5 (12%)	45,82,82	1.96	12 (26%)
4	IMD	C	502	2	3,5,5	0.52	0	4,5,5	0.70	0
2	HEM	C	501	1,4	41,50,50	1.38	4 (9%)	45,82,82	2.18	16 (35%)
3	PEG	D	503	-	6,6,6	0.46	0	5,5,5	0.13	0
4	IMD	D	504	2	3,5,5	0.53	0	4,5,5	0.64	0
5	FMT	B	505	-	2,2,2	0.74	0	1,1,1	0.69	0
4	IMD	B	504	2	3,5,5	0.38	0	4,5,5	0.61	0
4	IMD	A	503	2	3,5,5	0.47	0	4,5,5	0.56	0
3	PEG	B	501	-	6,6,6	0.54	0	5,5,5	0.67	0
5	FMT	A	504	-	2,2,2	0.78	0	1,1,1	0.69	0
3	PEG	D	501	-	6,6,6	0.58	0	5,5,5	0.59	0
2	HEM	A	501	1,4	41,50,50	1.41	6 (14%)	45,82,82	2.09	14 (31%)
3	PEG	A	502	-	6,6,6	0.63	0	5,5,5	0.45	0
3	PEG	D	505	-	6,6,6	0.60	0	5,5,5	0.39	0
3	PEG	B	503	-	6,6,6	0.53	0	5,5,5	0.22	0
5	FMT	C	503	-	2,2,2	0.73	0	1,1,1	0.74	0
2	HEM	B	502	1,4	41,50,50	1.42	6 (14%)	45,82,82	1.91	15 (33%)

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	D	502	1,4	-	0/12/54/54	-
4	IMD	C	502	2	-	-	0/1/1/1
2	HEM	C	501	1,4	-	0/12/54/54	-
3	PEG	D	503	-	-	2/4/4/4	-
4	IMD	D	504	2	-	-	0/1/1/1
4	IMD	B	504	2	-	-	0/1/1/1
4	IMD	A	503	2	-	-	0/1/1/1
3	PEG	B	501	-	-	2/4/4/4	-
3	PEG	D	501	-	-	2/4/4/4	-
2	HEM	A	501	1,4	-	0/12/54/54	-
3	PEG	A	502	-	-	2/4/4/4	-
3	PEG	D	505	-	-	3/4/4/4	-
3	PEG	B	503	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	502	1,4	-	0/12/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C1B-NB	-4.84	1.32	1.40
2	C	501	HEM	C1B-NB	-4.80	1.32	1.40
2	D	502	HEM	C1B-NB	-4.14	1.33	1.40
2	B	502	HEM	C1B-NB	-4.08	1.33	1.40
2	D	502	HEM	C4D-ND	-3.38	1.34	1.40
2	B	502	HEM	CHB-C1B	3.06	1.42	1.35
2	D	502	HEM	C4B-NB	-2.95	1.32	1.38
2	D	502	HEM	CHB-C1B	2.89	1.42	1.35
2	B	502	HEM	C4B-NB	-2.82	1.33	1.38
2	B	502	HEM	C4D-ND	-2.79	1.35	1.40
2	A	501	HEM	C4D-ND	-2.74	1.35	1.40
2	A	501	HEM	C4B-NB	-2.62	1.33	1.38
2	C	501	HEM	C4B-NB	-2.54	1.33	1.38
2	C	501	HEM	CHB-C1B	2.44	1.41	1.35
2	C	501	HEM	C4D-ND	-2.35	1.36	1.40
2	D	502	HEM	FE-NB	2.34	2.08	1.96
2	B	502	HEM	FE-NB	2.31	2.08	1.96
2	A	501	HEM	CHB-C1B	2.20	1.40	1.35
2	A	501	HEM	FE-NB	2.11	2.07	1.96
2	A	501	HEM	O1D-CGD	2.09	1.29	1.22
2	B	502	HEM	C1D-C2D	2.01	1.48	1.44

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CHC-C4B-NB	5.56	130.47	124.43
2	C	501	HEM	C1B-NB-C4B	5.28	110.52	105.07
2	A	501	HEM	C1B-NB-C4B	5.26	110.51	105.07
2	A	501	HEM	CHC-C4B-NB	5.21	130.09	124.43
2	D	502	HEM	C1B-NB-C4B	5.07	110.31	105.07
2	B	502	HEM	C1B-NB-C4B	4.71	109.94	105.07
2	A	501	HEM	CHD-C1D-ND	4.46	129.28	124.43
2	C	501	HEM	CHD-C1D-ND	4.29	129.09	124.43
2	B	502	HEM	CHD-C1D-ND	4.26	129.06	124.43
2	B	502	HEM	CHC-C4B-NB	4.03	128.81	124.43
2	D	502	HEM	CHC-C4B-NB	3.99	128.76	124.43
2	C	501	HEM	C4B-C3B-C2B	-3.78	104.11	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	HEM	CHD-C1D-ND	3.77	128.53	124.43
2	C	501	HEM	CBD-CAD-C3D	3.71	122.93	112.63
2	A	501	HEM	CAD-CBD-CGD	-3.64	105.78	113.60
2	A	501	HEM	C4B-C3B-C2B	-3.56	104.29	107.11
2	B	502	HEM	CHD-C1D-C2D	-3.54	119.46	124.98
2	C	501	HEM	CHA-C4D-C3D	-3.44	118.87	125.33
2	A	501	HEM	CHD-C1D-C2D	-3.42	119.64	124.98
2	A	501	HEM	CHA-C4D-ND	3.36	128.54	124.38
2	D	502	HEM	CHD-C1D-C2D	-3.30	119.82	124.98
2	C	501	HEM	CHA-C4D-ND	3.29	128.45	124.38
2	D	502	HEM	CAD-CBD-CGD	-3.19	106.73	113.60
2	D	502	HEM	O2D-CGD-CBD	3.07	123.91	114.03
2	D	502	HEM	CHA-C4D-ND	3.06	128.16	124.38
2	C	501	HEM	CAD-CBD-CGD	-2.94	107.28	113.60
2	D	502	HEM	CHB-C1B-NB	2.92	127.99	124.38
2	A	501	HEM	CBD-CAD-C3D	2.88	120.64	112.63
2	D	502	HEM	CMD-C2D-C1D	2.75	129.23	125.04
2	C	501	HEM	CMC-C2C-C3C	2.73	129.79	124.68
2	A	501	HEM	CHA-C4D-C3D	-2.70	120.25	125.33
2	B	502	HEM	CHA-C4D-ND	2.70	127.71	124.38
2	A	501	HEM	CHB-C1B-NB	2.68	127.69	124.38
2	B	502	HEM	C4B-C3B-C2B	-2.68	104.99	107.11
2	B	502	HEM	CHA-C4D-C3D	-2.64	120.38	125.33
2	D	502	HEM	O1D-CGD-CBD	-2.60	114.73	123.08
2	D	502	HEM	CHA-C4D-C3D	-2.56	120.52	125.33
2	B	502	HEM	CAD-CBD-CGD	-2.52	108.18	113.60
2	B	502	HEM	CAD-C3D-C4D	2.51	129.04	124.66
2	C	501	HEM	CHB-C1B-NB	2.46	127.43	124.38
2	B	502	HEM	CMD-C2D-C1D	2.45	128.77	125.04
2	C	501	HEM	CHD-C1D-C2D	-2.41	121.22	124.98
2	C	501	HEM	CAD-C3D-C4D	2.39	128.83	124.66
2	A	501	HEM	CMC-C2C-C3C	2.38	129.13	124.68
2	C	501	HEM	CHC-C4B-C3B	-2.33	121.00	124.57
2	B	502	HEM	CHB-C1B-NB	2.25	127.16	124.38
2	B	502	HEM	CMC-C2C-C3C	2.24	128.87	124.68
2	C	501	HEM	CBA-CAA-C2A	-2.24	108.80	112.62
2	C	501	HEM	C3D-C4D-ND	2.18	112.60	110.17
2	B	502	HEM	O2A-CGA-O1A	-2.17	117.89	123.30
2	A	501	HEM	CMD-C2D-C1D	2.16	128.32	125.04
2	B	502	HEM	CBD-CAD-C3D	2.13	118.54	112.63
2	D	502	HEM	CAD-C3D-C4D	2.11	128.34	124.66
2	C	501	HEM	CMA-C3A-C4A	-2.10	125.24	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	HEM	C4A-C3A-C2A	2.09	108.45	107.00
2	A	501	HEM	CHC-C4B-C3B	-2.05	121.43	124.57
2	A	501	HEM	CMA-C3A-C4A	-2.03	125.34	128.46

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PEG	O1-C1-C2-O2
3	A	502	PEG	O2-C3-C4-O4
3	B	501	PEG	O1-C1-C2-O2
3	B	503	PEG	O2-C3-C4-O4
3	B	503	PEG	O1-C1-C2-O2
3	D	503	PEG	O1-C1-C2-O2
3	D	501	PEG	O1-C1-C2-O2
3	D	505	PEG	O2-C3-C4-O4
3	D	501	PEG	C4-C3-O2-C2
3	D	505	PEG	C1-C2-O2-C3
3	D	503	PEG	O2-C3-C4-O4
3	B	503	PEG	C1-C2-O2-C3
3	D	505	PEG	O1-C1-C2-O2
3	B	501	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 9 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand IMD C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand IMD D 504

Bond lengths

Bond angles

Torsions

Rings

Ligand IMD B 504

Bond lengths

Bond angles

Torsions

Rings

Ligand IMD A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 502

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	449/460 (97%)	-0.05	3 (0%) 87	87	56, 78, 110, 156	0
1	B	448/460 (97%)	-0.04	3 (0%) 87	87	57, 80, 117, 153	0
1	C	449/460 (97%)	-0.04	3 (0%) 87	87	57, 77, 110, 153	0
1	D	447/460 (97%)	-0.04	4 (0%) 84	83	57, 80, 114, 168	0
All	All	1793/1840 (97%)	-0.04	13 (0%) 87	87	56, 79, 113, 168	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	GLU	4.7
1	D	276	GLU	4.5
1	D	487	HIS	3.1
1	B	276	GLU	2.9
1	C	277	GLN	2.9
1	D	67	TYR	2.7
1	B	487	HIS	2.6
1	A	334	PHE	2.5
1	B	90	PHE	2.5
1	A	277	GLN	2.2
1	C	66	GLN	2.2
1	A	488	HIS	2.0
1	D	272	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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	PEG	B	501	7/7	0.77	0.44	72,96,114,115	0
5	FMT	B	505	3/3	0.87	0.18	81,81,86,87	0
3	PEG	D	501	7/7	0.89	0.23	89,91,98,101	0
3	PEG	A	502	7/7	0.89	0.31	69,75,82,85	0
5	FMT	A	504	3/3	0.91	0.14	79,79,83,84	0
5	FMT	C	503	3/3	0.94	0.14	78,78,85,85	0
4	IMD	D	504	5/5	0.95	0.28	72,80,91,97	0
3	PEG	B	503	7/7	0.95	0.36	74,77,82,82	0
3	PEG	D	503	7/7	0.95	0.24	71,73,85,91	0
4	IMD	C	502	5/5	0.95	0.33	68,73,76,80	0
4	IMD	A	503	5/5	0.96	0.25	70,70,78,82	0
3	PEG	D	505	7/7	0.96	0.55	77,93,109,113	0
4	IMD	B	504	5/5	0.97	0.26	70,79,90,93	0
2	HEM	C	501	43/43	0.98	0.17	53,62,69,74	0
2	HEM	B	502	43/43	0.98	0.18	44,57,82,94	0
2	HEM	D	502	43/43	0.99	0.19	43,57,81,97	0
2	HEM	A	501	43/43	0.99	0.18	51,60,69,86	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 IMD D 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
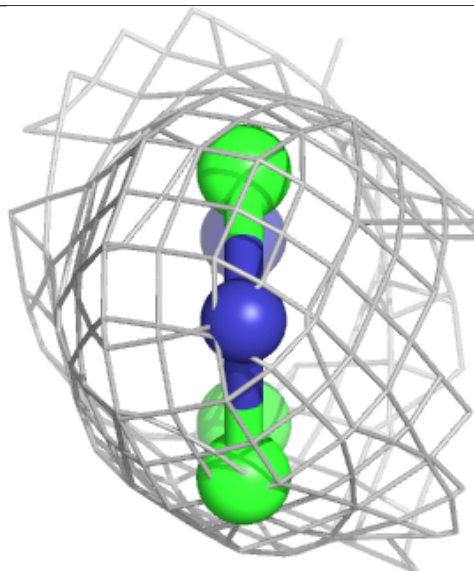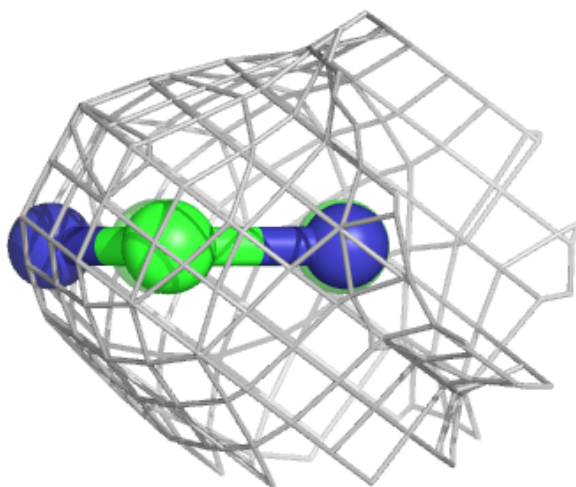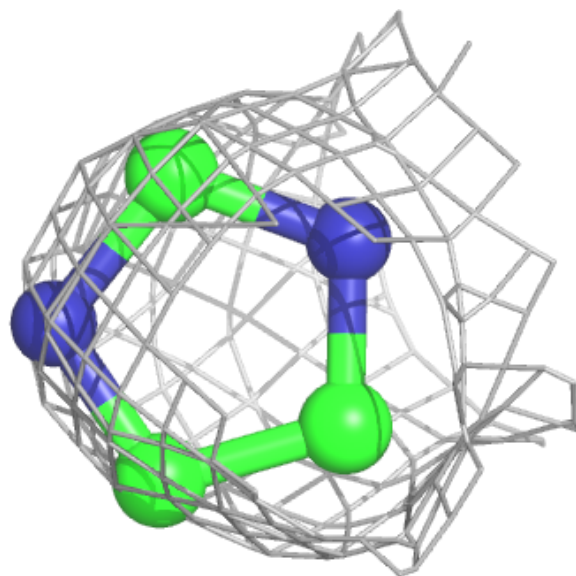
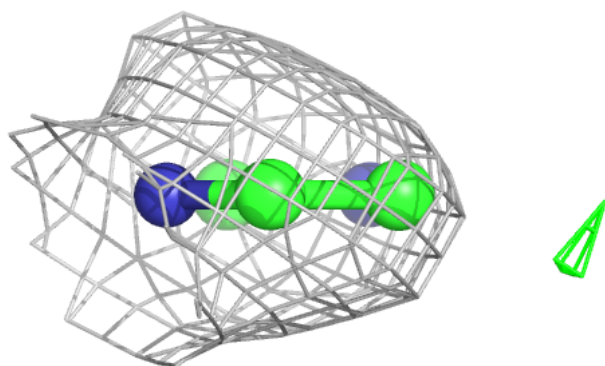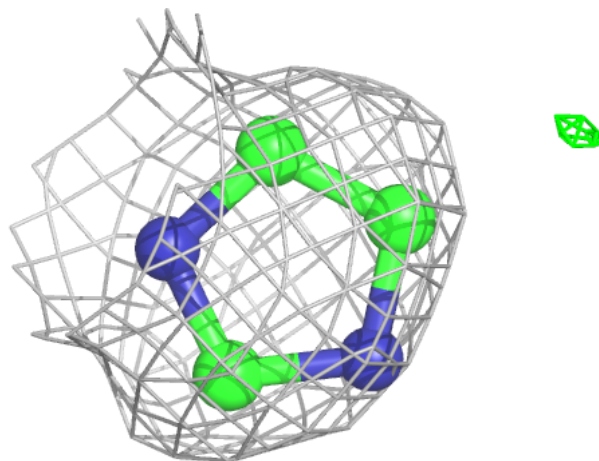**Electron density around IMD C 502:**

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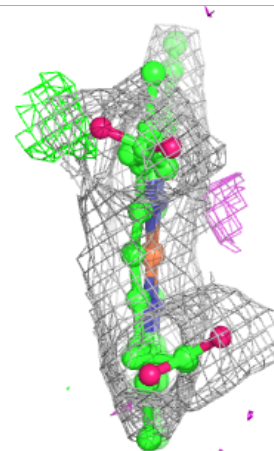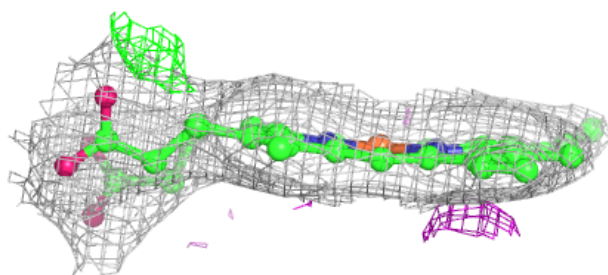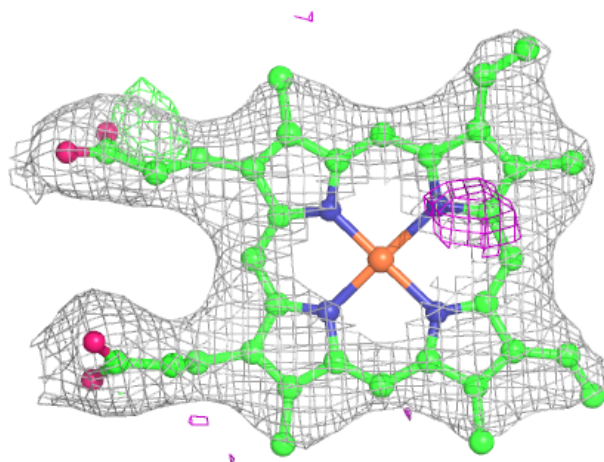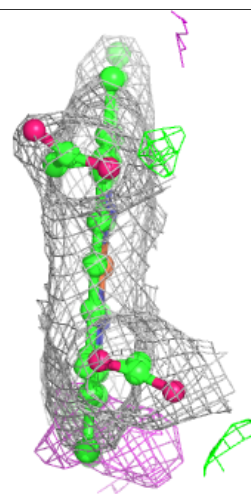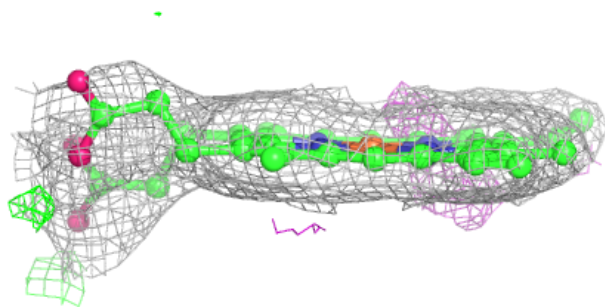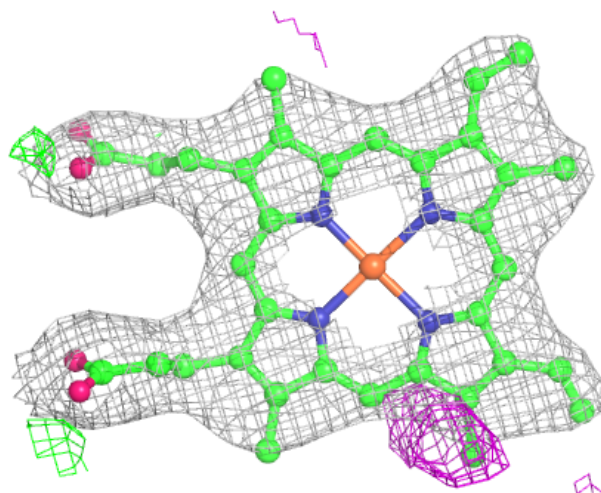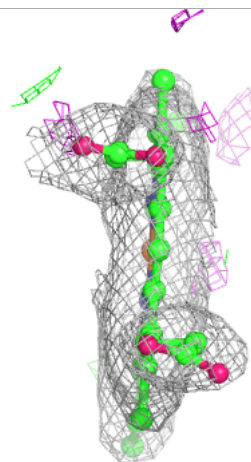and green (positive)

Electron density around IMD A 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
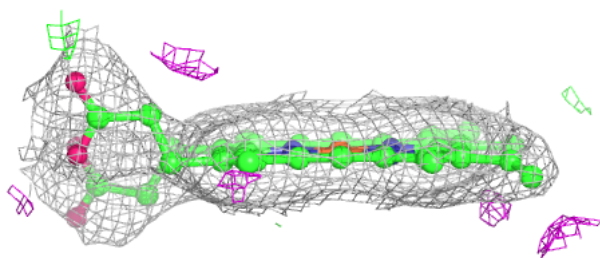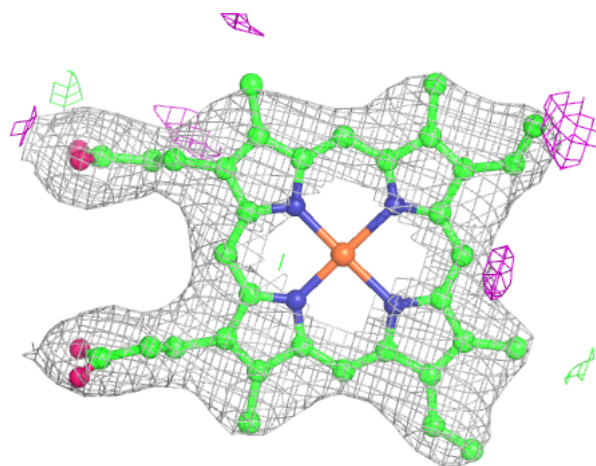and green (positive)
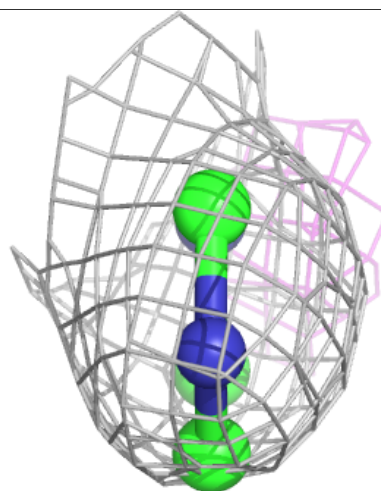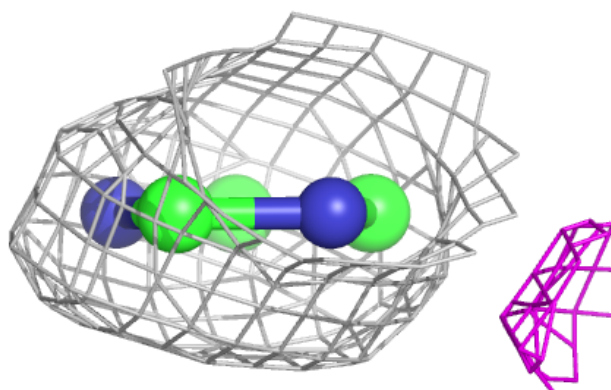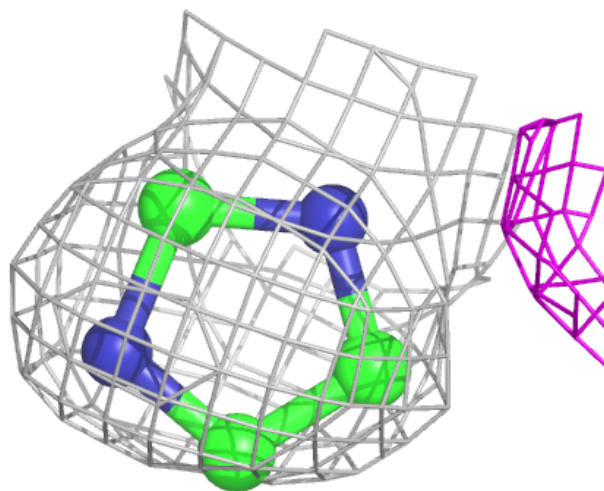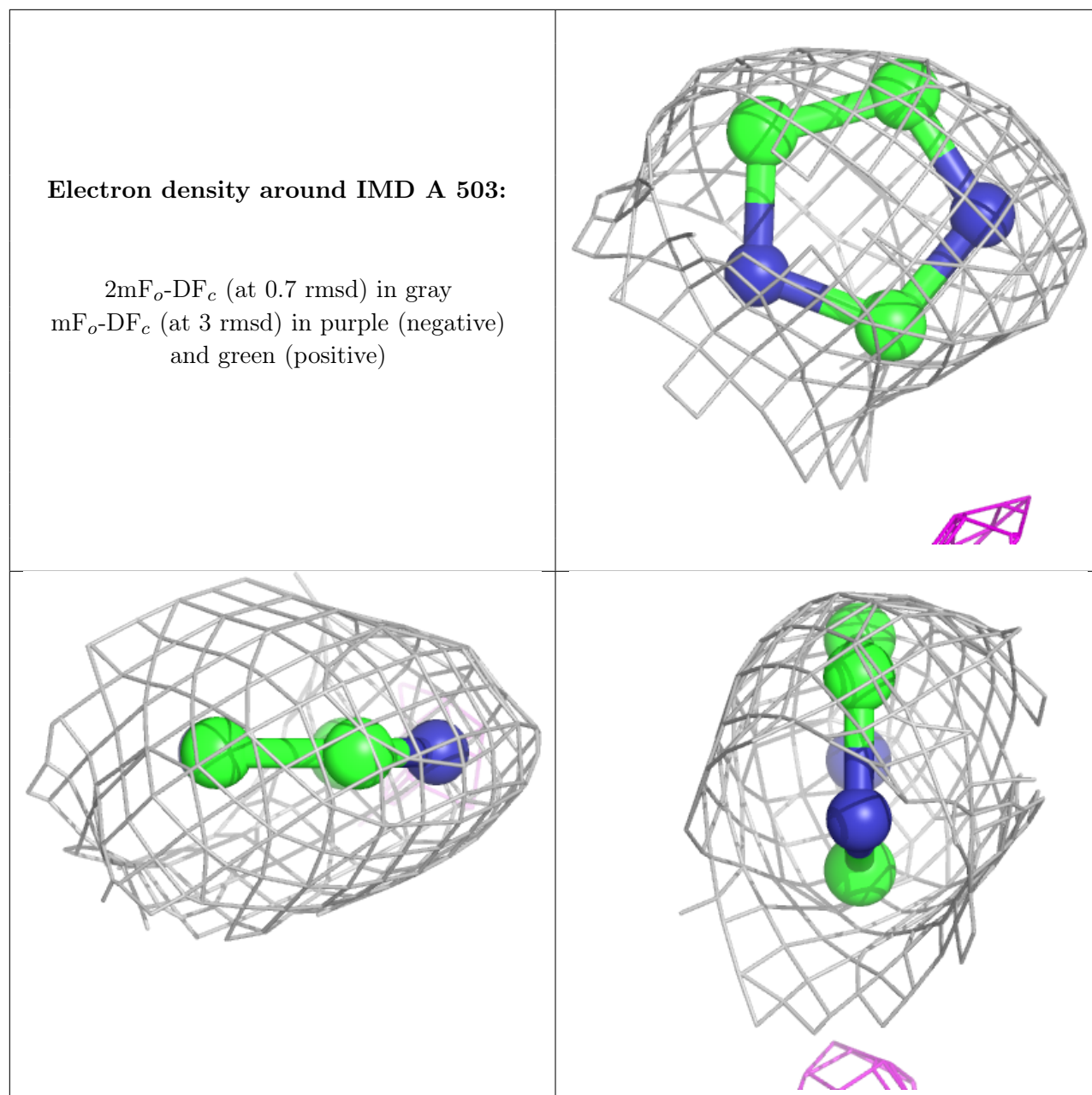
Electron density around IMD B 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
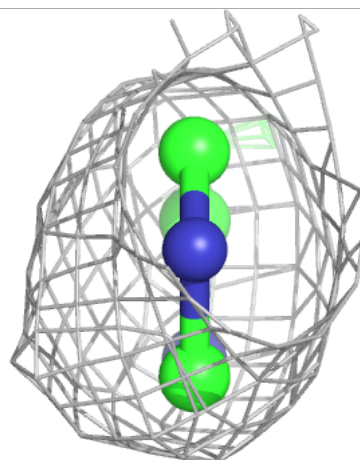
Electron density around HEM C 501:

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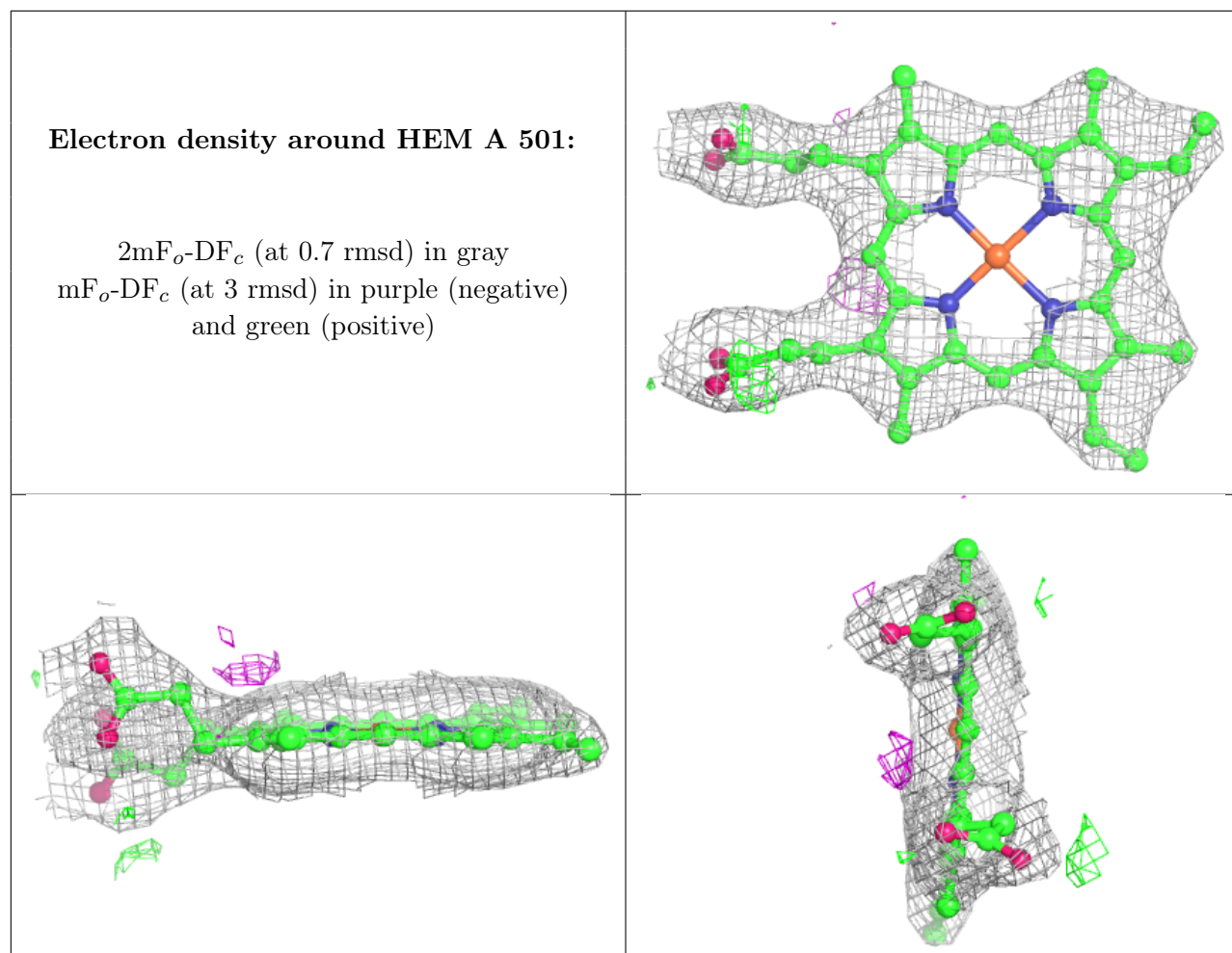and green (positive)

Electron density around HEM B 502:

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 502:

$2mF_o$-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 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.