



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2026 – 12:12 PM JST

PDB ID : 23UH / pdb_000023uh
Title : Structure of the CYP102A1 Heme Domain with 2-(undecylcarbamoyl)benzoic acid and benzene
Authors : Ishigami, M.; Sugimoto, H.; Shoji, O.
Deposited on : 2026-02-18
Resolution : 1.48 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

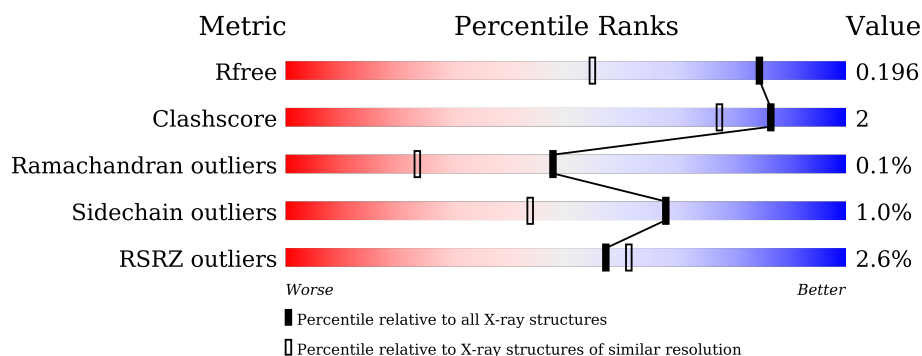
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	B	456	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

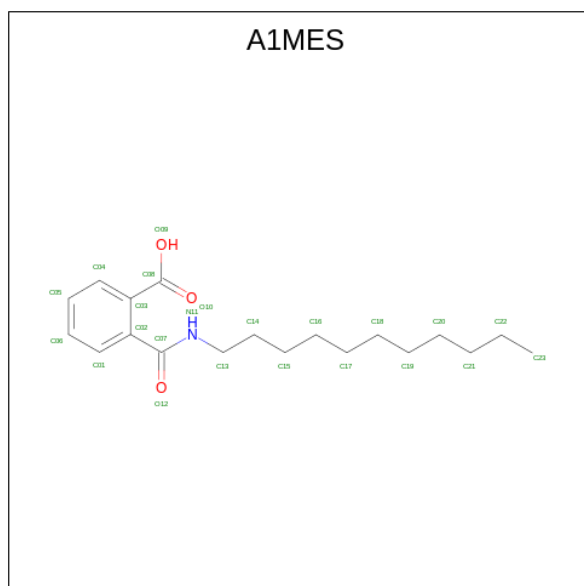
There are 5 unique types of molecules in this entry. The entry contains 15909 atoms, of which 7529 are hydrogens and 0 are deuteriums.

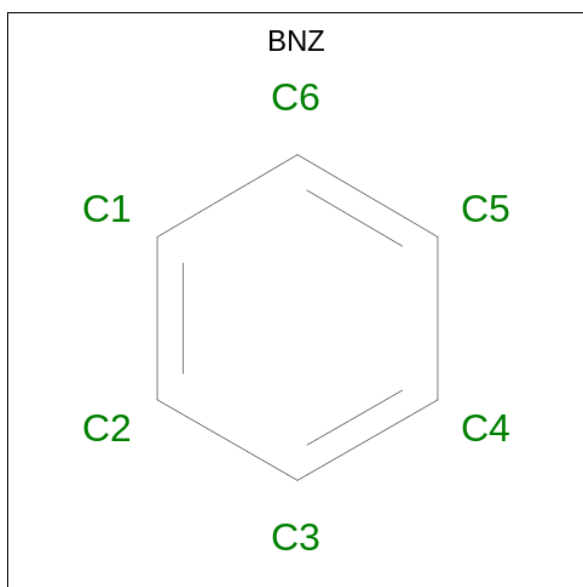
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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	82	14	0
			7445	2378	3719	631	698	19			
1	B	455	Total	C	H	N	O	S	81	6	0
			7376	2359	3682	626	692	17			

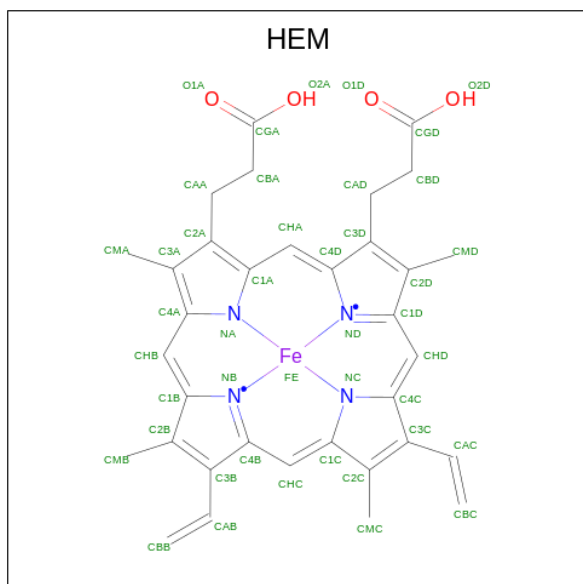
- Molecule 2 is 2-(undecylcarbamoyl)benzoic acid (CCD ID: A1MES) (formula: C₁₉H₂₉NO₃) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 12	C 6	H 6	0	0
3	B	1	Total 12	C 6	H 6	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



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

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

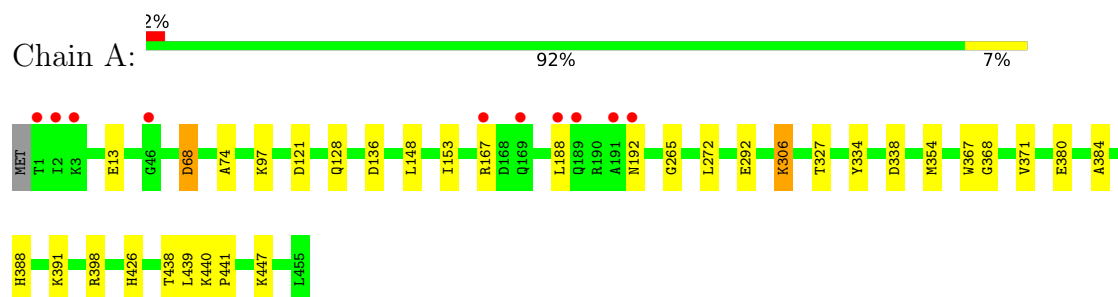
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	426	Total	O	0	0
			426	426		
5	B	390	Total	O	0	0
			390	390		

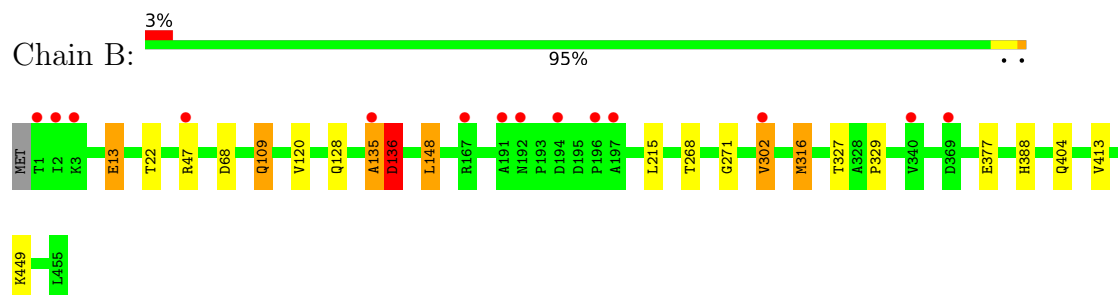
3 Residue-property plots [i](#)

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	58.71Å 128.61Å 148.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 1.48 46.10 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.10-1.48) 99.9 (46.10-1.48)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.176 , 0.199 0.174 , 0.196	Depositor DCC
R_{free} test set	9377 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15909	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 45.92 % 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 1.2323e-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: A1MES, HEM, BNZ

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	0.74	1/3876 (0.0%)	1.13	12/5239 (0.2%)
1	B	0.74	1/3802 (0.0%)	1.15	8/5141 (0.2%)
All	All	0.74	2/7678 (0.0%)	1.14	20/10380 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	HIS	CG-CD2	-6.21	1.29	1.35
1	A	292	GLU	CD-OE1	5.03	1.34	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ASP	CA-CB-CG	9.28	121.88	112.60
1	B	302	VAL	N-CA-CB	-7.97	103.92	112.37
1	A	292	GLU	CG-CD-OE1	7.42	135.46	118.40
1	B	13	GLU	CB-CG-CD	6.58	123.79	112.60
1	A	398	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	B	109	GLN	CB-CA-C	6.25	121.16	110.79
1	A	292	GLU	CG-CD-OE2	-6.03	104.53	118.40
1	B	68	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	136	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	68	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	316	MET	CG-SD-CE	5.66	113.35	100.90
1	B	109	GLN	N-CA-CB	-5.65	101.81	110.12
1	A	338	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	13	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	441	PRO	CB-CA-C	-5.29	102.83	111.56
1	A	121	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	135	ALA	N-CA-C	-5.16	102.64	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ALA	CA-C-N	-5.13	118.90	122.59
1	A	384	ALA	C-N-CA	-5.13	118.90	122.59
1	A	167	ARG	CD-NE-CZ	5.03	131.44	124.40

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	3726	3719	3639	17	0
1	B	3694	3682	3641	15	0
2	A	23	28	0	0	0
2	B	23	28	0	0	0
3	A	6	6	6	0	0
3	B	6	6	6	0	0
4	A	43	30	30	0	0
4	B	43	30	30	1	0
5	A	426	0	0	5	0
5	B	390	0	0	3	0
All	All	8380	7529	7352	32	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 (32) 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:380:GLU:HB3	5:A:814:HOH:O	1.67	0.93
1:A:440:LYS:HG3	5:A:649:HOH:O	1.90	0.70
1:B:109:GLN:HE21	1:B:404:GLN:HG2	1.62	0.63
1:A:354[A]:MET:HA	1:A:354[A]:MET:HE3	1.81	0.60
1:B:47:ARG:NH2	5:B:602:HOH:O	2.34	0.60
1:B:128:GLN:NE2	5:B:601:HOH:O	2.34	0.59
1:A:426:HIS:CD2	1:A:447:LYS:HE3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLU:H	1:B:13:GLU:CD	2.10	0.58
1:B:135:ALA:O	1:B:136:ASP:CB	2.52	0.58
1:A:128[A]:GLN:NE2	5:A:602:HOH:O	2.27	0.57
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.88	0.56
1:A:272:LEU:N	1:A:327[A]:THR:HG21	2.24	0.53
1:B:135:ALA:O	1:B:136:ASP:HB3	2.08	0.52
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.90	0.52
1:B:316:MET:CE	1:B:377:GLU:HA	2.43	0.48
1:A:153:ILE:HG21	1:A:265:GLY:HA3	1.94	0.48
1:B:316:MET:HE3	1:B:377:GLU:HA	1.96	0.48
1:A:327[A]:THR:O	1:A:438:THR:HB	2.13	0.47
1:A:354[A]:MET:HE3	1:A:354[A]:MET:CA	2.41	0.47
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.98	0.46
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.97	0.46
1:A:74:ALA:HB2	1:A:188:LEU:HD11	1.98	0.46
1:B:271:GLY:C	1:B:327[A]:THR:HG21	2.42	0.45
1:A:97:LYS:HE3	5:A:675:HOH:O	2.17	0.45
1:A:368:GLY:O	1:A:371:VAL:HG13	2.16	0.45
1:A:306:LYS:HG2	5:A:989:HOH:O	2.17	0.44
1:B:271:GLY:HA3	1:B:327[A]:THR:HG21	2.00	0.43
1:B:327[A]:THR:HG23	5:B:650:HOH:O	2.18	0.42
1:B:268:THR:HB	4:B:503:HEM:C2C	2.55	0.42
1:B:327[A]:THR:O	1:B:329:PRO:HD3	2.20	0.42
1:A:327[B]:THR:HG23	1:A:439:LEU:O	2.19	0.41
1:A:68:ASP:HB3	1:A:334:TYR:CZ	2.56	0.41

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	467/456 (102%)	453 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	459/456 (101%)	445 (97%)	13 (3%)	1 (0%)	43	22
All	All	926/912 (102%)	898 (97%)	27 (3%)	1 (0%)	48	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	ASP

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	412/400 (103%)	409 (99%)	3 (1%)	76	56
1	B	404/400 (101%)	399 (99%)	5 (1%)	63	36
All	All	816/800 (102%)	808 (99%)	8 (1%)	68	43

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	192	ASN
1	A	306	LYS
1	B	22	THR
1	B	136	ASP
1	B	148	LEU
1	B	215	LEU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	186	ASN

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Mol	Chain	Res	Type
1	A	204	GLN
1	A	359	GLN
1	B	70	ASN
1	B	110	GLN
1	B	186	ASN
1	B	204	GLN
1	B	359	GLN
1	B	403	GLN

5.3.3 RNA [i](#)

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](#)

6 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	BNZ	A	502	-	6,6,6	0.54	0	6,6,6	0.15	0
4	HEM	B	503	1	50,50,50	1.50	5 (10%)	66,82,82	1.51	10 (15%)
2	A1MES	A	501	-	23,23,23	1.38	2 (8%)	27,27,27	1.19	3 (11%)
2	A1MES	B	501	-	23,23,23	1.18	2 (8%)	27,27,27	1.20	2 (7%)
4	HEM	A	503	1	50,50,50	1.52	9 (18%)	66,82,82	1.43	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BNZ	B	502	-	6,6,6	0.72	0	6,6,6	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	503	1	-	2/14/54/54	-
3	BNZ	A	502	-	-	-	0/1/1/1
2	A1MES	A	501	-	-	5/20/20/20	0/1/1/1
2	A1MES	B	501	-	-	5/20/20/20	0/1/1/1
4	HEM	A	503	1	-	2/14/54/54	-
3	BNZ	B	502	-	-	-	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	HEM	FE-ND	4.80	2.09	1.94
2	A	501	A1MES	C07-N11	4.80	1.44	1.33
4	A	503	HEM	FE-ND	4.61	2.09	1.94
4	B	503	HEM	FE-NA	4.56	2.10	1.95
4	B	503	HEM	FE-NB	4.00	2.07	1.94
2	B	501	A1MES	C07-N11	3.75	1.42	1.33
4	A	503	HEM	C3C-C4C	-3.60	1.39	1.46
4	A	503	HEM	FE-NA	3.60	2.07	1.95
4	B	503	HEM	C3C-C4C	-3.15	1.40	1.46
4	A	503	HEM	FE-NB	3.02	2.04	1.94
4	A	503	HEM	FE-NC	2.88	2.04	1.95
4	A	503	HEM	C3B-C4B	-2.80	1.39	1.44
2	A	501	A1MES	C03-C08	2.68	1.55	1.49
4	B	503	HEM	C3B-C4B	-2.61	1.39	1.44
4	A	503	HEM	C1A-C2A	-2.54	1.39	1.44
2	B	501	A1MES	O09-C08	-2.29	1.23	1.30
4	A	503	HEM	C1D-C2D	-2.13	1.40	1.44
4	A	503	HEM	O2A-CGA	-2.09	1.23	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	HEM	C4C-NC-C1C	-4.59	100.85	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	HEM	C4B-C3B-C2B	4.52	110.70	107.11
4	A	503	HEM	CHC-C1C-NC	-4.02	120.09	124.44
4	B	503	HEM	C4A-NA-C1A	4.01	109.27	105.35
4	A	503	HEM	CHC-C4B-NB	-3.47	120.65	124.42
4	B	503	HEM	C2A-C1A-NA	-3.26	106.51	110.15
4	A	503	HEM	CHD-C1D-ND	-3.05	121.10	124.42
4	A	503	HEM	C1C-CHC-C4B	2.95	132.42	126.06
4	B	503	HEM	CHB-C1B-NB	-2.82	120.89	124.37
4	B	503	HEM	C3B-C2B-C1B	-2.79	104.42	106.49
4	A	503	HEM	C2A-C1A-NA	-2.70	107.13	110.15
2	B	501	A1MES	C01-C02-C03	2.49	122.03	119.26
4	B	503	HEM	CHA-C1A-C2A	2.37	130.53	125.36
2	A	501	A1MES	O09-C08-C03	2.34	122.04	115.31
4	B	503	HEM	CHC-C1C-NC	-2.32	121.93	124.44
4	A	503	HEM	C4C-CHD-C1D	2.26	130.92	126.06
2	A	501	A1MES	C01-C02-C03	2.19	121.69	119.26
4	A	503	HEM	C4A-NA-C1A	2.18	107.48	105.35
4	A	503	HEM	C1A-C2A-C3A	2.18	110.32	106.89
4	A	503	HEM	C3B-C2B-C1B	-2.17	104.88	106.49
2	B	501	A1MES	O09-C08-O10	-2.15	118.57	123.35
4	B	503	HEM	C2C-C1C-NC	2.15	113.65	109.69
4	B	503	HEM	C3C-C2C-C1C	-2.10	105.07	107.08
4	A	503	HEM	C4B-C3B-C2B	2.03	108.73	107.11
2	A	501	A1MES	O09-C08-O10	-2.02	118.87	123.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	A1MES	C20-C21-C22-C23
2	A	501	A1MES	C20-C21-C22-C23
2	A	501	A1MES	C15-C16-C17-C18
4	A	503	HEM	CAA-CBA-CGA-O1A
4	B	503	HEM	CAA-CBA-CGA-O1A
2	A	501	A1MES	C14-C15-C16-C17
4	B	503	HEM	CAA-CBA-CGA-O2A
2	A	501	A1MES	C16-C17-C18-C19
4	A	503	HEM	CAA-CBA-CGA-O2A
2	B	501	A1MES	C04-C03-C08-O09
2	B	501	A1MES	C04-C03-C08-O10
2	B	501	A1MES	C15-C16-C17-C18
2	A	501	A1MES	C04-C03-C08-O10

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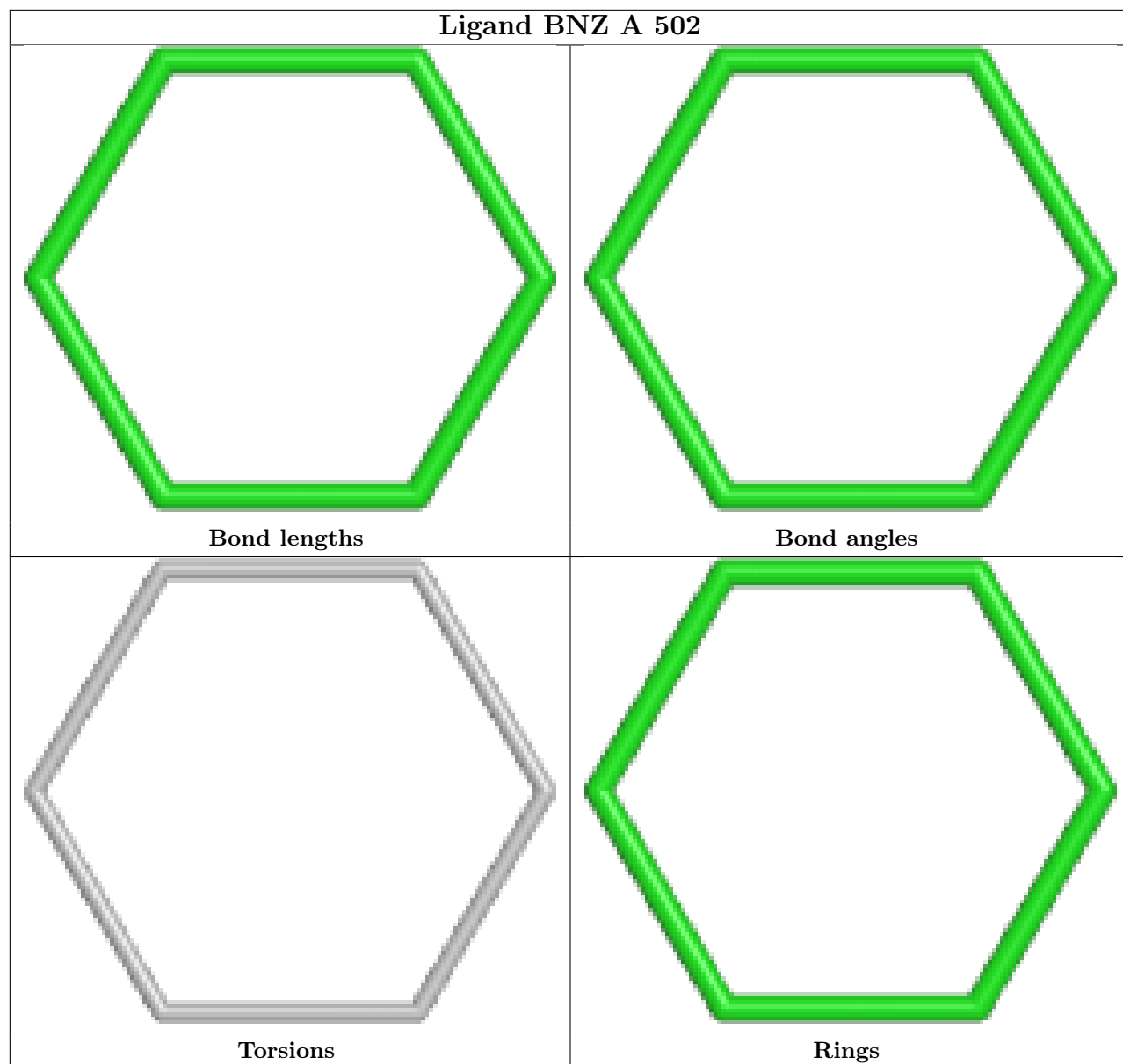
Mol	Chain	Res	Type	Atoms
2	B	501	A1MES	C14-C15-C16-C17

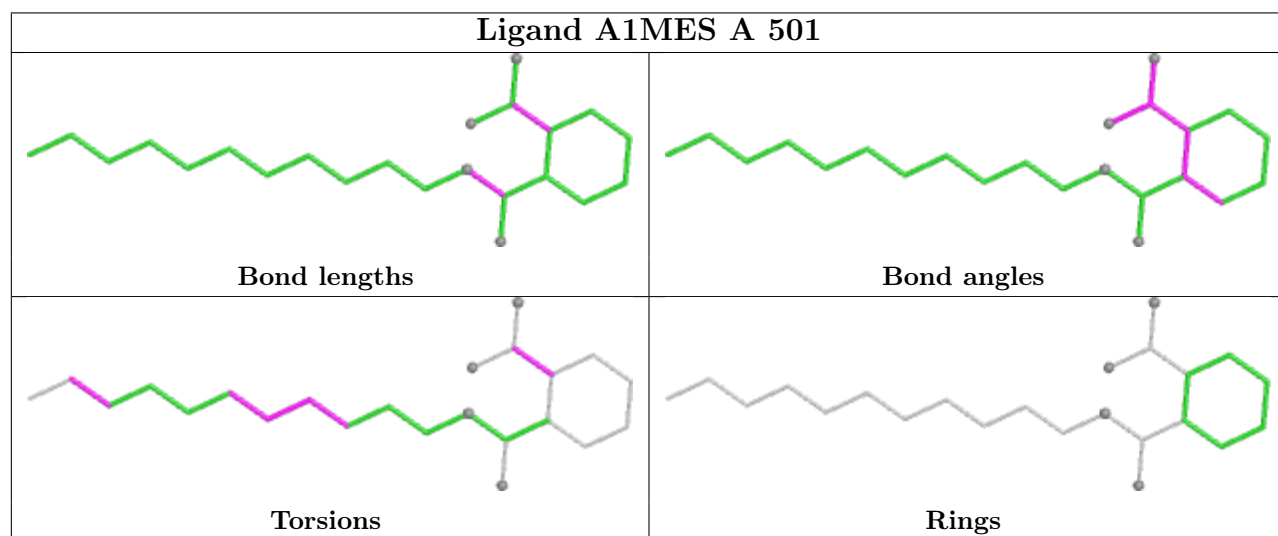
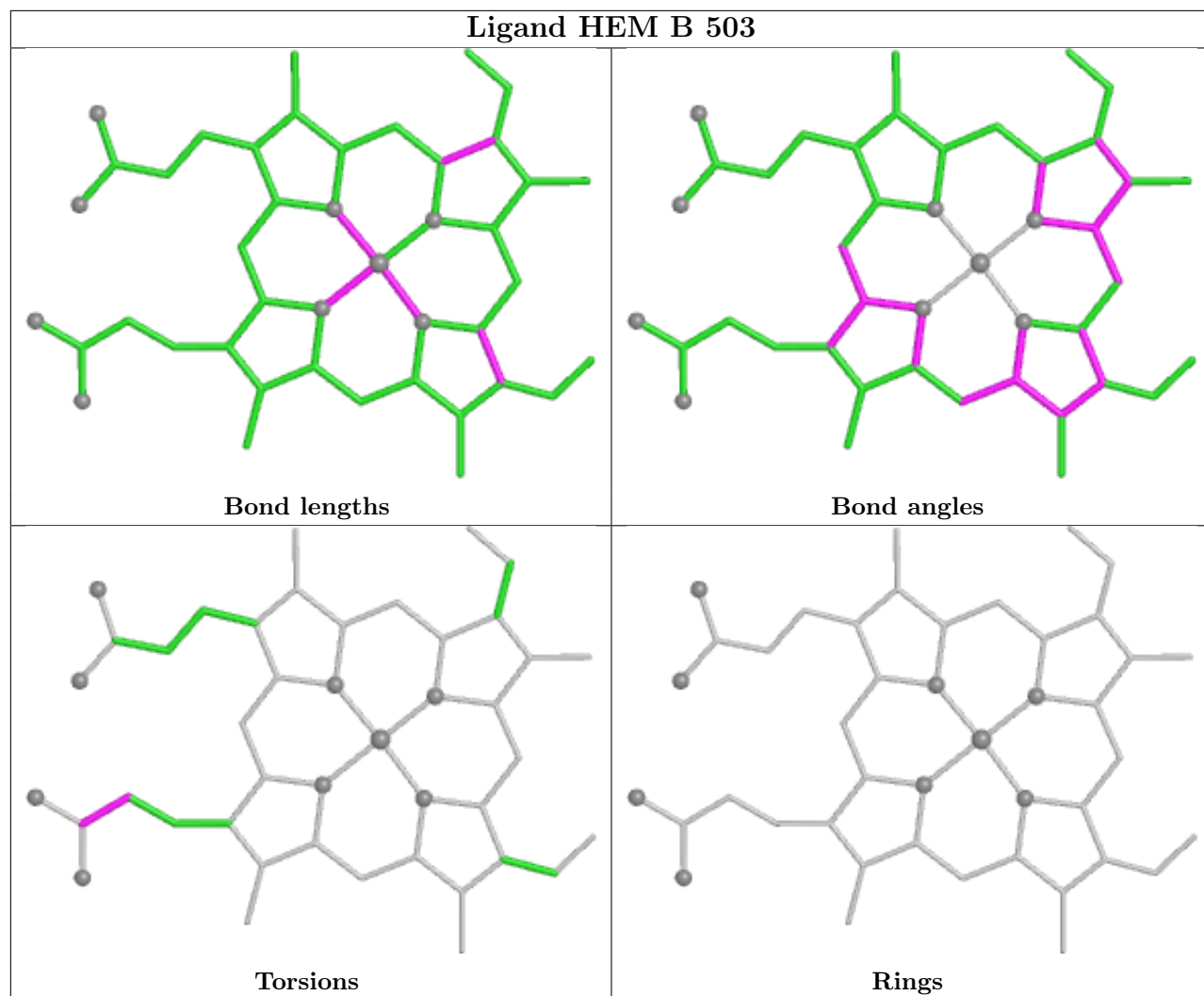
There are no ring outliers.

1 monomer is involved in 1 short contact:

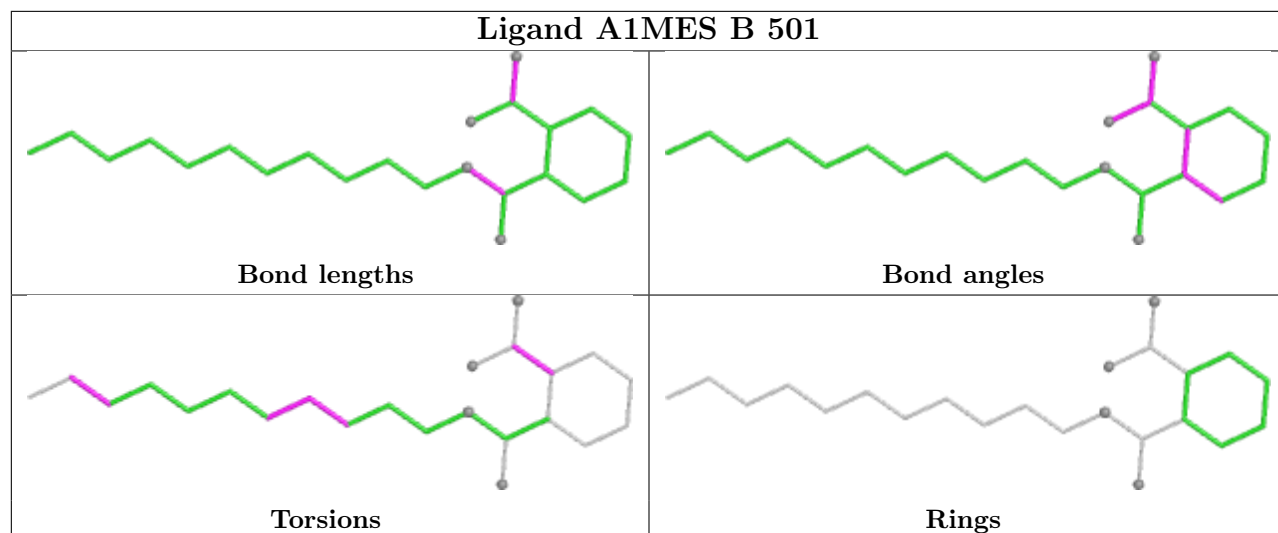
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	HEM	1	0

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.

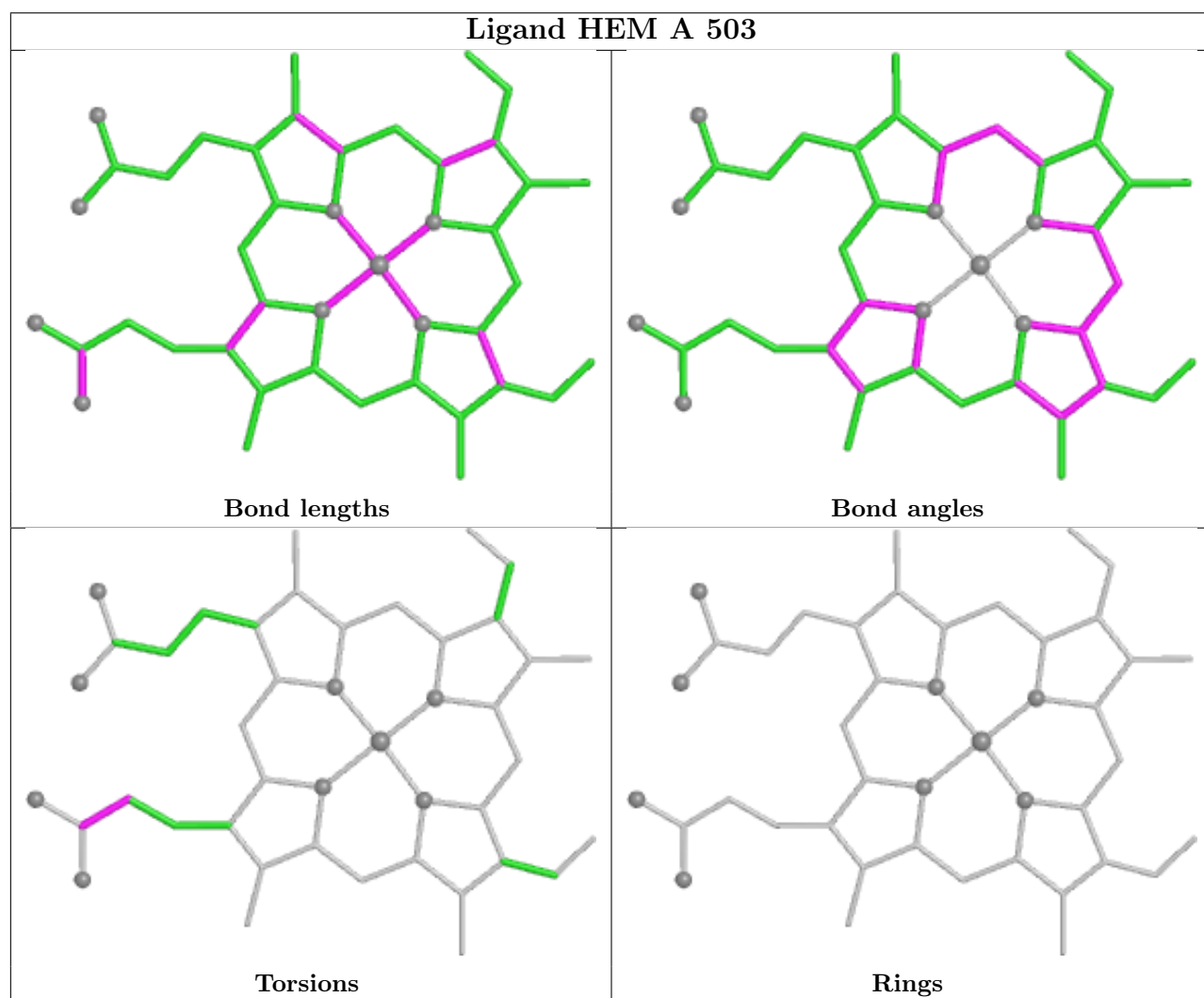


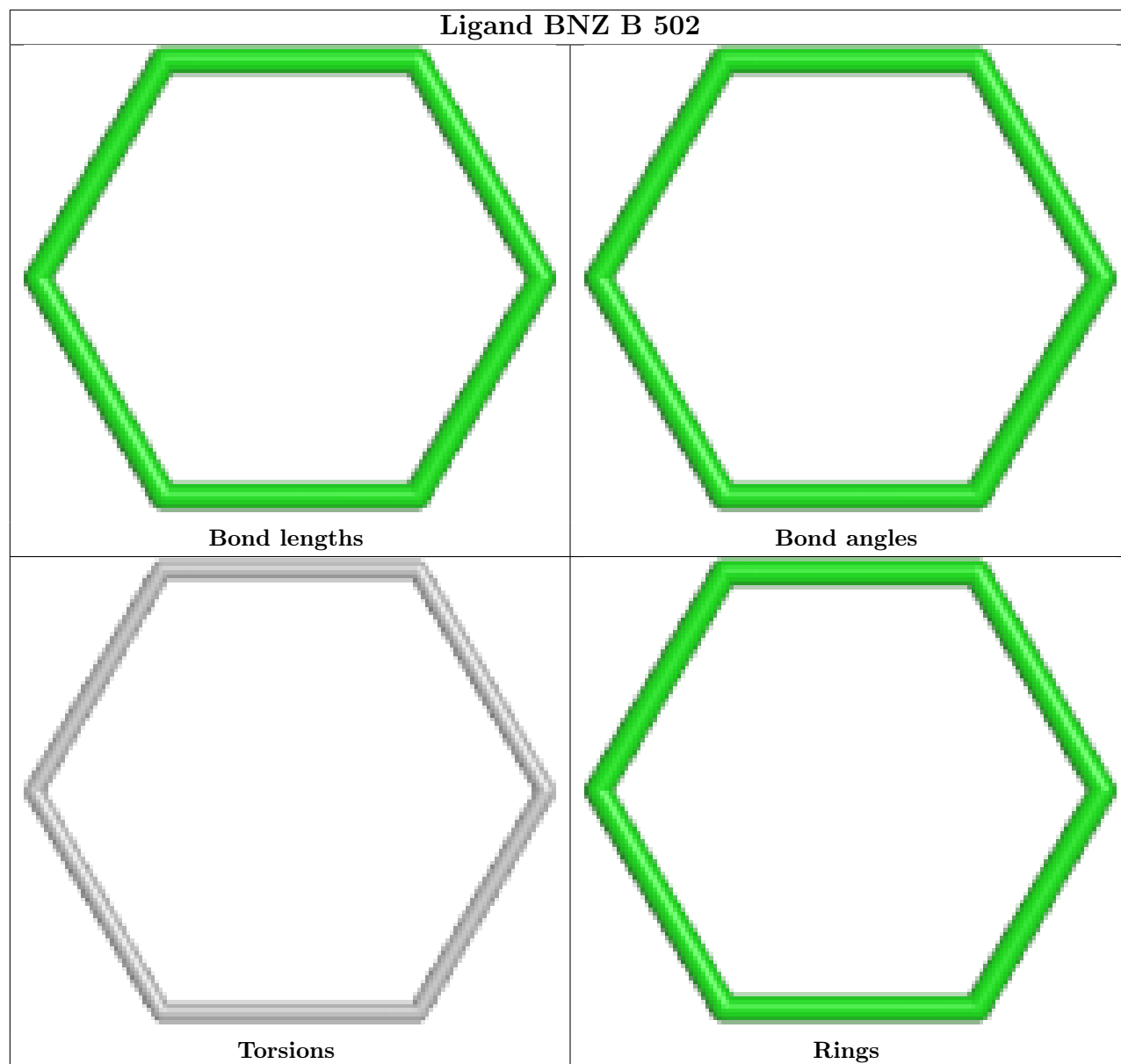


Ligand A1MES B 501



Ligand HEM A 503





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%)	-0.39	10 (2%) 62 66	4, 11, 27, 58	7 (1%)
1	B	455/456 (99%)	-0.25	14 (3%) 51 56	5, 12, 30, 63	3 (0%)
All	All	910/912 (99%)	-0.32	24 (2%) 57 61	4, 12, 28, 63	10 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	6.1
1	A	1	THR	4.8
1	B	1	THR	4.8
1	A	2	ILE	4.7
1	B	135	ALA	3.5
1	A	188	LEU	3.4
1	A	192	ASN	3.3
1	A	167	ARG	3.1
1	B	167	ARG	3.0
1	B	302	VAL	2.9
1	B	191	ALA	2.9
1	A	191	ALA	2.6
1	B	3	LYS	2.6
1	B	197	ALA	2.6
1	B	47	ARG	2.6
1	A	46	GLY	2.6
1	B	340	VAL	2.3
1	B	192	ASN	2.3
1	A	189	GLN	2.3
1	A	169	GLN	2.1
1	A	3	LYS	2.0
1	B	196	PRO	2.0
1	B	194	ASP	2.0
1	B	369	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

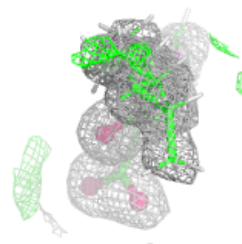
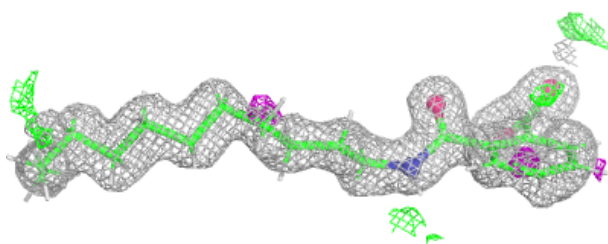
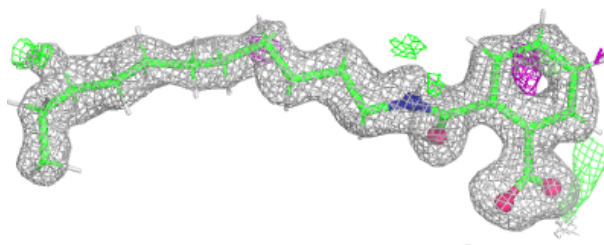
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1MES	A	501	23/23	0.94	0.08	18,20,23,25	0
2	A1MES	B	501	23/23	0.94	0.08	15,19,22,23	0
3	BNZ	B	502	6/6	0.96	0.08	13,15,16,17	0
3	BNZ	A	502	6/6	0.97	0.08	15,16,17,18	0
4	HEM	A	503	43/43	0.99	0.04	5,6,11,15	12
4	HEM	B	503	43/43	0.99	0.04	5,7,12,17	12

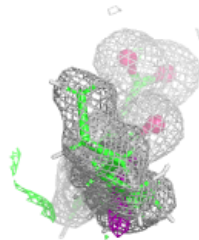
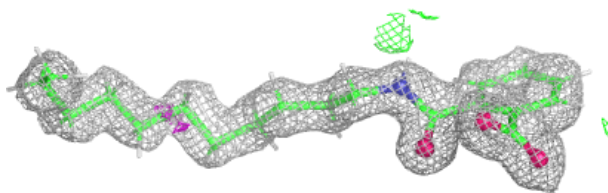
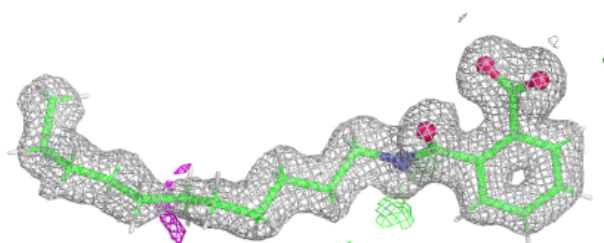
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1MES 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)

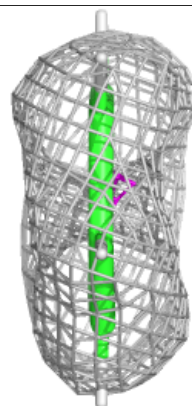
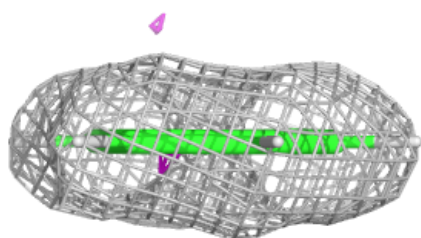
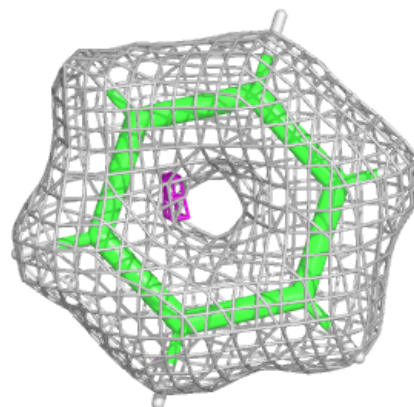
**Electron density around A1MES B 501:**

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

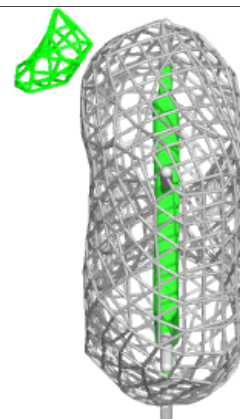
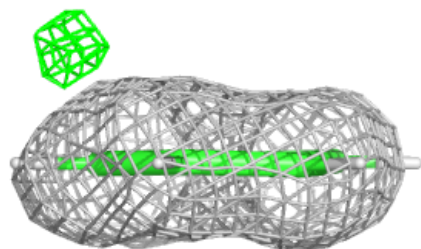
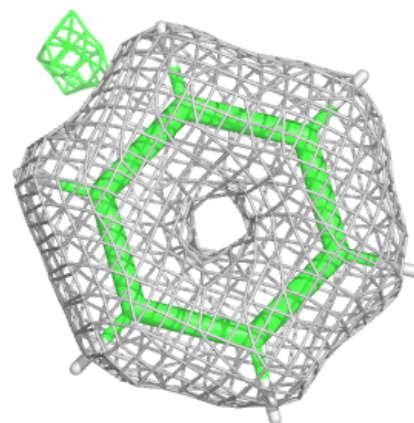


Electron density around BNZ B 502:

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

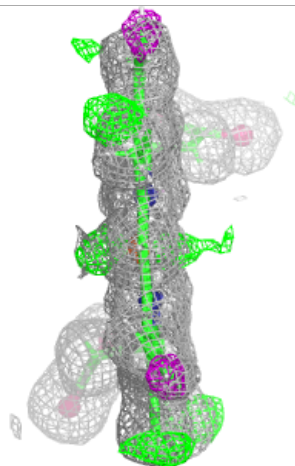
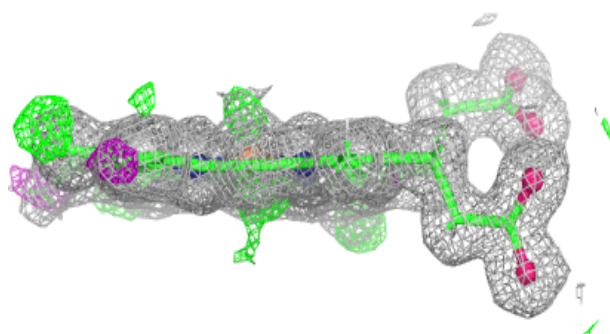
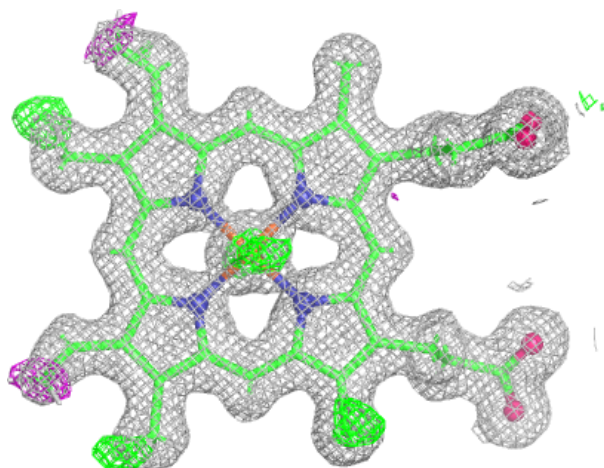
**Electron density around BNZ A 502:**

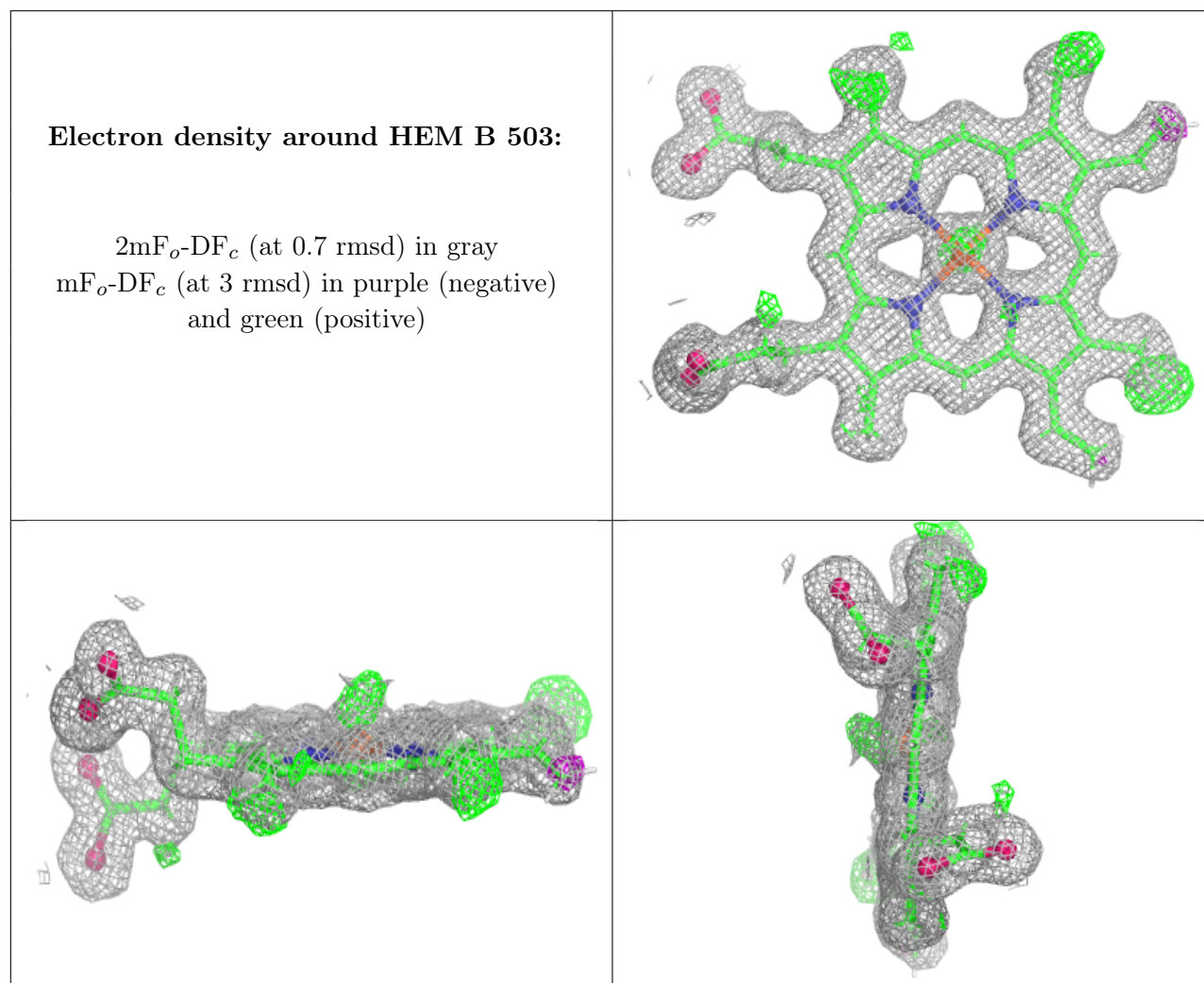
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 503:

$2mF_o-DF_c$ (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.