



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2026 – 12:11 PM JST

PDB ID : 23UB / pdb_000023ub
Title : Structure of the CYP102A1 Heme Domain with 2-(undecylcarbamoyl)benzoic acid
Authors : Ishigami, M.; Sugimoto, H.; Shoji, O.
Deposited on : 2026-02-17
Resolution : 1.63 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	:	1.8.5 (274361), CSD as541be (2020)
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

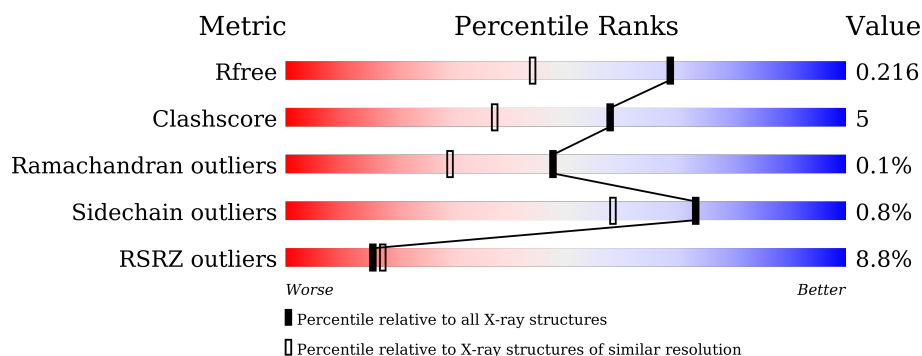
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

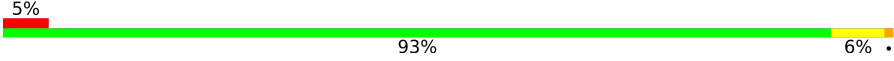

The reported resolution of this entry is 1.63 Å.

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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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 $\leq 5\%$. 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	456	
1	B	456	

2 Entry composition [i](#)

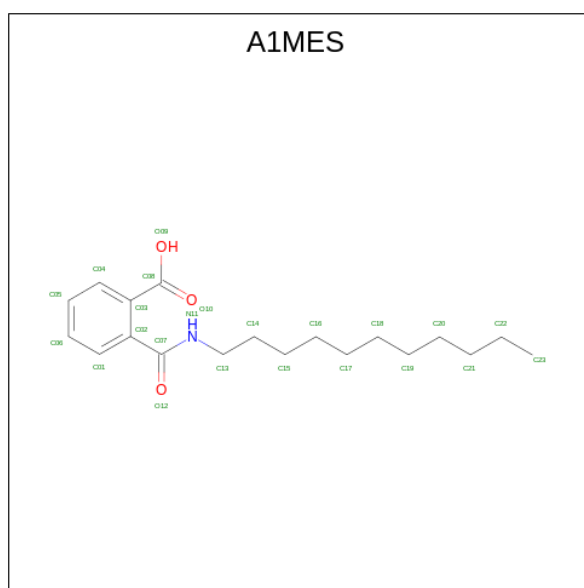
There are 4 unique types of molecules in this entry. The entry contains 15635 atoms, of which 7507 are hydrogens and 0 are deuteriums.

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.

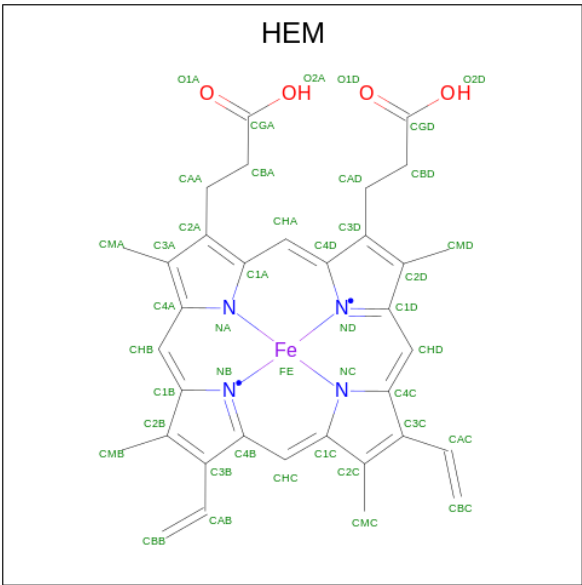
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	H	N	O	S	81	8	0
			7395	2367	3689	628	694	17			
1	B	455	Total	C	H	N	O	S	80	7	0
			7411	2371	3702	630	690	18			

- Molecule 2 is 2-(undecylcarbamoyl)benzoic acid (CCD ID: A1MES) (formula: $C_{19}H_{29}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			51	19	28	1	3		
2	B	1	Total	C	H	N	O	0	0
			51	19	28	1	3		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	12	0
			73	34	1	30	4	4		
3	B	1	Total	C	Fe	H	N	O	12	0
			73	34	1	30	4	4		

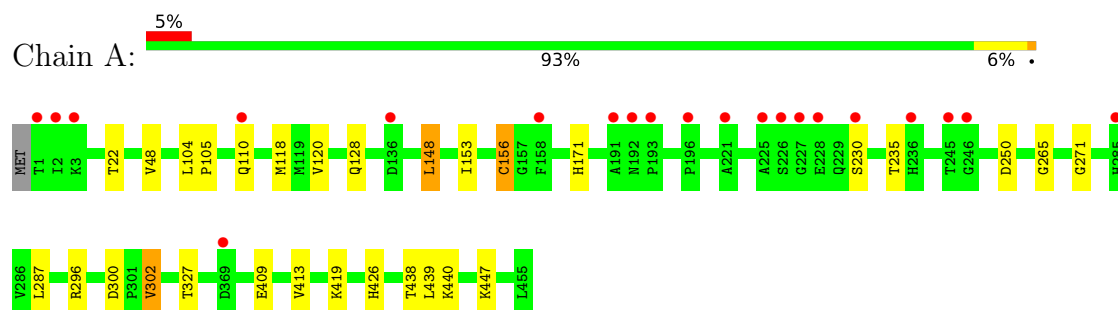
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	283	Total	O	0	0
			283	283		
4	B	298	Total	O	0	0
			298	298		

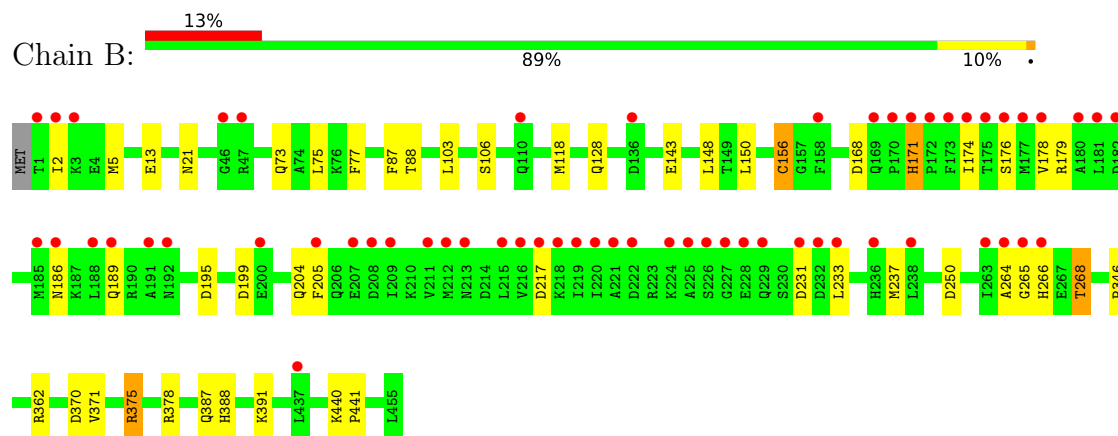
3 Residue-property plots [i](#)

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: Bifunctional cytochrome P450/NADPH-P450 reductase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.08Å 129.48Å 149.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.40 – 1.63 46.40 – 1.63	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.40-1.63) 100.0 (46.40-1.63)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.188 , 0.216 0.188 , 0.216	Depositor DCC
R_{free} test set	7312 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15635	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1728e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, A1MES

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	0.68	0/3822	1.14	6/5168 (0.1%)
1	B	0.69	0/3820	1.18	14/5162 (0.3%)
All	All	0.69	0/7642	1.16	20/10330 (0.2%)

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

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	195	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	250	ASP	CA-CB-CG	6.99	119.58	112.60
1	B	13	GLU	CB-CG-CD	6.15	123.05	112.60
1	B	231	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	217	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	302	VAL	N-CA-CB	-5.79	104.09	111.39
1	A	235	THR	CA-CB-OG1	-5.63	101.15	109.60
1	B	5	MET	CB-CA-C	5.54	116.39	108.68
1	B	231	ASP	CB-CA-C	-5.43	104.49	111.50
1	B	156	CYS	CA-C-N	5.42	126.66	120.70
1	B	156	CYS	C-N-CA	5.42	126.66	120.70
1	B	199	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	143	GLU	CB-CG-CD	5.38	121.74	112.60
1	A	250	ASP	CA-CB-CG	5.36	117.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	LEU	N-CA-CB	-5.21	102.46	110.12
1	B	205	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	268	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	110	GLN	CB-CA-C	-5.11	102.30	110.79
1	B	378	ARG	CB-CA-C	-5.06	101.27	110.63
1	A	156	CYS	N-CA-C	-5.04	105.79	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	375[A]	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3706	3689	3638	20	0
1	B	3709	3702	3664	46	0
2	A	23	28	0	0	0
2	B	23	28	0	2	0
3	A	43	30	30	0	0
3	B	43	30	30	1	0
4	A	283	0	0	7	0
4	B	298	0	0	21	0
All	All	8128	7507	7362	68	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 5.

All (68) 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:375[A]:ARG:CZ	4:B:601:HOH:O	1.78	1.31
1:B:370:ASP:OD2	1:B:375[B]:ARG:NH1	1.65	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:PRO:C	4:B:602:HOH:O	1.83	1.21
1:B:204:GLN:HG3	4:B:607:HOH:O	1.30	1.20
1:B:375[A]:ARG:NH1	4:B:601:HOH:O	1.73	1.10
1:A:118:MET:HE1	4:A:612:HOH:O	1.69	0.92
1:B:375[A]:ARG:HH11	1:B:375[A]:ARG:HG2	1.36	0.91
1:B:179:ARG:HB3	4:B:731:HOH:O	1.70	0.89
1:A:118:MET:HG2	4:A:862:HOH:O	1.77	0.83
1:B:375[B]:ARG:NE	4:B:604:HOH:O	2.13	0.81
1:B:375[A]:ARG:NH1	4:B:605:HOH:O	2.19	0.75
1:B:375[A]:ARG:HH11	1:B:375[A]:ARG:CG	2.01	0.74
1:A:440:LYS:HG3	4:A:614:HOH:O	1.88	0.73
1:B:75:LEU:HD21	1:B:87:PHE:CZ	2.24	0.73
2:B:501:A1MES:C01	4:B:846:HOH:O	2.38	0.71
1:A:171:HIS:HB2	4:A:720:HOH:O	1.93	0.67
1:B:176:SER:HA	4:B:731:HOH:O	1.96	0.65
1:B:150:LEU:HD21	1:B:174:ILE:HD11	1.82	0.62
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.83	0.60
1:B:204:GLN:C	4:B:607:HOH:O	2.45	0.59
1:B:441:PRO:O	4:B:602:HOH:O	2.00	0.59
1:A:409:GLU:OE1	4:A:601:HOH:O	2.17	0.59
1:B:179:ARG:CB	4:B:731:HOH:O	2.40	0.58
1:B:375[A]:ARG:NH1	1:B:375[A]:ARG:HG2	2.12	0.57
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.87	0.57
1:A:271:GLY:HA3	1:A:327[A]:THR:HG21	1.86	0.57
1:A:128:GLN:NE2	4:A:607:HOH:O	2.40	0.54
1:B:103:LEU:HD21	1:B:237:MET:HG2	1.91	0.52
1:B:73:GLN:HG3	1:B:77:PHE:CE2	2.46	0.51
1:A:271:GLY:C	1:A:327[A]:THR:HG21	2.35	0.50
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.92	0.50
1:B:171:HIS:H	1:B:174:ILE:HD12	1.75	0.50
1:B:21:ASN:CG	4:B:606:HOH:O	2.56	0.48
1:B:174:ILE:O	1:B:178:VAL:HG23	2.14	0.48
1:B:362:ARG:HA	1:B:371:VAL:HG21	1.96	0.48
1:B:440:LYS:HD2	4:B:844:HOH:O	2.13	0.48
1:A:153:ILE:HG21	1:A:265:GLY:HA3	1.95	0.47
1:B:128:GLN:NE2	4:B:610:HOH:O	2.42	0.46
3:B:502:HEM:HBC2	3:B:502:HEM:HMC2	1.98	0.46
1:B:128:GLN:NE2	4:B:616:HOH:O	2.49	0.46
1:B:268:THR:OG1	4:B:603:HOH:O	2.06	0.46
1:A:271:GLY:CA	1:A:327[A]:THR:HG21	2.47	0.45
1:B:264:ALA:HB2	2:B:501:A1MES:C23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD21	1:B:237:MET:CG	2.46	0.45
1:A:426:HIS:CD2	1:A:447:LYS:HE3	2.52	0.44
1:B:118[B]:MET:HE2	4:B:659:HOH:O	2.17	0.44
1:B:75:LEU:HD22	1:B:88:THR:HG22	1.98	0.44
1:B:387:GLN:HG2	1:B:388:HIS:CD2	2.53	0.44
1:B:362:ARG:HA	1:B:371:VAL:CG2	2.47	0.44
1:B:2:ILE:HG23	1:B:346:PRO:HD3	2.00	0.44
1:B:150:LEU:HD21	1:B:174:ILE:CD1	2.48	0.43
1:A:118:MET:HE3	1:A:156:CYS:HA	2.01	0.43
1:B:186:ASN:O	1:B:189:GLN:HG2	2.19	0.42
1:B:179:ARG:CZ	4:B:731:HOH:O	2.68	0.42
1:B:204:GLN:CG	4:B:607:HOH:O	2.17	0.42
1:A:300:ASP:O	1:A:419:LYS:NZ	2.52	0.42
1:A:118:MET:CE	1:A:156:CYS:HA	2.49	0.42
1:A:296:ARG:NH2	4:A:602:HOH:O	2.24	0.42
1:B:118[B]:MET:HE3	1:B:156:CYS:HA	2.01	0.42
1:A:327[A]:THR:HG22	1:A:439:LEU:O	2.19	0.42
1:B:168:ASP:HA	4:B:622:HOH:O	2.19	0.42
1:A:327[B]:THR:HG22	1:A:438:THR:HB	2.01	0.42
1:B:171:HIS:HB2	1:B:174:ILE:HD12	2.01	0.42
1:A:104:LEU:HB3	1:A:105:PRO:HD3	2.03	0.41
1:B:75:LEU:HA	1:B:75:LEU:HD23	1.73	0.41
1:B:106:SER:HB3	1:B:233:LEU:HD23	2.03	0.41
1:B:264:ALA:O	1:B:265:GLY:C	2.62	0.41
1:B:118[B]:MET:CE	1:B:156:CYS:HA	2.51	0.41

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	461/456 (101%)	448 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	460/456 (101%)	444 (96%)	15 (3%)	1 (0%)	43	27
All	All	921/912 (101%)	892 (97%)	28 (3%)	1 (0%)	48	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	HIS

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	406/400 (102%)	402 (99%)	4 (1%)	68	49
1	B	406/400 (102%)	404 (100%)	2 (0%)	81	71
All	All	812/800 (102%)	806 (99%)	6 (1%)	73	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	48	VAL
1	A	148	LEU
1	A	230	SER
1	B	148	LEU
1	B	171	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	128	GLN
1	A	186	ASN
1	A	359	GLN

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Mol	Chain	Res	Type
1	B	70	ASN
1	B	110	GLN
1	B	128	GLN
1	B	186	ASN
1	B	189	GLN
1	B	359	GLN
1	B	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	A1MES	A	501	-	23,23,23	1.11	1 (4%)	27,27,27	1.33	4 (14%)
2	A1MES	B	501	-	23,23,23	1.51	3 (13%)	27,27,27	0.88	1 (3%)
3	HEM	A	502	1	50,50,50	1.62	12 (24%)	66,82,82	1.27	10 (15%)
3	HEM	B	502	1	50,50,50	1.81	15 (30%)	66,82,82	1.15	5 (7%)

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	A1MES	A	501	-	-	4/20/20/20	0/1/1/1
2	A1MES	B	501	-	-	4/20/20/20	0/1/1/1
3	HEM	A	502	1	-	2/14/54/54	-
3	HEM	B	502	1	-	2/14/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1MES	C07-N11	5.43	1.45	1.33
3	A	502	HEM	FE-ND	5.36	2.11	1.94
3	B	502	HEM	FE-NA	5.08	2.12	1.95
2	A	501	A1MES	C07-N11	4.37	1.43	1.33
3	B	502	HEM	FE-ND	4.12	2.07	1.94
3	A	502	HEM	C3C-C4C	-3.91	1.39	1.46
3	B	502	HEM	C3C-C4C	-3.64	1.39	1.46
3	B	502	HEM	FE-NB	3.11	2.04	1.94
3	A	502	HEM	FE-NA	3.05	2.05	1.95
3	B	502	HEM	C1B-C2B	-2.98	1.38	1.44
3	B	502	HEM	C3B-C4B	-2.91	1.39	1.44
3	A	502	HEM	FE-NB	2.79	2.03	1.94
3	B	502	HEM	C3B-C2B	2.78	1.42	1.37
3	A	502	HEM	C1B-NB	-2.76	1.35	1.40
3	A	502	HEM	C4D-ND	-2.66	1.35	1.40
3	B	502	HEM	C4D-C3D	-2.61	1.40	1.45
2	B	501	A1MES	O12-C07	-2.61	1.18	1.23
3	A	502	HEM	C1A-C2A	-2.57	1.39	1.44
3	B	502	HEM	C1D-C2D	-2.50	1.39	1.44
3	B	502	HEM	C4A-NA	-2.47	1.35	1.39
3	B	502	HEM	FE-NC	2.41	2.03	1.95
3	A	502	HEM	C3B-C4B	-2.21	1.40	1.44
3	B	502	HEM	CBA-CGA	2.14	1.55	1.50
3	A	502	HEM	C1C-C2C	-2.11	1.41	1.45
3	B	502	HEM	C4D-ND	-2.09	1.36	1.40
3	A	502	HEM	FE-NC	2.09	2.02	1.95
3	B	502	HEM	C1B-NB	-2.06	1.36	1.40
3	A	502	HEM	C1D-C2D	-2.05	1.40	1.44
3	B	502	HEM	C1A-C2A	-2.03	1.40	1.44
3	A	502	HEM	C4D-C3D	-2.02	1.41	1.45
2	B	501	A1MES	C03-C08	2.01	1.53	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1MES	O09-C08-C03	3.53	125.46	115.31
3	B	502	HEM	C4C-C3C-C2C	3.23	109.40	106.75
3	B	502	HEM	C4A-NA-C1A	2.94	108.23	105.35
3	A	502	HEM	C1D-C2D-C3D	-2.69	104.13	106.96
3	A	502	HEM	C3C-C2C-C1C	-2.61	104.58	107.08
3	A	502	HEM	C4D-C3D-C2D	2.55	110.61	106.90
3	A	502	HEM	CHD-C1D-ND	-2.54	121.65	124.42
2	A	501	A1MES	O09-C08-O10	-2.49	117.83	123.35
3	A	502	HEM	C3D-C4D-ND	-2.43	107.46	110.17
3	A	502	HEM	C4C-CHD-C1D	2.41	131.26	126.06
3	B	502	HEM	C3C-C2C-C1C	-2.31	104.87	107.08
3	B	502	HEM	CAD-CBD-CGD	2.28	118.50	113.60
2	B	501	A1MES	C14-C13-N11	-2.23	105.82	112.21
2	A	501	A1MES	O10-C08-C03	-2.23	116.52	121.94
3	A	502	HEM	C3B-C2B-C1B	-2.21	104.85	106.49
3	A	502	HEM	CHC-C4B-NB	-2.15	122.08	124.42
3	B	502	HEM	CHD-C1D-ND	-2.15	122.08	124.42
2	A	501	A1MES	C17-C16-C15	-2.08	103.87	114.42
3	A	502	HEM	CHA-C4D-C3D	2.05	129.18	125.33
3	A	502	HEM	CAD-CBD-CGD	2.01	117.93	113.60

There are no chirality outliers.

All (12) torsion outliers are listed below:

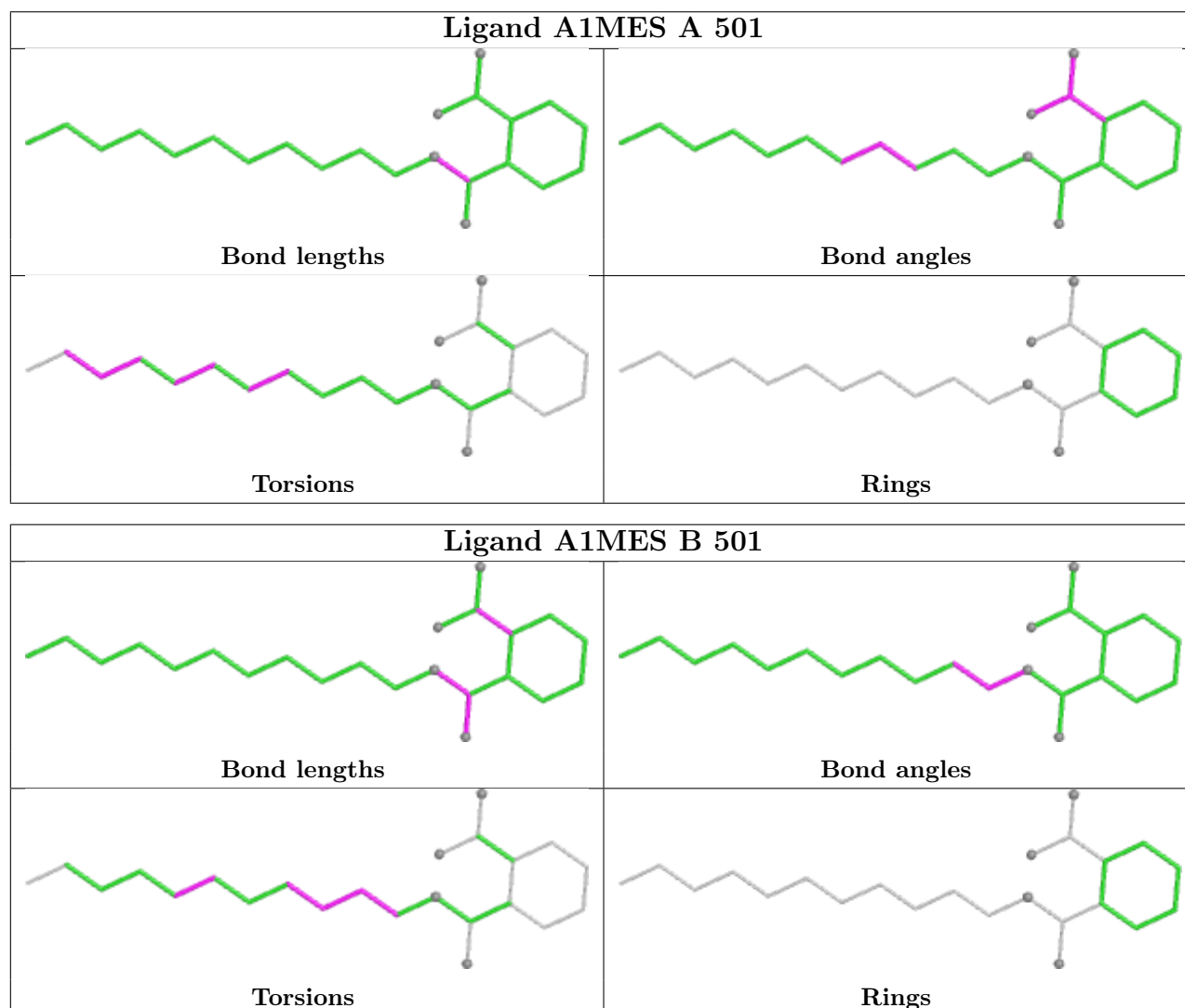
Mol	Chain	Res	Type	Atoms
2	B	501	A1MES	N11-C13-C14-C15
2	A	501	A1MES	C17-C18-C19-C20
2	A	501	A1MES	C19-C20-C21-C22
2	A	501	A1MES	C20-C21-C22-C23
2	B	501	A1MES	C13-C14-C15-C16
2	B	501	A1MES	C17-C18-C19-C20
2	A	501	A1MES	C15-C16-C17-C18
3	A	502	HEM	CAA-CBA-CGA-O1A
3	B	502	HEM	CAA-CBA-CGA-O1A
3	A	502	HEM	CAA-CBA-CGA-O2A
3	B	502	HEM	CAA-CBA-CGA-O2A
2	B	501	A1MES	C14-C15-C16-C17

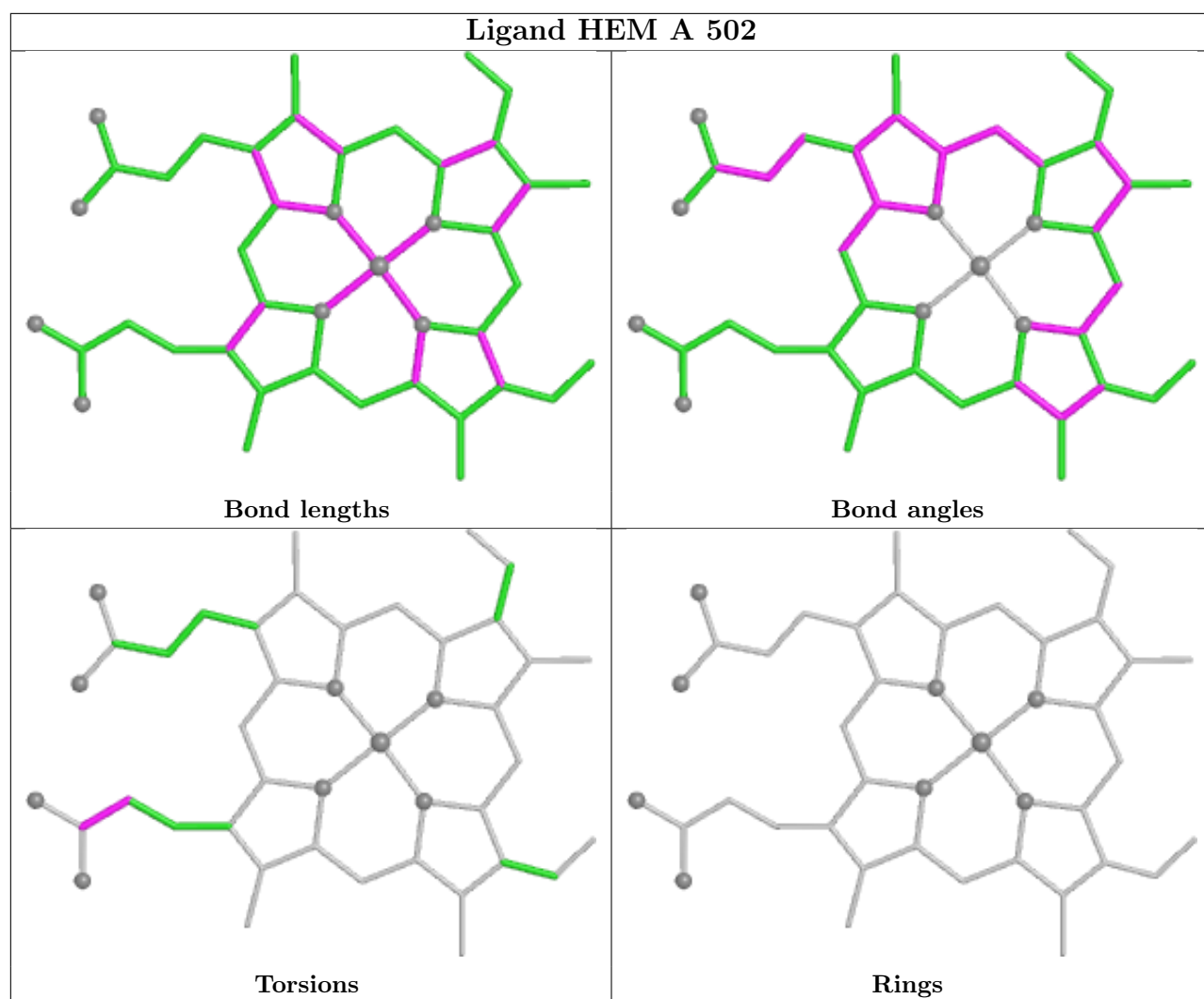
There are no ring outliers.

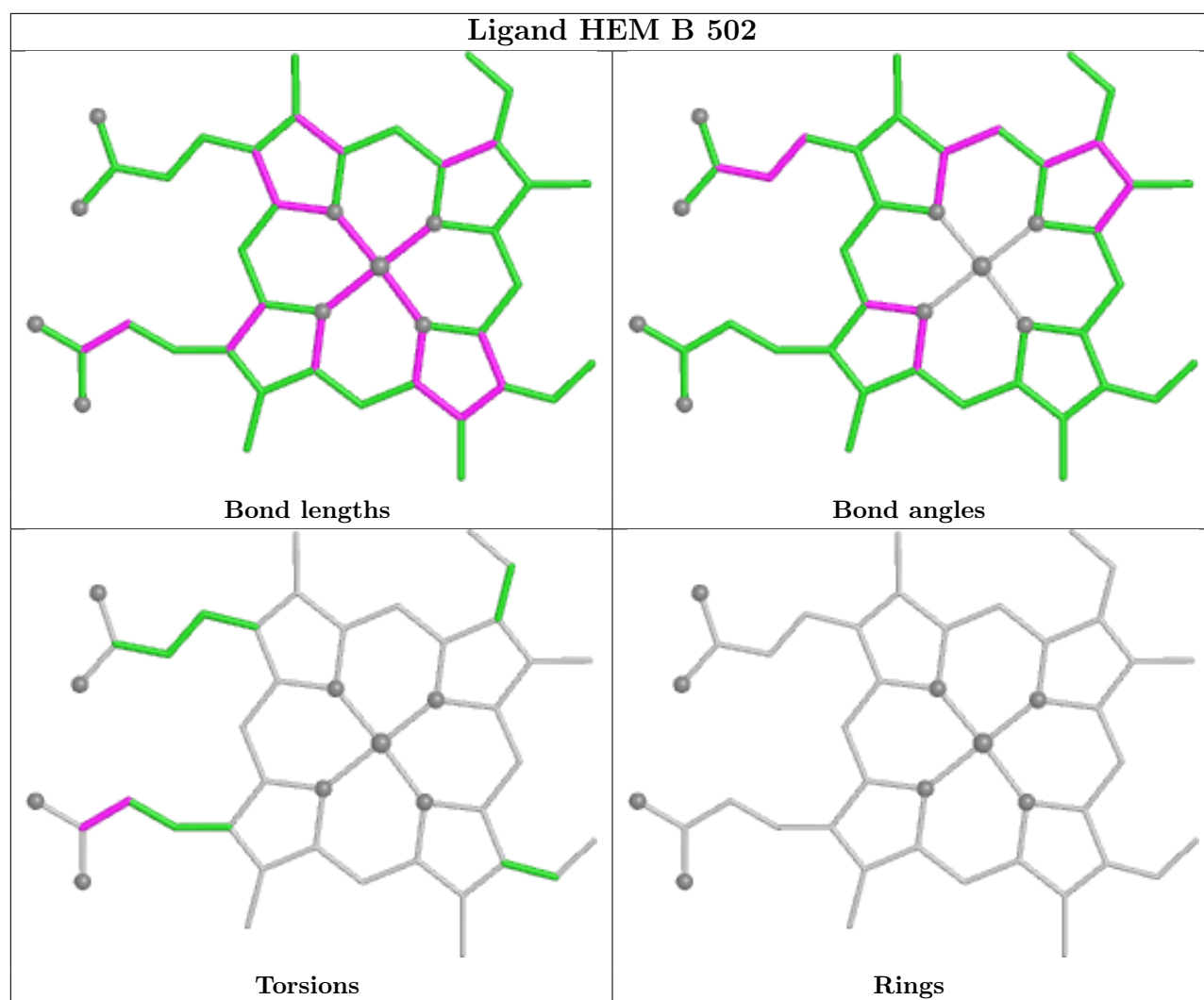
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	A1MES	2	0
3	B	502	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	455/456 (99%)	0.05	21 (4%) 37 42	6, 18, 44, 73	4 (0%)
1	B	455/456 (99%)	0.21	59 (12%) 7 8	5, 17, 51, 86	4 (0%)
All	All	910/912 (99%)	0.13	80 (8%) 15 17	5, 18, 49, 86	8 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	GLY	6.5
1	A	2	ILE	6.1
1	B	2	ILE	6.1
1	B	173	PHE	5.9
1	B	220	ILE	5.6
1	B	1	THR	5.5
1	B	227	GLY	5.5
1	B	215	LEU	5.4
1	B	266	HIS	5.1
1	A	1	THR	4.8
1	B	225	ALA	4.8
1	B	211	VAL	4.8
1	B	221	ALA	4.7
1	B	158[A]	PHE	4.4
1	B	219	ILE	4.4
1	B	170	PRO	4.3
1	B	174	ILE	4.3
1	B	236	HIS	4.2
1	B	224	LYS	4.0
1	B	212	MET	4.0
1	B	226	SER	3.9
1	B	171	HIS	3.9
1	B	188	LEU	3.8
1	A	227	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	216	VAL	3.7
1	A	225	ALA	3.6
1	B	172	PRO	3.6
1	A	158[A]	PHE	3.5
1	B	178	VAL	3.5
1	B	136	ASP	3.4
1	B	192	ASN	3.4
1	B	191	ALA	3.4
1	B	231	ASP	3.4
1	B	264	ALA	3.3
1	B	209	ILE	3.3
1	B	238	LEU	3.2
1	B	175	THR	3.1
1	B	207	GLU	3.1
1	B	169	GLN	3.1
1	B	180	ALA	3.0
1	B	217	ASP	3.0
1	B	185	MET	2.9
1	B	47	ARG	2.9
1	B	228	GLU	2.9
1	B	437	LEU	2.8
1	A	191	ALA	2.7
1	A	193	PRO	2.7
1	B	177	MET	2.7
1	A	369	ASP	2.7
1	B	213	ASN	2.7
1	B	208	ASP	2.7
1	B	229	GLN	2.6
1	B	218	LYS	2.6
1	A	110	GLN	2.6
1	B	189	GLN	2.6
1	B	200	GLU	2.6
1	A	196	PRO	2.5
1	A	246	GLY	2.5
1	A	136	ASP	2.5
1	A	245	THR	2.5
1	B	176	SER	2.4
1	B	222	ASP	2.4
1	B	232	ASP	2.4
1	A	228	GLU	2.4
1	A	236	HIS	2.4
1	B	46	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	205	PHE	2.3
1	B	263	ILE	2.3
1	A	226	SER	2.3
1	A	285	HIS	2.3
1	A	192	ASN	2.3
1	B	182	ASP	2.3
1	B	186	ASN	2.2
1	B	181	LEU	2.1
1	B	233	LEU	2.1
1	B	3	LYS	2.1
1	B	110	GLN	2.0
1	A	3	LYS	2.0
1	A	221	ALA	2.0
1	A	230	SER	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](#)

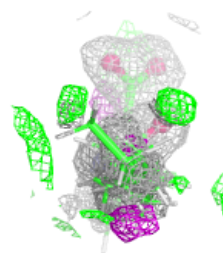
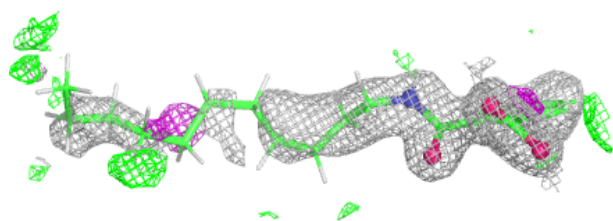
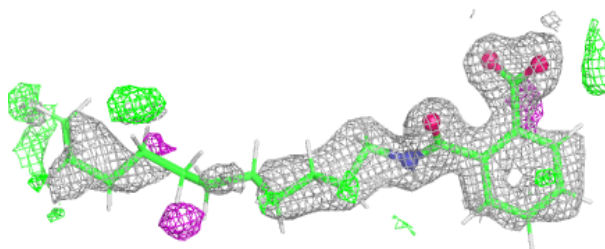
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1MES	B	501	23/23	0.83	0.17	28,39,56,59	0
2	A1MES	A	501	23/23	0.90	0.11	22,29,31,33	0
3	HEM	A	502	43/43	0.98	0.06	8,9,15,17	12
3	HEM	B	502	43/43	0.98	0.06	9,10,17,22	12

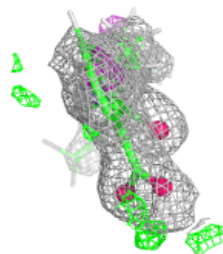
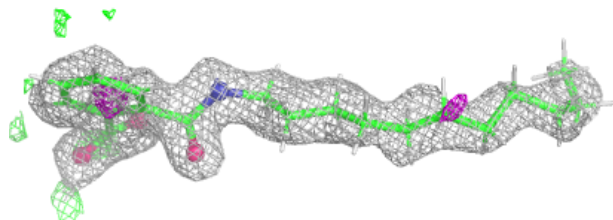
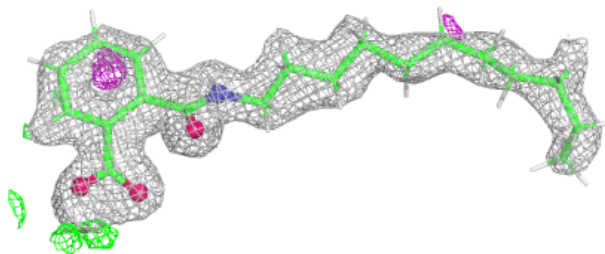
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1MES 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)

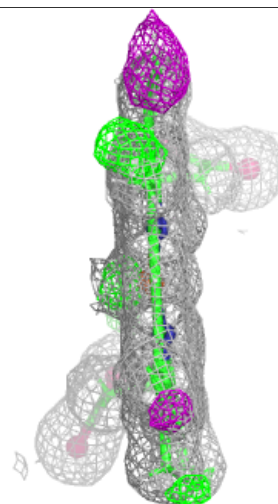
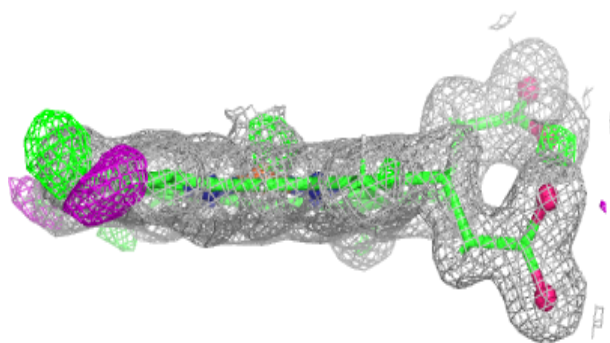
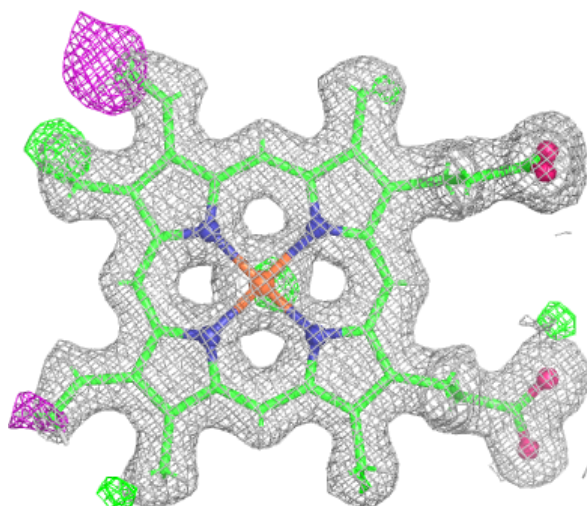
**Electron density around A1MES A 501:**

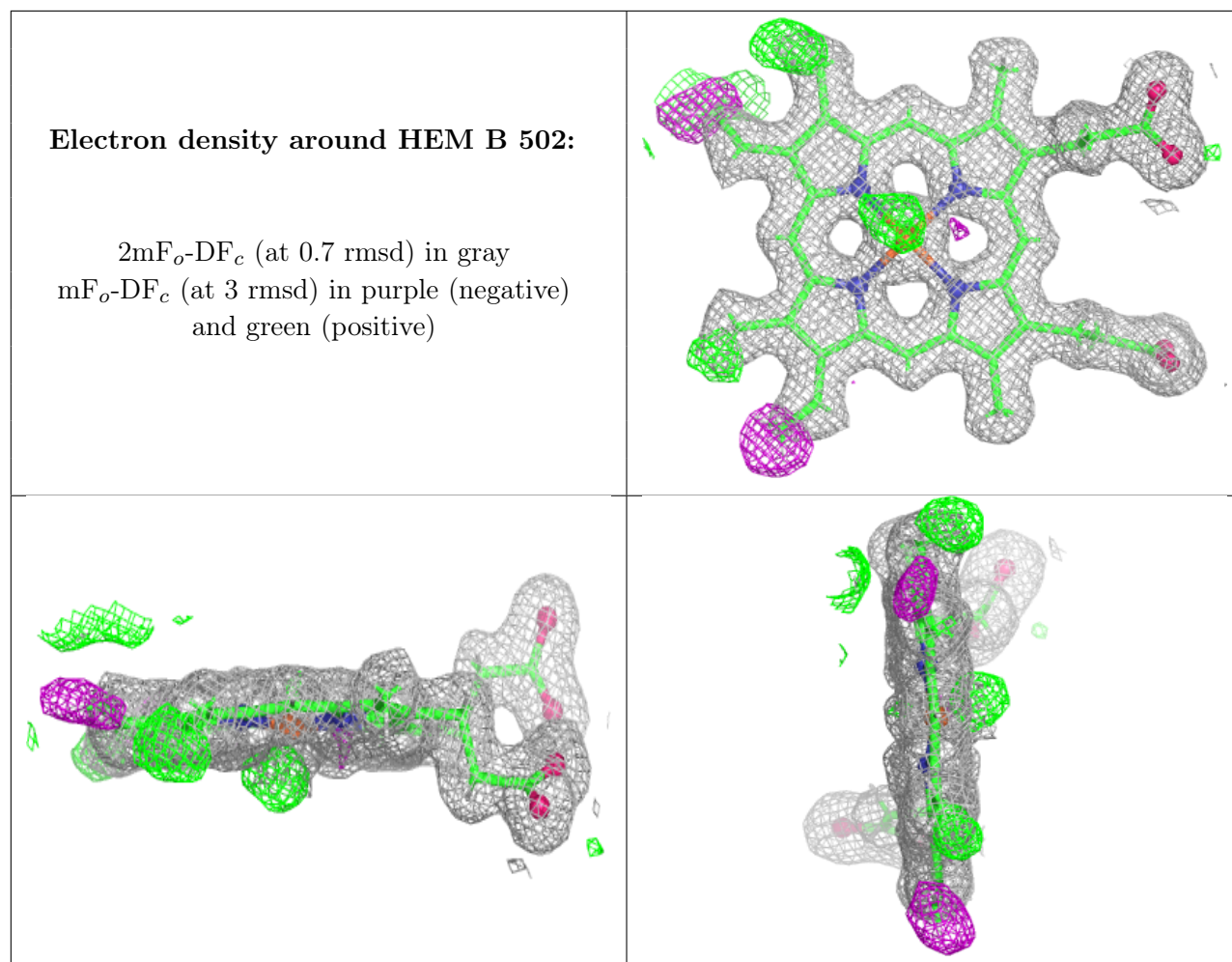
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.