



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 08:57 PM EST

PDB ID : 4KEW
Title : structure of the A82F BM3 heme domain in complex with omeprazole
Authors : Leys, D.
Deposited on : 2013-04-26
Resolution : 1.89 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

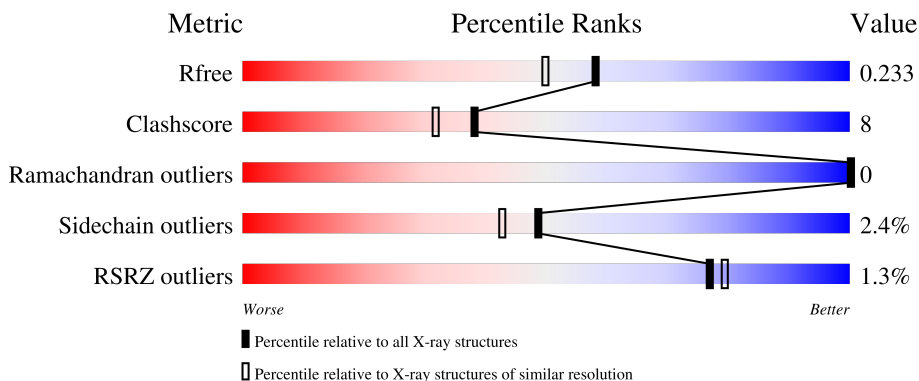
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


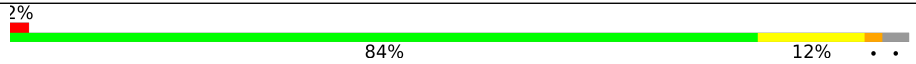
The reported resolution of this entry is 1.89 Å.

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	455	 87% 11% ..
1	B	455	 2% 84% 12% ..

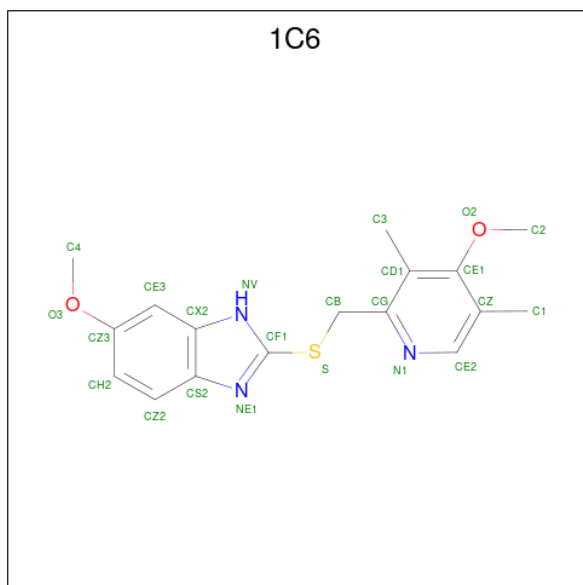
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1C6	A	502	-	-	X	-

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

- Molecule 3 is 6-methoxy-2-[[[(4-methoxy-3,5-dimethylpyridin-2-yl)methyl]sulfonyl]-1H-benzimidazole (three-letter code: 1C6) (formula: C₁₇H₁₉N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	23	17	3	2	1	0	0
3	B	1	23	17	3	2	1	0	0


- Molecule 4 is water.

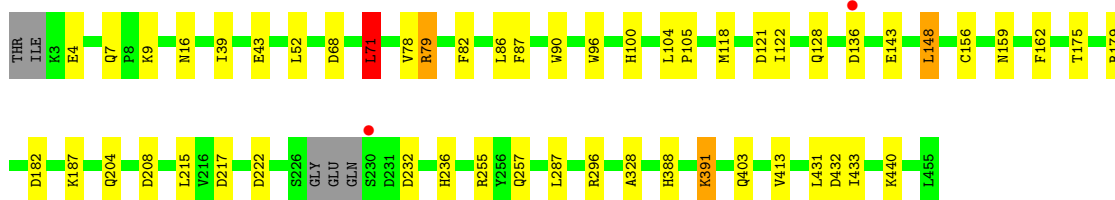
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	418	418	418	0	0
4	B	329	329	329	0	0

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.

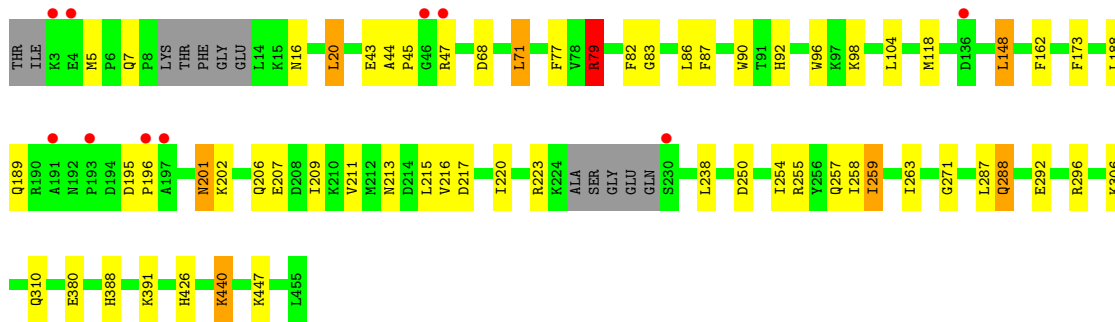
- Molecule 1: Bifunctional P-450/NADPH-P450 reductase

Chain A:  87% 11% ..



- Molecule 1: Bifunctional P-450/NADPH-P450 reductase

Chain B:  84% 12% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.43Å 129.51Å 145.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.75 – 1.89 64.75 – 1.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.75-1.89) 99.4 (64.75-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.188 , 0.237 0.191 , 0.233	Depositor DCC
R_{free} test set	4503 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8159	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1C6, 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	1.06	2/3755 (0.1%)	0.97	14/5077 (0.3%)
1	B	0.97	1/3695 (0.0%)	0.90	8/4995 (0.2%)
All	All	1.02	3/7450 (0.0%)	0.94	22/10072 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	GLN	CG-CD	6.53	1.66	1.51
1	A	143	GLU	CG-CD	5.92	1.60	1.51
1	A	9	LYS	CE-NZ	5.31	1.62	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASP	CB-CG-OD1	8.16	125.64	118.30
1	A	79	ARG	CG-CD-NE	7.90	128.39	111.80
1	A	79	ARG	N-CA-CB	7.73	124.51	110.60
1	B	79	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	79	ARG	CB-CA-C	-6.96	96.49	110.40
1	A	68	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	79	ARG	CA-CB-CG	6.71	128.16	113.40
1	A	68	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	71	LEU	CB-CG-CD1	6.62	122.25	111.00
1	B	20	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	296	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	79	ARG	CA-CB-CG	6.14	126.90	113.40
1	B	287	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	68	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	432	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	296	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	79	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	B	96	TRP	CA-CB-CG	-5.11	104.00	113.70
1	A	96	TRP	CA-CB-CG	-5.08	104.05	113.70
1	B	250	ASP	CB-CG-OD1	5.02	122.81	118.30
1	A	391	LYS	CD-CE-NZ	-5.01	100.18	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3669	0	3614	46	0
1	B	3611	0	3565	59	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	23	0	19	12	0
3	B	23	0	19	6	0
4	A	418	0	0	11	0
4	B	329	0	0	14	0
All	All	8159	0	7277	112	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 8.

All (112) 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:292:GLU:OE1	1:B:296:ARG:NH1	1.73	1.18
1:A:78:VAL:CG1	1:A:82:PHE:CD2	2.40	1.05
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.22	1.02
3:A:502:1C6:H10	4:A:756:HOH:O	1.59	1.01
1:A:217:ASP:OD1	1:A:255:ARG:NH1	1.98	0.96
1:B:20:LEU:HD23	4:B:651:HOH:O	1.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:502:1C6:H10	4:B:861:HOH:O	1.65	0.95
1:B:211:VAL:HG23	4:B:824:HOH:O	1.68	0.94
3:A:502:1C6:H3	3:A:502:1C6:H8	1.50	0.93
1:B:7:GLN:HE21	1:B:16:ASN:HD21	1.21	0.89
1:B:292:GLU:CD	1:B:296:ARG:NH1	2.27	0.87
1:A:78:VAL:CG1	1:A:82:PHE:HD2	1.86	0.87
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.08	0.86
1:A:7:GLN:HE21	1:A:16:ASN:HD21	1.25	0.84
1:B:217:ASP:OD1	1:B:255:ARG:NH1	2.11	0.83
1:B:310[A]:GLN:OE1	4:B:912:HOH:O	1.97	0.82
1:B:16:ASN:HD22	1:B:43:GLU:H	1.23	0.81
1:B:306:LYS:O	1:B:310[B]:GLN:HG2	1.80	0.81
1:B:86:LEU:H	1:B:257:GLN:HE22	1.29	0.81
1:A:118:MET:HE1	4:A:620:HOH:O	1.81	0.80
1:A:78:VAL:HG12	1:A:82:PHE:HD2	1.45	0.79
1:A:118:MET:HE2	4:A:645:HOH:O	1.82	0.79
1:B:207:GLU:O	4:B:824:HOH:O	2.01	0.78
1:A:16:ASN:HD22	1:A:43:GLU:H	1.32	0.76
1:B:92:HIS:HD2	4:B:665:HOH:O	1.68	0.75
1:A:78:VAL:HG12	1:A:82:PHE:CD2	2.20	0.75
3:A:502:1C6:C1	4:A:756:HOH:O	2.23	0.73
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.24	0.73
1:A:78:VAL:HG11	1:A:82:PHE:CD2	2.24	0.73
1:A:86:LEU:H	1:A:257:GLN:HE22	1.37	0.72
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.69	0.72
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.56	0.70
1:B:71:LEU:HD22	1:B:90:TRP:CE2	2.26	0.70
1:A:7:GLN:HE21	1:A:16:ASN:ND2	1.89	0.69
1:B:5:MET:HE3	4:B:688:HOH:O	1.92	0.69
1:A:136:ASP:OD1	4:A:989:HOH:O	2.13	0.66
1:A:179:ARG:NH1	1:A:204:GLN:OE1	2.28	0.65
1:B:82:PHE:HE1	1:B:263:ILE:HD12	1.62	0.65
1:A:175:THR:HG22	1:A:179:ARG:HH21	1.62	0.65
1:A:217:ASP:OD2	4:A:975:HOH:O	2.14	0.64
1:B:292:GLU:OE2	1:B:296:ARG:NH1	2.27	0.64
1:A:100:HIS:CE1	1:A:104:LEU:HD11	2.33	0.64
1:B:292:GLU:CD	1:B:296:ARG:HH11	2.00	0.60
1:B:209:ILE:CG2	1:B:213:ASN:HD21	2.13	0.60
1:A:78:VAL:HG11	1:A:82:PHE:CE2	2.36	0.60
1:A:87[A]:PHE:HZ	3:A:502:1C6:CE2	2.16	0.58
1:B:220:ILE:HD11	1:B:258:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASN:HD22	1:B:201:ASN:N	2.02	0.58
1:B:209:ILE:HG22	1:B:213:ASN:ND2	2.19	0.57
1:B:271:GLY:HA2	1:B:440:LYS:HG3	1.85	0.57
1:A:78:VAL:HG13	1:A:82:PHE:CD2	2.38	0.57
1:A:87[A]:PHE:CZ	3:A:502:1C6:CE2	2.88	0.57
1:B:263:ILE:HG22	3:B:502:1C6:H6	1.85	0.56
1:B:173:PHE:CD1	1:B:215:LEU:HD23	2.40	0.56
1:A:162:PHE:HE1	1:A:215:LEU:CD2	2.19	0.56
3:A:502:1C6:H3	3:A:502:1C6:C2	2.31	0.56
1:A:128:GLN:HG2	4:A:684:HOH:O	2.07	0.55
1:A:71:LEU:HD22	1:A:90:TRP:CE2	2.42	0.54
1:A:182[A]:ASP:OD2	4:A:828:HOH:O	2.18	0.53
1:A:78:VAL:CG1	1:A:82:PHE:CE2	2.89	0.53
1:A:431:LEU:HD21	1:A:433:ILE:HD11	1.91	0.52
1:B:87[A]:PHE:CZ	3:B:502:1C6:CE2	2.94	0.51
1:A:87[A]:PHE:CE1	3:A:502:1C6:H11	2.46	0.51
1:B:86:LEU:N	1:B:257:GLN:HE22	2.06	0.51
1:A:87[A]:PHE:CE1	3:A:502:1C6:C1	2.94	0.51
1:A:179:ARG:NH1	1:A:208:ASP:OD1	2.44	0.50
1:B:195:ASP:CG	1:B:196:PRO:HD2	2.33	0.49
1:A:104:LEU:N	1:A:105:PRO:CD	2.75	0.49
1:A:128:GLN:NE2	4:A:684:HOH:O	2.43	0.49
1:B:220:ILE:HD11	1:B:258:ILE:CD1	2.42	0.49
3:B:502:1C6:C1	4:B:861:HOH:O	2.38	0.49
1:B:77:PHE:HE2	1:B:188:LEU:HD23	1.77	0.49
1:B:118:MET:CE	4:B:616:HOH:O	2.60	0.49
1:B:209:ILE:CG2	1:B:213:ASN:ND2	2.76	0.49
1:A:232:ASP:O	1:A:236:HIS:HD2	1.96	0.49
1:B:207:GLU:HG2	4:B:824:HOH:O	2.12	0.49
1:A:87[A]:PHE:HE1	3:A:502:1C6:C1	2.26	0.48
1:A:403:GLN:NE2	4:A:734:HOH:O	2.46	0.48
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.95	0.48
1:B:148:LEU:O	1:B:148:LEU:HG	2.14	0.48
1:A:87[A]:PHE:CE1	3:A:502:1C6:CZ	2.97	0.48
1:B:118:MET:HE1	4:B:616:HOH:O	2.13	0.48
1:B:77:PHE:CE2	1:B:188:LEU:HD23	2.49	0.47
1:A:118:MET:HE3	1:A:156:CYS:HA	1.95	0.47
1:B:209:ILE:HG23	1:B:213:ASN:HD21	1.79	0.47
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.44	0.47
1:A:39:ILE:HD12	1:A:52:LEU:CD2	2.46	0.46
1:B:195:ASP:OD2	1:B:196:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87[A]:PHE:CZ	3:A:502:1C6:CZ	2.99	0.45
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.98	0.45
1:B:220:ILE:CD1	1:B:258:ILE:CD1	2.94	0.45
1:B:259:ILE:HD12	1:B:259:ILE:HG21	1.75	0.44
1:B:380:GLU:O	1:B:380:GLU:HG3	2.16	0.44
1:B:16:ASN:ND2	1:B:43:GLU:H	2.02	0.44
1:B:87[A]:PHE:HZ	3:B:502:1C6:CE2	2.29	0.44
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.99	0.44
1:A:328:ALA:HB1	3:A:502:1C6:N1	2.33	0.44
1:B:216:VAL:O	1:B:220:ILE:HG12	2.17	0.44
1:B:207:GLU:C	4:B:824:HOH:O	2.52	0.44
1:B:118:MET:HG2	4:B:841:HOH:O	2.17	0.44
1:B:209:ILE:O	1:B:213:ASN:ND2	2.51	0.43
1:A:79:ARG:HG3	4:A:746:HOH:O	2.17	0.43
1:B:79:ARG:HD3	1:B:83:GLY:O	2.18	0.43
1:B:306:LYS:O	1:B:310[B]:GLN:CG	2.61	0.43
1:B:44:ALA:HB1	1:B:45:PRO:CD	2.50	0.42
1:B:426:HIS:CD2	1:B:447:LYS:HE3	2.54	0.42
1:B:82:PHE:CE1	1:B:263:ILE:HD12	2.48	0.42
1:B:87[A]:PHE:CE1	3:B:502:1C6:C1	3.03	0.41
1:B:202:LYS:O	1:B:206:GLN:HG2	2.20	0.41
1:B:209:ILE:HG22	1:B:213:ASN:HD21	1.80	0.41
1:B:20:LEU:CD2	4:B:651:HOH:O	2.43	0.41
1:B:238:LEU:HD23	1:B:254:ILE:HD13	2.02	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	450/455 (99%)	439 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/455 (97%)	420 (96%)	20 (4%)	0	100	100
All	All	890/910 (98%)	859 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/400 (99%)	389 (98%)	8 (2%)	55	51
1	B	392/400 (98%)	381 (97%)	11 (3%)	43	36
All	All	789/800 (99%)	770 (98%)	19 (2%)	49	43

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	71	LEU
1	A	148	LEU
1	A	159	ASN
1	A	187	LYS
1	A	222	ASP
1	A	287	LEU
1	A	440	LYS
1	B	47	ARG
1	B	71	LEU
1	B	79	ARG
1	B	98	LYS
1	B	104	LEU
1	B	148	LEU
1	B	189	GLN
1	B	201	ASN
1	B	259	ILE
1	B	288	GLN

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Mol	Chain	Res	Type
1	B	440	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	95	ASN
1	A	159	ASN
1	A	189	GLN
1	A	201	ASN
1	A	236	HIS
1	A	253	ASN
1	A	257	GLN
1	A	388	HIS
1	A	403	GLN
1	B	16	ASN
1	B	73	GLN
1	B	95	ASN
1	B	159	ASN
1	B	213	ASN
1	B	253	ASN
1	B	257	GLN
1	B	283	ASN
1	B	288	GLN
1	B	381	ASN
1	B	388	HIS
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 monosaccharides 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	HEM	B	501	1	41,50,50	2.00	8 (19%)	45,82,82	2.48	16 (35%)
2	HEM	A	501	1	41,50,50	1.88	6 (14%)	45,82,82	2.11	13 (28%)
3	1C6	B	502	-	23,25,25	3.63	7 (30%)	28,35,35	2.30	8 (28%)
3	1C6	A	502	-	23,25,25	3.25	7 (30%)	28,35,35	2.45	11 (39%)

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	B	501	1	-	3/12/54/54	-
2	HEM	A	501	1	-	2/12/54/54	-
3	1C6	B	502	-	-	2/7/9/9	0/3/3/3
3	1C6	A	502	-	-	6/7/9/9	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	1C6	CD1-CG	11.53	1.50	1.39
3	A	502	1C6	CD1-CG	10.95	1.50	1.39
2	B	501	HEM	C3D-C2D	7.28	1.52	1.36
2	A	501	HEM	C3D-C2D	6.75	1.51	1.36
3	B	502	1C6	CE1-CZ	6.63	1.51	1.40
3	A	502	1C6	CE1-CD1	6.39	1.50	1.39
3	B	502	1C6	CE1-CD1	6.26	1.50	1.39
3	B	502	1C6	CB-S	-6.17	1.68	1.82
2	A	501	HEM	C3C-C2C	-5.34	1.33	1.40
3	A	502	1C6	CE1-CZ	5.16	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	1C6	CB-S	-4.89	1.71	1.82
2	B	501	HEM	FE-ND	4.24	2.17	1.96
2	B	501	HEM	C3C-CAC	4.13	1.56	1.47
3	B	502	1C6	CF1-S	-4.11	1.67	1.75
3	B	502	1C6	CE3-CZ3	3.86	1.43	1.37
2	B	501	HEM	CMD-C2D	3.33	1.57	1.50
2	B	501	HEM	CMB-C2B	3.04	1.57	1.50
2	B	501	HEM	C3C-C2C	-2.68	1.36	1.40
2	A	501	HEM	O1A-CGA	2.55	1.30	1.22
2	B	501	HEM	CAA-C2A	2.52	1.55	1.52
2	A	501	HEM	C4D-ND	-2.33	1.36	1.40
3	A	502	1C6	CF1-S	-2.31	1.71	1.75
3	B	502	1C6	CS2-CX2	2.30	1.50	1.42
3	A	502	1C6	CZ2-CS2	-2.18	1.38	1.41
2	B	501	HEM	CMC-C2C	2.12	1.56	1.51
2	A	501	HEM	CMD-C2D	2.10	1.55	1.50
2	A	501	HEM	C1A-CHA	-2.05	1.35	1.41
3	A	502	1C6	CE3-CZ3	2.01	1.40	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4D-ND-C1D	8.36	113.70	105.07
2	A	501	HEM	C4D-ND-C1D	6.23	111.51	105.07
3	A	502	1C6	CE2-N1-CG	5.59	124.80	117.75
3	B	502	1C6	CE2-N1-CG	5.50	124.68	117.75
3	B	502	1C6	CD1-CG-N1	-5.36	118.69	123.95
3	B	502	1C6	CZ-CE1-CD1	-5.19	117.16	121.53
2	B	501	HEM	C1B-NB-C4B	5.12	110.36	105.07
3	A	502	1C6	CD1-CG-N1	-5.00	119.05	123.95
2	A	501	HEM	C4C-CHD-C1D	4.65	128.70	122.56
2	B	501	HEM	CHC-C4B-NB	4.57	129.39	124.43
3	A	502	1C6	CZ-CE1-CD1	-4.52	117.72	121.53
3	A	502	1C6	CB-CG-CD1	4.45	124.47	120.29
3	A	502	1C6	O2-CE1-CD1	4.44	125.06	118.83
2	B	501	HEM	CMA-C3A-C4A	-4.33	121.81	128.46
2	B	501	HEM	C4A-C3A-C2A	4.28	109.98	107.00
2	A	501	HEM	CHA-C4D-ND	4.04	129.38	124.38
2	A	501	HEM	CBA-CAA-C2A	-3.85	106.05	112.62
2	A	501	HEM	CMA-C3A-C4A	-3.71	122.76	128.46
2	B	501	HEM	C4B-C3B-C2B	3.62	109.99	107.11
2	B	501	HEM	C4B-CHC-C1C	3.57	127.28	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3D-C4D-ND	-3.55	106.22	110.17
2	A	501	HEM	CBD-CAD-C3D	-3.29	103.50	112.63
3	B	502	1C6	CG-CB-S	3.13	116.92	109.96
3	A	502	1C6	CZ-CE2-N1	-3.02	122.02	125.11
3	A	502	1C6	CB-S-CF1	-3.02	99.10	102.42
2	A	501	HEM	C4B-C3B-C2B	3.00	109.50	107.11
3	B	502	1C6	CE3-CX2-NV	2.99	139.38	130.83
3	B	502	1C6	CB-CG-CD1	2.93	123.05	120.29
2	B	501	HEM	C2C-C3C-C4C	2.82	108.87	106.90
2	B	501	HEM	CHA-C4D-ND	2.72	127.75	124.38
2	B	501	HEM	CBD-CAD-C3D	-2.72	105.06	112.63
2	B	501	HEM	C1D-C2D-C3D	-2.72	104.10	106.96
2	B	501	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
2	A	501	HEM	O1A-CGA-CBA	-2.70	114.40	123.08
3	A	502	1C6	C4-O3-CZ3	2.61	123.16	117.51
3	A	502	1C6	CE3-CX2-NV	2.52	138.03	130.83
2	A	501	HEM	C4B-CHC-C1C	2.48	125.83	122.56
2	A	501	HEM	CMA-C3A-C2A	2.35	129.37	124.94
2	A	501	HEM	C1B-NB-C4B	2.34	107.49	105.07
3	A	502	1C6	CE2-CZ-CE1	2.25	118.99	116.27
2	B	501	HEM	C4C-CHD-C1D	2.18	125.44	122.56
2	A	501	HEM	C1D-C2D-C3D	-2.17	104.68	106.96
2	A	501	HEM	CBB-CAB-C3B	-2.15	116.94	127.62
3	A	502	1C6	C3-CD1-CG	-2.08	120.88	122.69
3	B	502	1C6	CB-CG-N1	2.07	118.22	116.03
2	B	501	HEM	O1A-CGA-CBA	-2.06	116.46	123.08
2	B	501	HEM	CHD-C1D-ND	2.03	126.64	124.43
3	B	502	1C6	C1-CZ-CE1	2.02	124.08	120.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	1C6	CD1-CE1-O2-C2
3	A	502	1C6	CH2-CZ3-O3-C4
3	A	502	1C6	CE3-CZ3-O3-C4
3	A	502	1C6	S-CB-CG-N1
3	B	502	1C6	S-CB-CG-CD1
3	A	502	1C6	CZ-CE1-O2-C2
3	B	502	1C6	S-CB-CG-N1
3	A	502	1C6	S-CB-CG-CD1
2	A	501	HEM	CAD-CBD-CGD-O2D

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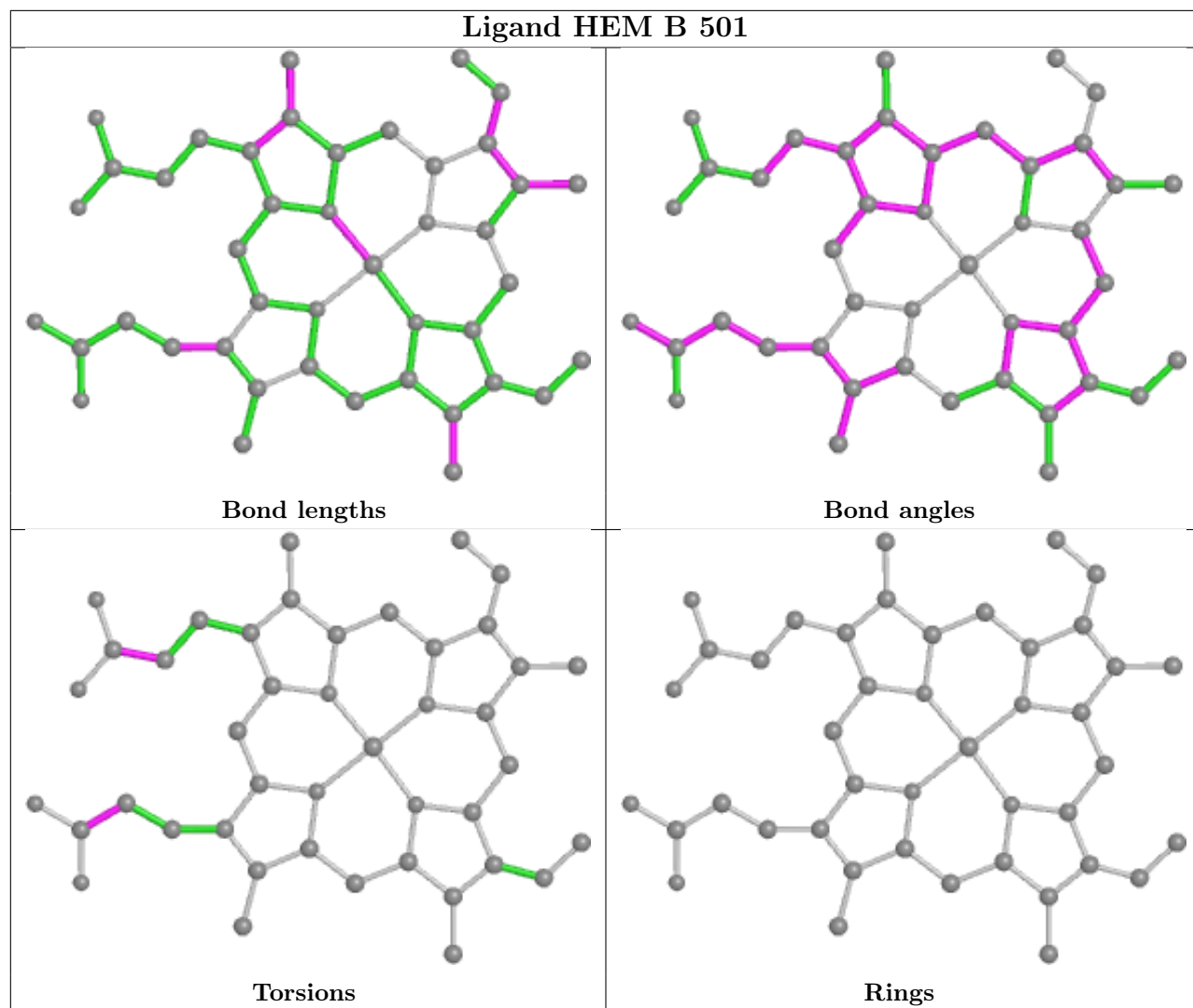
Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O1D

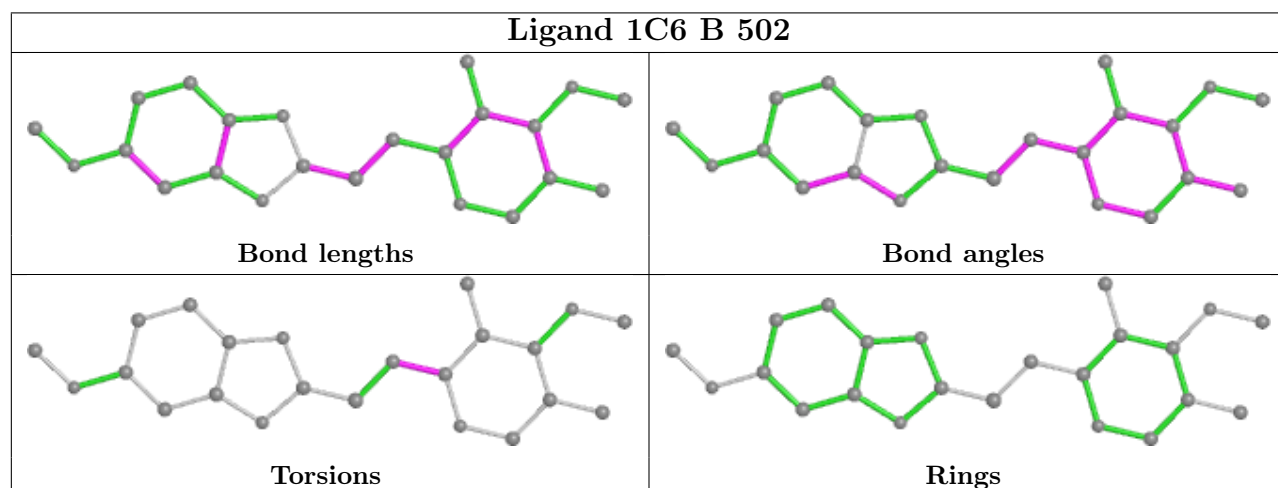
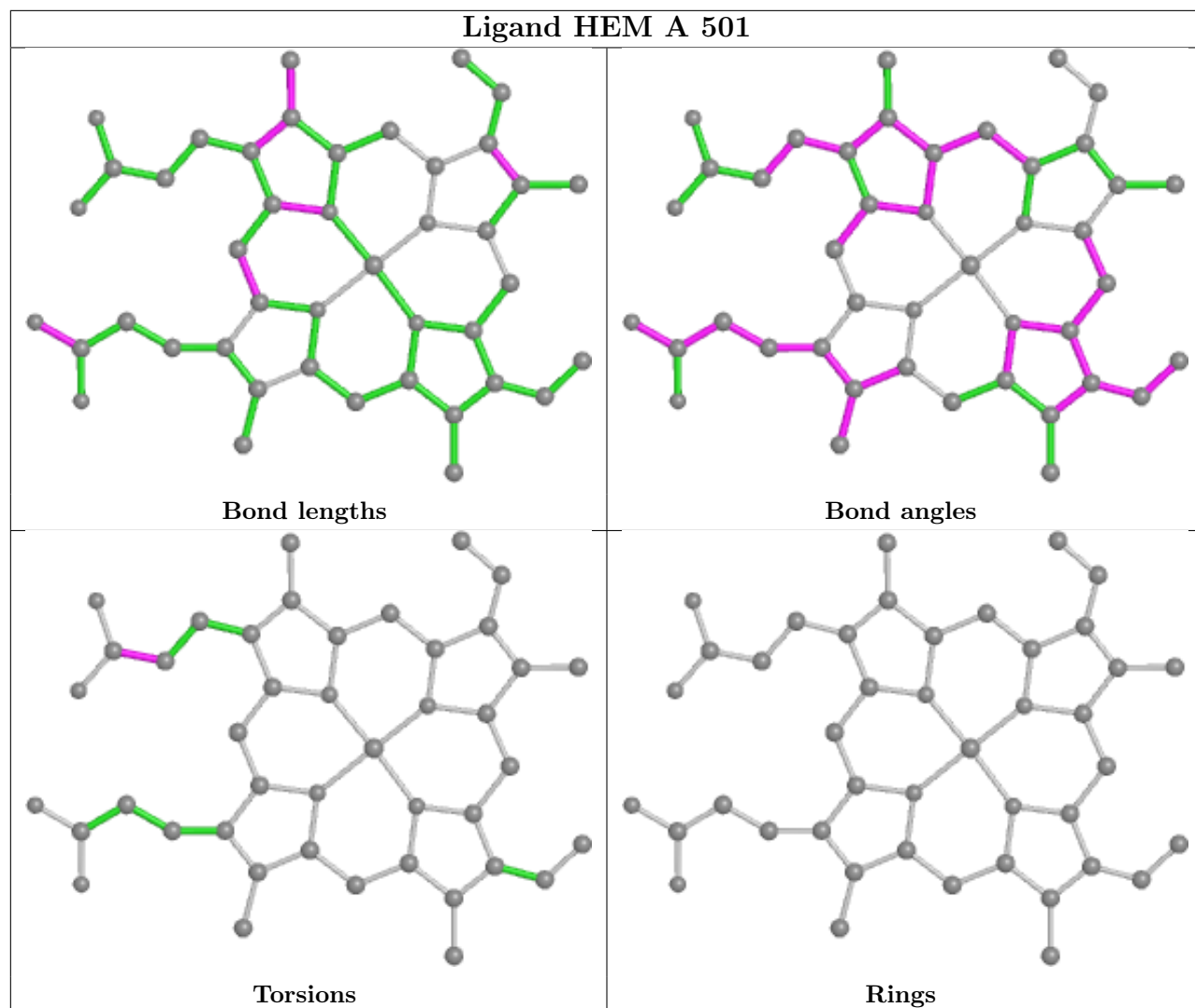
There are no ring outliers.

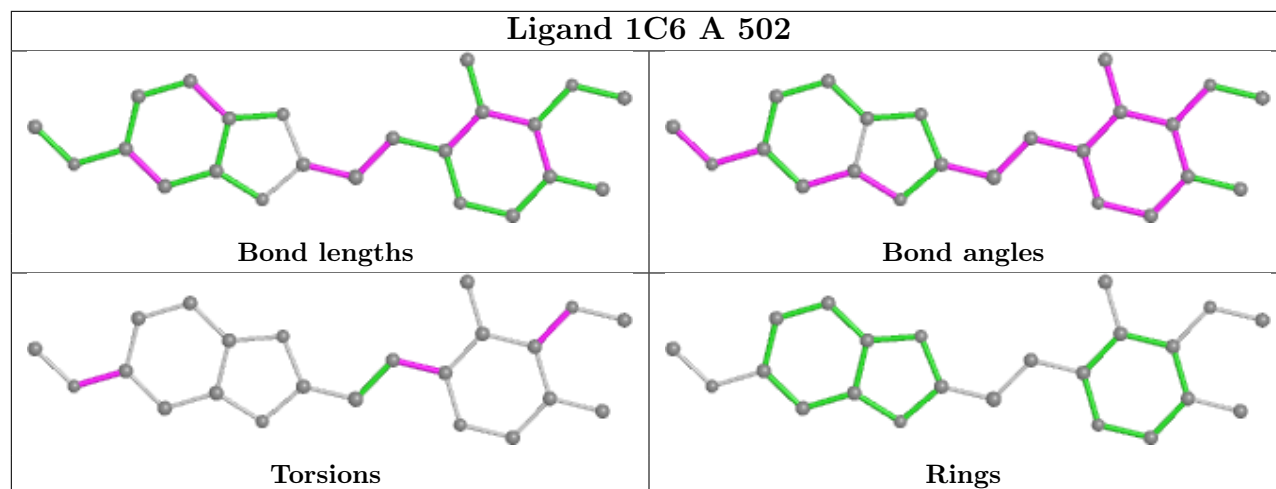
3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	1	0
3	B	502	1C6	6	0
3	A	502	1C6	12	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	450/455 (98%)	-0.24	2 (0%) 92 93	10, 18, 36, 50	0
1	B	443/455 (97%)	-0.06	10 (2%) 60 63	14, 25, 53, 72	0
All	All	893/910 (98%)	-0.15	12 (1%) 77 79	10, 21, 47, 72	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	4.9
1	B	191	ALA	4.5
1	B	196	PRO	3.9
1	B	197	ALA	3.5
1	B	193	PRO	3.3
1	A	136	ASP	2.6
1	B	136	ASP	2.6
1	B	4	GLU	2.5
1	B	3	LYS	2.5
1	B	47	ARG	2.3
1	B	230	SER	2.1
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](#)

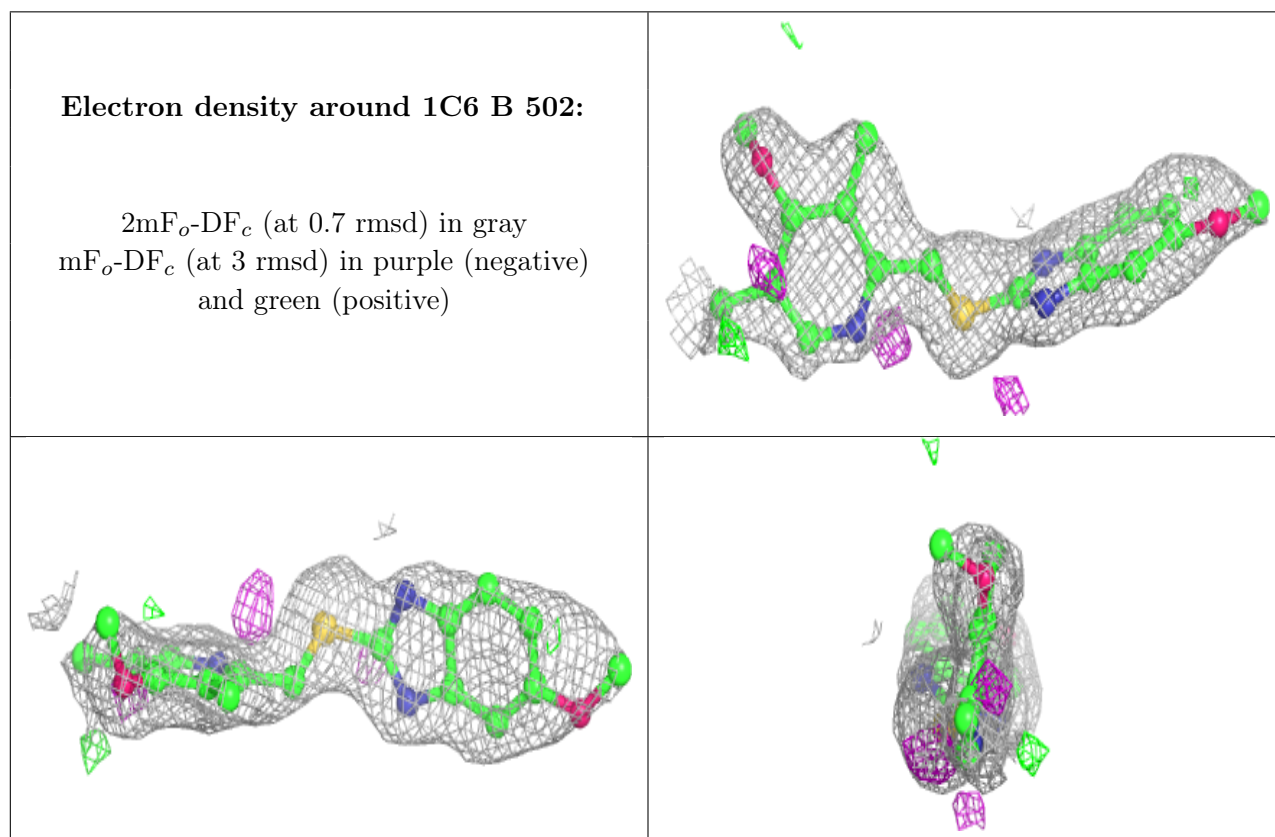
There are no monosaccharides in this entry.

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.

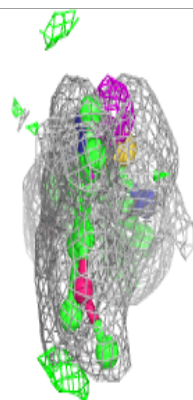
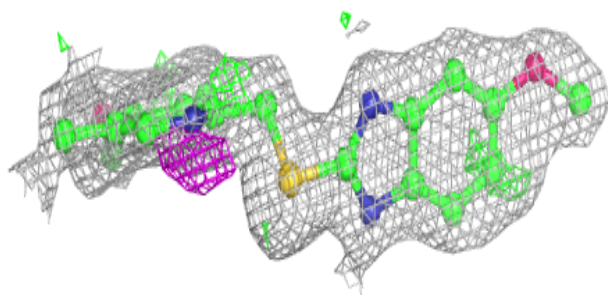
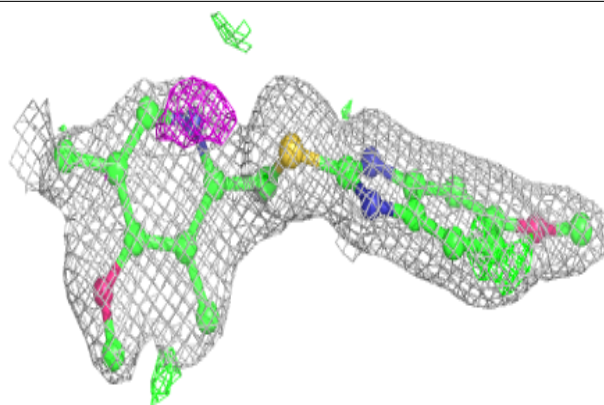
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	1C6	B	502	23/23	0.85	0.20	47,50,52,56	0
3	1C6	A	502	23/23	0.91	0.13	24,31,42,43	0
2	HEM	B	501	43/43	0.97	0.09	11,16,20,25	0
2	HEM	A	501	43/43	0.98	0.10	6,10,13,14	0

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.



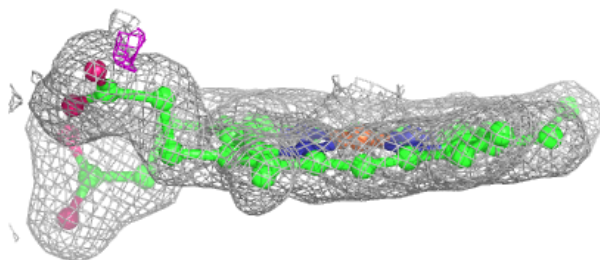
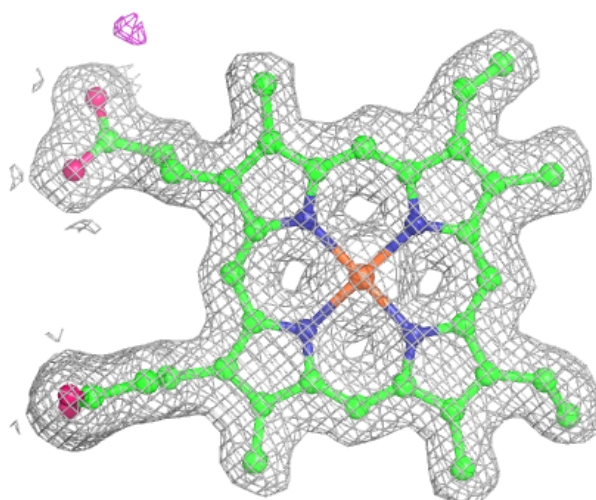
Electron density around 1C6 A 502:

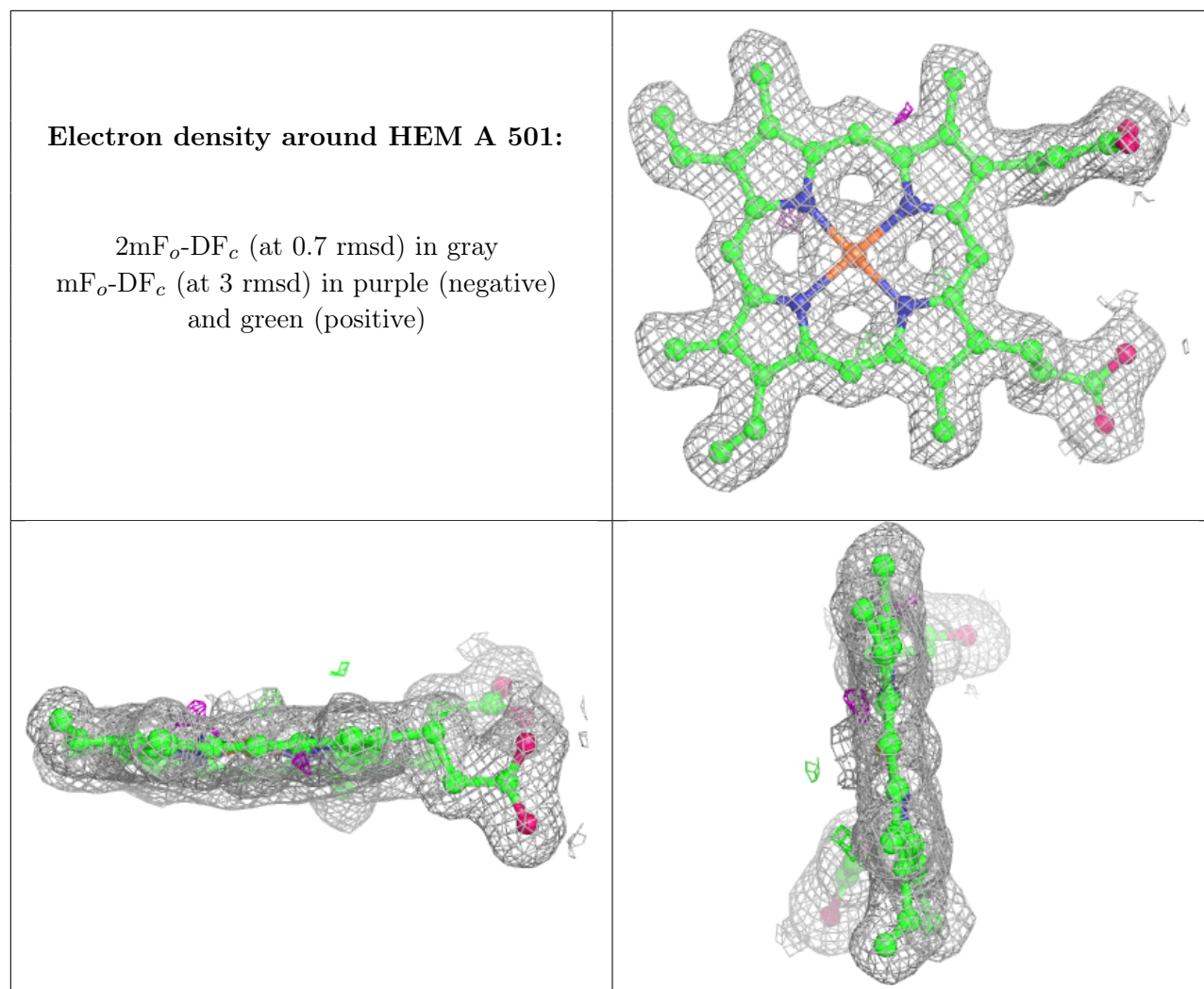
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.