



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 12:14 PM EDT

PDB ID : 6Q2C
Title : Domain-swapped dimer of Acanthamoeba castellanii CYP51
Authors : Sharma, V.; Podust, L.M.
Deposited on : 2019-08-07
Resolution : 1.80 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 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 : 2.14.6
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) : 2.14.6

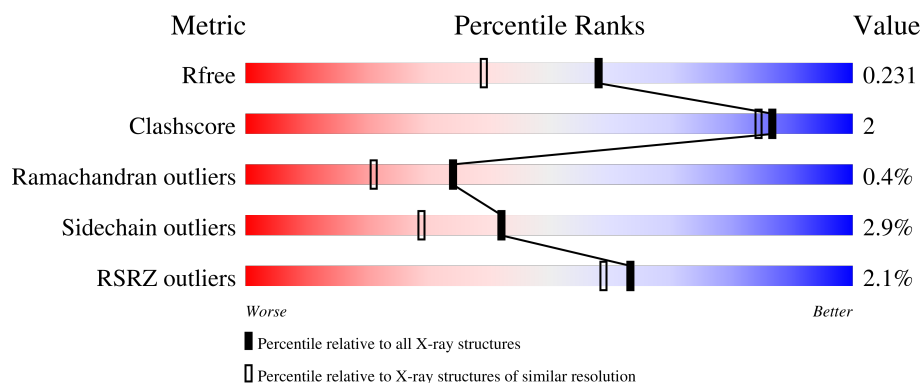
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	460	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 90%, yellow 90%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 90% 7% . </div> </div>
1	B	460	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 90%, yellow 90%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 90% 7% .. </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7890 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	4	0
			3601	2327	600	656	18			
1	B	449	Total	C	N	O	S	0	3	0
			3583	2317	597	651	18			

There are 32 discrepancies between the modelled and reference sequences:

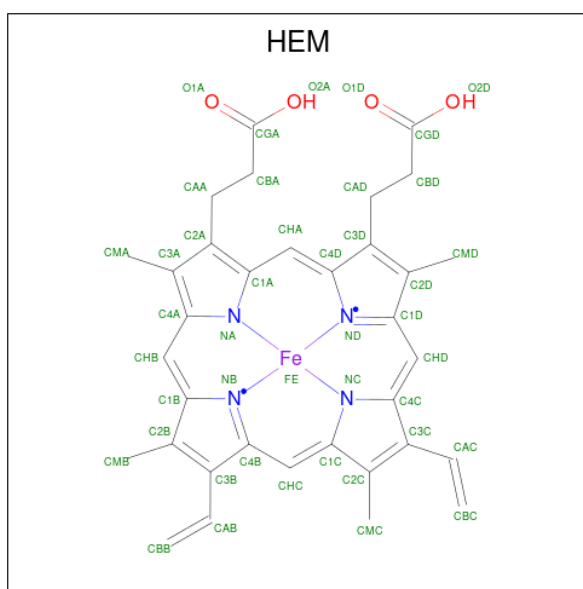
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	expression tag	UNP L8GJB3
A	34	ALA	-	expression tag	UNP L8GJB3
A	35	LYS	-	expression tag	UNP L8GJB3
A	36	LYS	-	expression tag	UNP L8GJB3
A	37	THR	-	expression tag	UNP L8GJB3
A	38	SER	-	expression tag	UNP L8GJB3
A	39	SER	-	expression tag	UNP L8GJB3
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	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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





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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	279	Total	O	0	0
			279	279		

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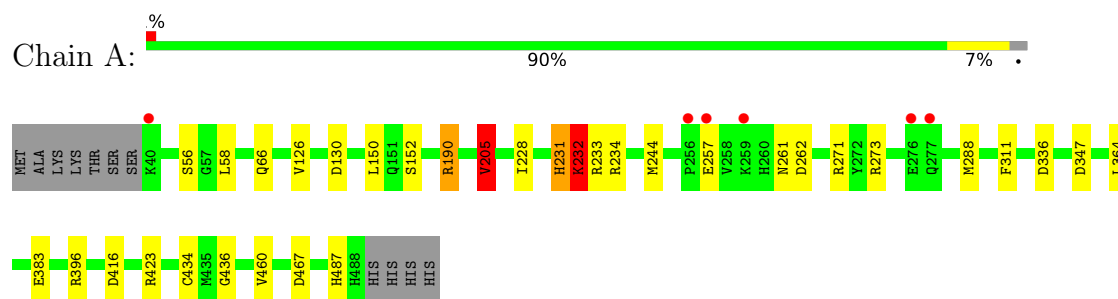
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	231	Total 231	O 231	0	0

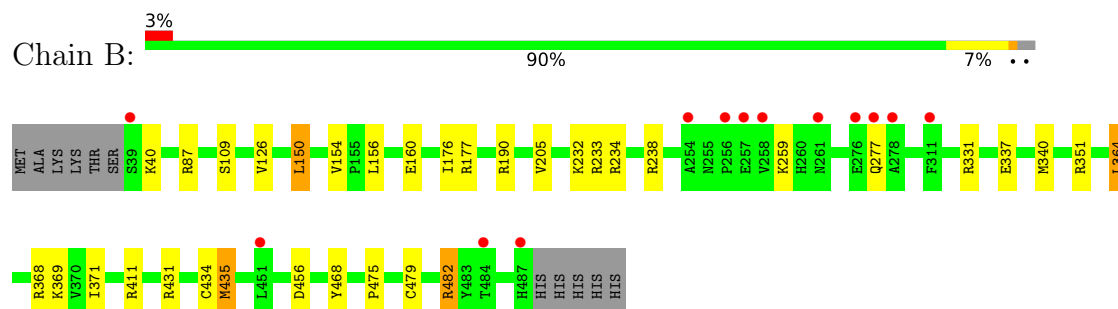
3 Residue-property plots [i](#)

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: Obtusifoliol 14alphademethylase



• Molecule 1: Obtusifoliol 14alphademethylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.35Å 101.57Å 123.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.51 – 1.80 71.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (78.51-1.80) 98.1 (71.39-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.185 , 0.227 0.193 , 0.231	Depositor DCC
R_{free} test set	5783 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7890	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.98	2/3690 (0.1%)	1.02	19/4996 (0.4%)
1	B	0.95	0/3672	0.99	17/4974 (0.3%)
All	All	0.97	2/7362 (0.0%)	1.01	36/9970 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	LYS	N-CA	6.31	1.58	1.46
1	A	311	PHE	CB-CG	-5.68	1.41	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ARG	NE-CZ-NH2	10.30	125.45	120.30
1	B	233	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	B	238	ARG	NE-CZ-NH2	9.13	124.87	120.30
1	A	273	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	B	435	MET	CG-SD-CE	7.86	112.78	100.20
1	A	232	LYS	N-CA-CB	7.42	123.95	110.60
1	B	238	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	233	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	B	368	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	190	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	347	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	482	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	467	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	130	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	233	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	87	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	190	ARG	NE-CZ-NH1	-6.24	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	368	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	190	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	A	467	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	271	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	234	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	288	MET	CG-SD-CE	-5.56	91.30	100.20
1	B	411	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	396	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	231	HIS	N-CA-C	-5.20	96.97	111.00
1	B	87	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	351	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	234	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	205	VAL	CB-CA-C	-5.10	101.71	111.40
1	B	331	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	416	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	273	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	364	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	A	423	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	3601	0	3560	11	0
1	B	3583	0	3528	11	0
2	A	86	0	60	6	0
2	B	86	0	60	8	0
3	A	14	0	20	0	0
3	B	7	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	1	0	0	0	0
6	A	279	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	231	0	0	1	0
All	All	7890	0	7238	30	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 (30) 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:160[B]:GLU:OE2	1:B:160[B]:GLU:HA	1.50	1.10
1:A:205:VAL:HG13	1:A:244:MET:SD	2.29	0.72
1:A:231:HIS:O	1:A:232:LYS:CB	2.32	0.71
1:B:160[B]:GLU:OE2	1:B:160[B]:GLU:CA	2.30	0.71
2:B:501[B]:HEM:HBC2	2:B:501[B]:HEM:HMC2	1.79	0.65
2:B:501[B]:HEM:HHA	2:B:501[B]:HEM:HBD1	1.80	0.64
1:A:434:CYS:HA	2:A:501[B]:HEM:CHA	2.29	0.62
1:A:228:ILE:O	1:A:231:HIS:O	2.18	0.61
2:A:501[B]:HEM:HMC2	2:A:501[B]:HEM:HBC2	1.83	0.61
1:A:231:HIS:O	1:A:232:LYS:HB3	2.02	0.59
2:A:501[A]:HEM:HMC2	2:A:501[A]:HEM:HBC2	1.85	0.58
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:HMC2	1.87	0.57
1:A:152:SER:HB3	1:A:261:ASN:ND2	2.22	0.54
1:B:369:LYS:NZ	6:B:603:HOH:O	2.41	0.54
1:A:434:CYS:HA	2:A:501[B]:HEM:C4D	2.44	0.52
2:A:501[B]:HEM:CMC	2:A:501[B]:HEM:HBC2	2.40	0.51
1:A:205:VAL:CG1	1:A:244:MET:SD	2.99	0.49
2:B:501[B]:HEM:HMB2	2:B:501[B]:HEM:HBB2	1.96	0.48
1:B:109:SER:HB2	1:B:371:ILE:HD11	1.96	0.47
2:B:501[B]:HEM:CMB	2:B:501[B]:HEM:HBB2	2.44	0.46
1:A:66[B]:GLN:OE1	1:B:232:LYS:CE	2.65	0.45
1:B:177:ARG:NH1	1:B:475:PRO:O	2.50	0.43
1:A:460:VAL:O	6:A:601:HOH:O	2.21	0.42
2:B:501[B]:HEM:HBC2	2:B:501[B]:HEM:CMC	2.47	0.41
1:B:150:LEU:C	1:B:340:MET:HE1	2.41	0.41
1:B:434:CYS:HA	2:B:501[A]:HEM:C4D	2.56	0.41
1:B:154:VAL:HG21	1:B:340:MET:HE2	2.02	0.41
1:B:435:MET:HE2	2:B:501[A]:HEM:HBD2	2.03	0.41
1:A:436:GLY:HA3	2:A:501[B]:HEM:C3C	2.56	0.40
1:B:364:LEU:HD21	1:B:468:TYR:CE1	2.57	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	451/460 (98%)	443 (98%)	6 (1%)	2 (0%)	34	21
1	B	450/460 (98%)	442 (98%)	6 (1%)	2 (0%)	34	21
All	All	901/920 (98%)	885 (98%)	12 (1%)	4 (0%)	34	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	LYS
1	A	126	VAL
1	B	126	VAL
1	B	259	LYS

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%)	372 (97%)	10 (3%)	46	32
1	B	377/397 (95%)	365 (97%)	12 (3%)	39	25
All	All	759/794 (96%)	737 (97%)	22 (3%)	42	29

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	150	LEU
1	A	190	ARG
1	A	205	VAL
1	A	257	GLU
1	A	262	ASP
1	A	336	ASP
1	A	383	GLU
1	A	487	HIS
1	B	40	LYS
1	B	150	LEU
1	B	156	LEU
1	B	176	ILE
1	B	205	VAL
1	B	277	GLN
1	B	337	GLU
1	B	364	LEU
1	B	431	ARG
1	B	456	ASP
1	B	479	CYS
1	B	482	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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	A	501[B]	1,6	27,50,50	0.86	0	17,82,82	1.65	5 (29%)
3	PEG	B	502	-	6,6,6	1.01	0	5,5,5	1.26	0
2	HEM	A	501[A]	1,6	27,50,50	0.91	1 (3%)	17,82,82	1.65	3 (17%)
3	PEG	A	502	-	6,6,6	0.84	0	5,5,5	0.84	0
2	HEM	B	501[A]	1,6	27,50,50	0.95	2 (7%)	17,82,82	1.32	2 (11%)
3	PEG	A	503	-	6,6,6	0.61	0	5,5,5	0.72	0
2	HEM	B	501[B]	1,6	27,50,50	1.05	2 (7%)	17,82,82	1.76	4 (23%)

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	A	501[B]	1,6	-	0/6/54/54	-
3	PEG	B	502	-	-	1/4/4/4	-
2	HEM	A	501[A]	1,6	-	0/6/54/54	-
3	PEG	A	502	-	-	2/4/4/4	-
2	HEM	B	501[A]	1,6	-	0/6/54/54	-
3	PEG	A	503	-	-	2/4/4/4	-
2	HEM	B	501[B]	1,6	-	2/6/54/54	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501[B]	HEM	C3B-C2B	-3.35	1.35	1.40
2	A	501[A]	HEM	C4D-C3D	2.99	1.49	1.42
2	B	501[A]	HEM	C4D-C3D	2.68	1.48	1.42
2	B	501[B]	HEM	C4D-C3D	2.59	1.48	1.42
2	B	501[A]	HEM	C3B-C2B	-2.29	1.37	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[A]	HEM	CAD-CBD-CGD	3.64	118.78	112.67
2	B	501[B]	HEM	CAA-CBA-CGA	-3.51	106.79	112.67
2	B	501[B]	HEM	CBD-CAD-C3D	3.45	118.83	112.48
2	A	501[B]	HEM	CBD-CAD-C3D	3.41	118.76	112.48
2	A	501[A]	HEM	CBA-CAA-C2A	3.10	118.21	112.49
2	A	501[B]	HEM	CMC-C2C-C3C	2.66	129.65	124.68
2	B	501[A]	HEM	CMC-C2C-C3C	2.62	129.58	124.68
2	B	501[A]	HEM	CBA-CAA-C2A	2.56	117.20	112.49
2	A	501[A]	HEM	CMC-C2C-C3C	2.49	129.33	124.68
2	B	501[B]	HEM	CMC-C2C-C3C	2.49	129.33	124.68
2	A	501[B]	HEM	CMB-C2B-C3B	2.43	129.22	124.68
2	A	501[B]	HEM	C3C-C4C-NC	-2.08	107.02	110.94
2	A	501[B]	HEM	C4C-C3C-C2C	2.07	108.34	106.90
2	B	501[B]	HEM	CAD-CBD-CGD	-2.06	109.22	112.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501[B]	HEM	C2D-C3D-CAD-CBD
2	B	501[B]	HEM	C4D-C3D-CAD-CBD
3	B	502	PEG	C1-C2-O2-C3
3	A	502	PEG	O1-C1-C2-O2
3	A	503	PEG	O1-C1-C2-O2
3	A	503	PEG	C4-C3-O2-C2
3	A	502	PEG	O2-C3-C4-O4

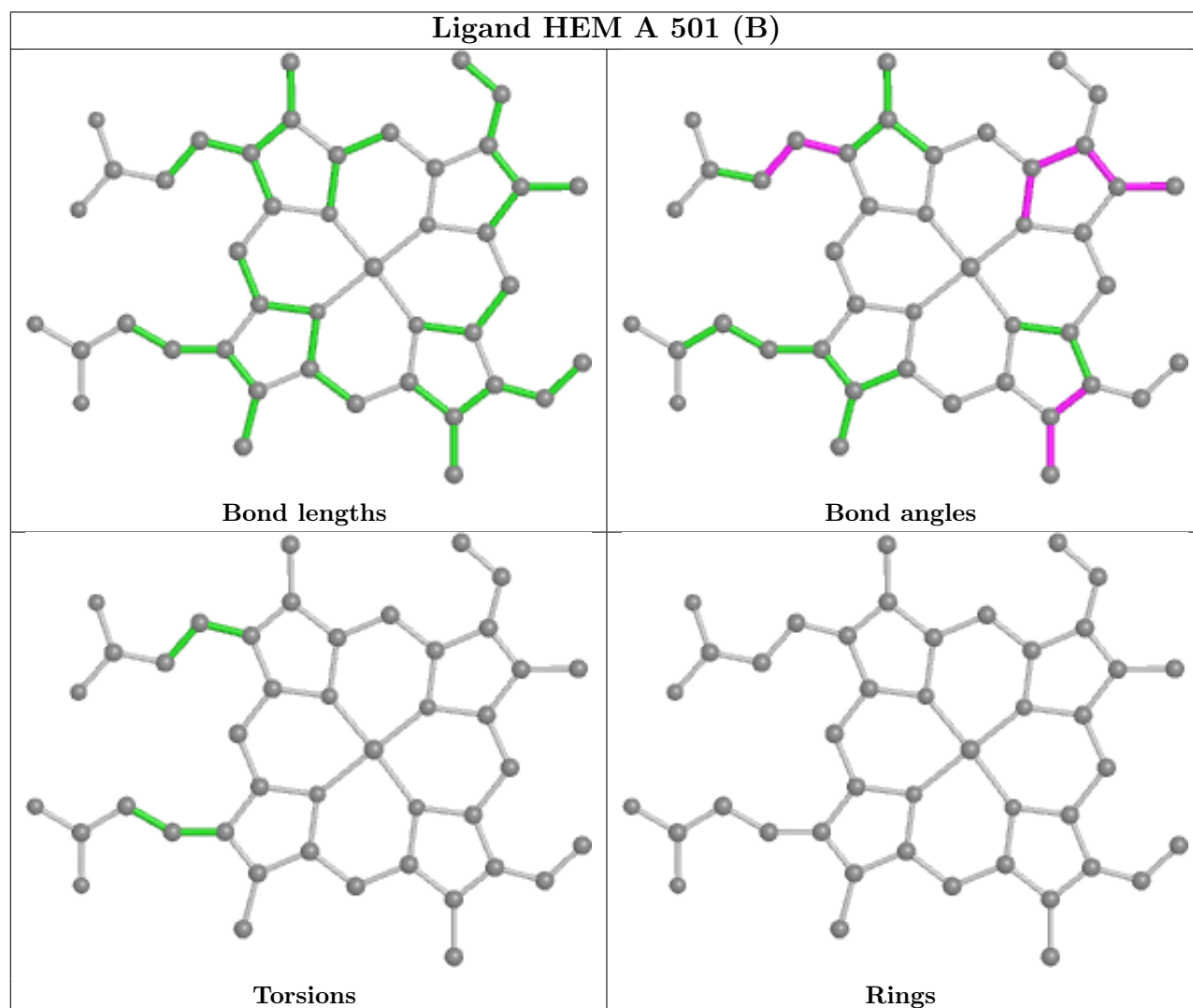
There are no ring outliers.

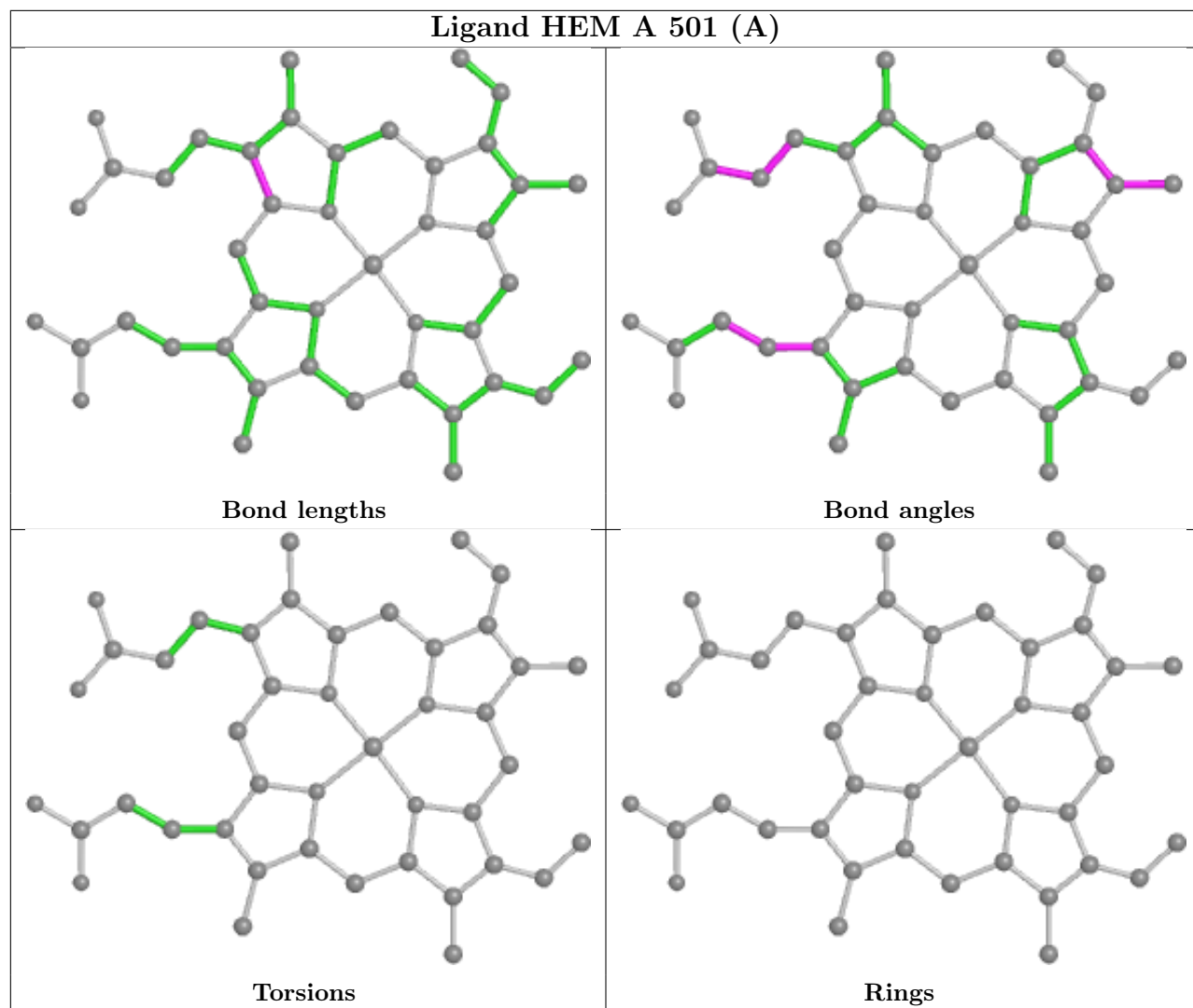
4 monomers are involved in 14 short contacts:

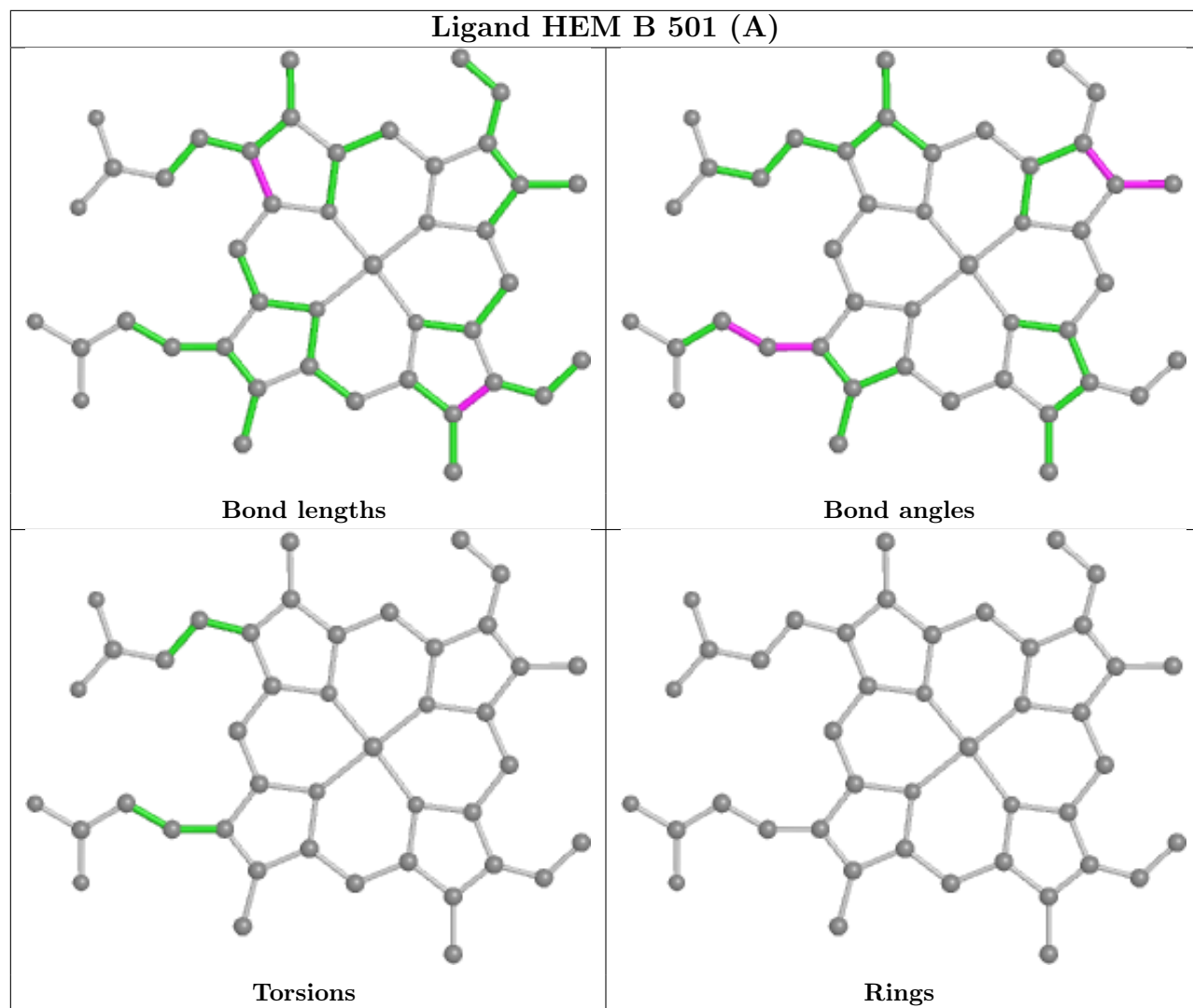
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[B]	HEM	5	0
2	A	501[A]	HEM	1	0
2	B	501[A]	HEM	3	0
2	B	501[B]	HEM	5	0

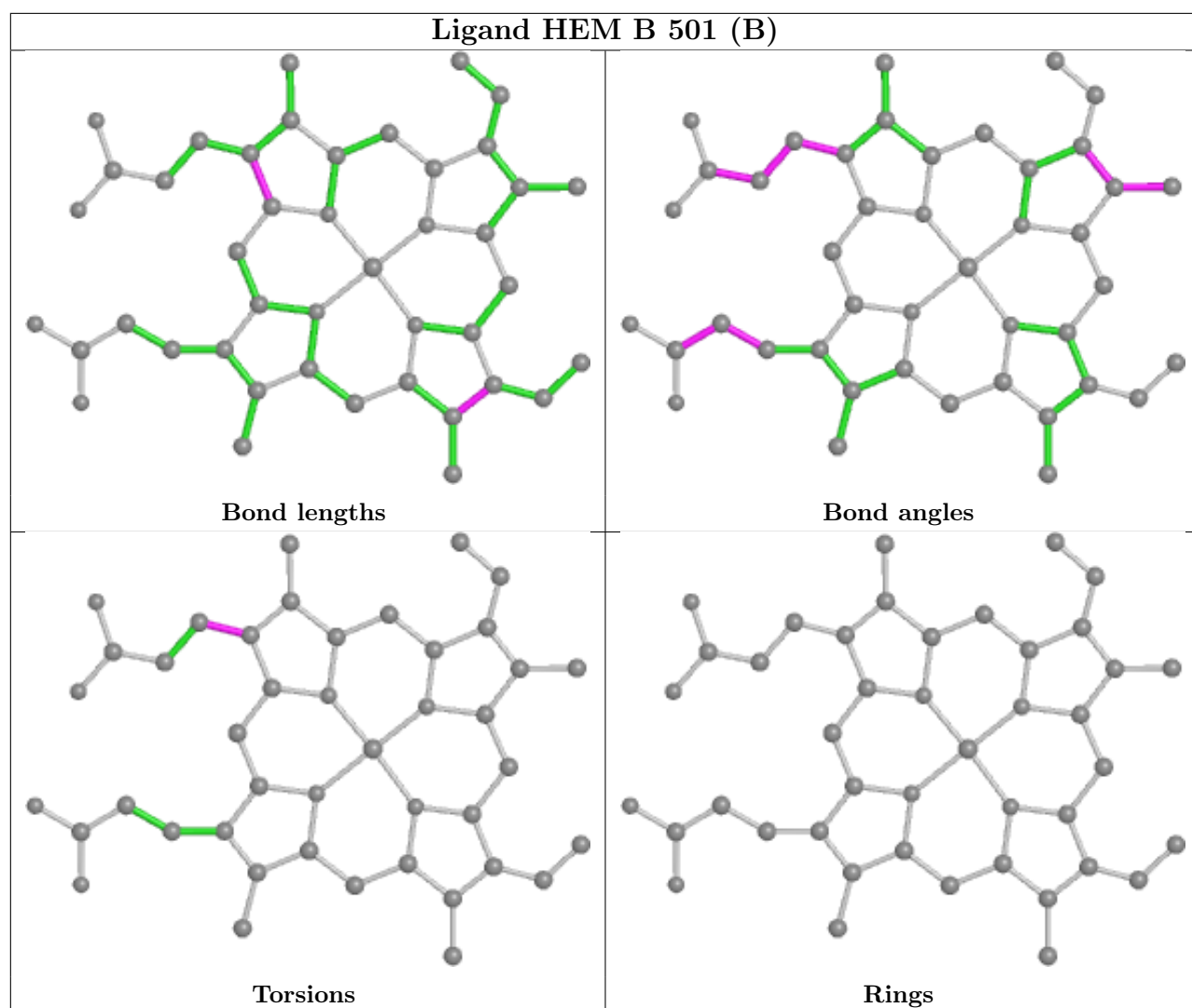
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	449/460 (97%)	-0.17	6 (1%) 77 74	33, 45, 66, 100	0
1	B	449/460 (97%)	0.02	13 (2%) 51 46	36, 50, 77, 116	0
All	All	898/920 (97%)	-0.08	19 (2%) 63 59	33, 47, 73, 116	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	HIS	4.1
1	A	276	GLU	3.5
1	B	278	ALA	3.4
1	B	261	ASN	3.2
1	B	276	GLU	3.0
1	B	257	GLU	2.9
1	B	277	GLN	2.9
1	B	254	ALA	2.8
1	A	257	GLU	2.7
1	B	484	THR	2.7
1	A	40	LYS	2.6
1	B	258	VAL	2.4
1	B	451	LEU	2.4
1	B	256	PRO	2.3
1	B	311	PHE	2.2
1	B	39	SER	2.2
1	A	277	GLN	2.2
1	A	259	LYS	2.2
1	A	256	PRO	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](#)

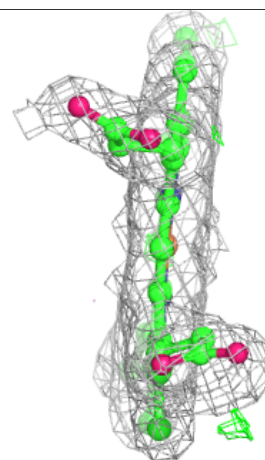
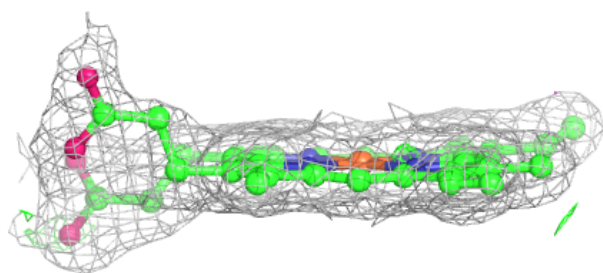
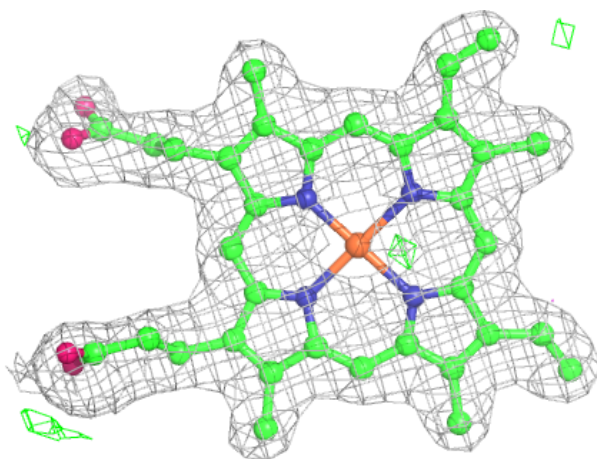
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEG	B	502	7/7	0.71	0.30	61,66,76,77	0
3	PEG	A	502	7/7	0.73	0.22	61,66,73,80	0
5	CL	B	503	1/1	0.76	0.29	77,77,77,77	0
4	K	B	504	1/1	0.91	0.04	86,86,86,86	0
3	PEG	A	503	7/7	0.92	0.32	64,66,74,79	0
4	K	A	504	1/1	0.97	0.20	88,88,88,88	0
2	HEM	B	501[A]	43/43	0.98	0.11	30,33,38,40	43
2	HEM	A	501[B]	43/43	0.98	0.09	29,33,36,42	43
2	HEM	A	501[A]	43/43	0.98	0.09	29,34,43,48	43
2	HEM	B	501[B]	43/43	0.98	0.11	33,36,41,47	43

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

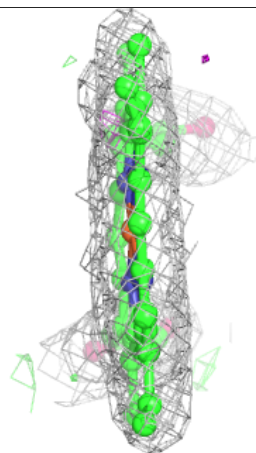
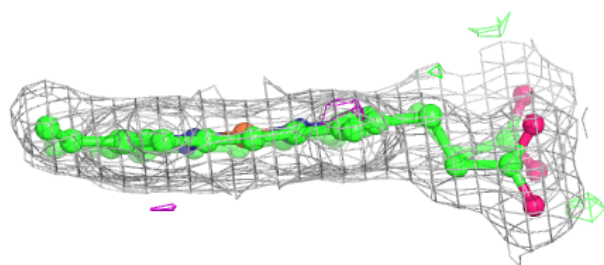
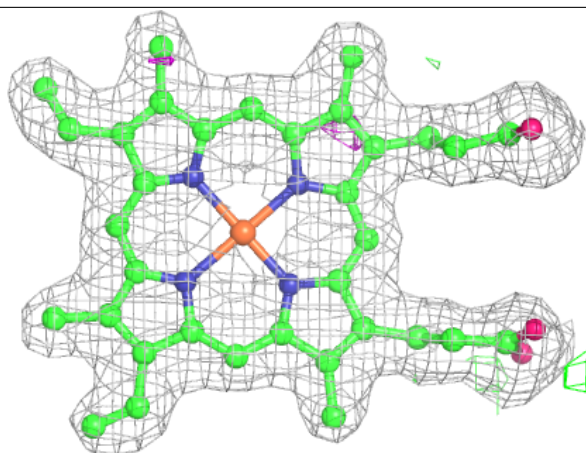
Electron density around HEM B 501 (A):

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



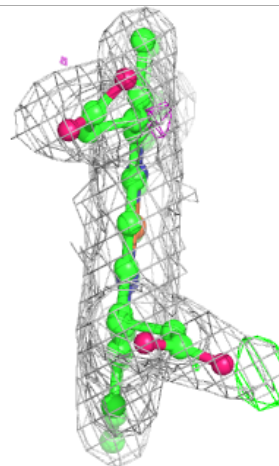
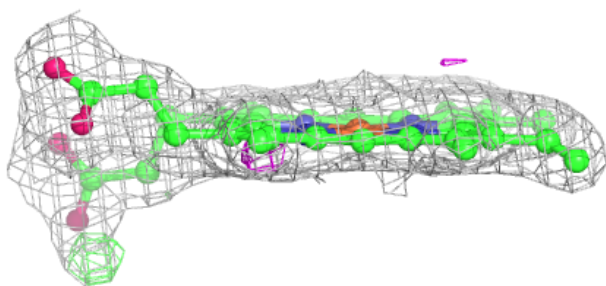
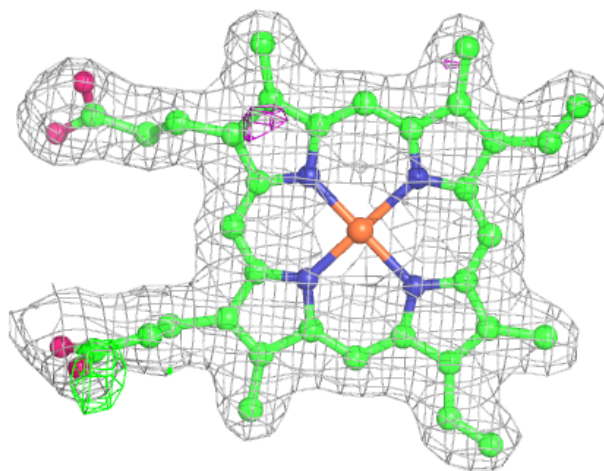
Electron density around HEM A 501 (B):

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



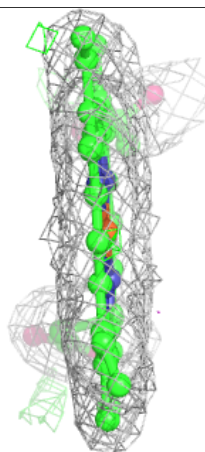
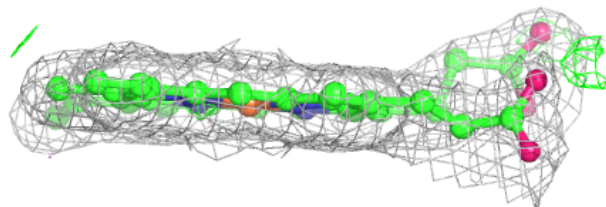
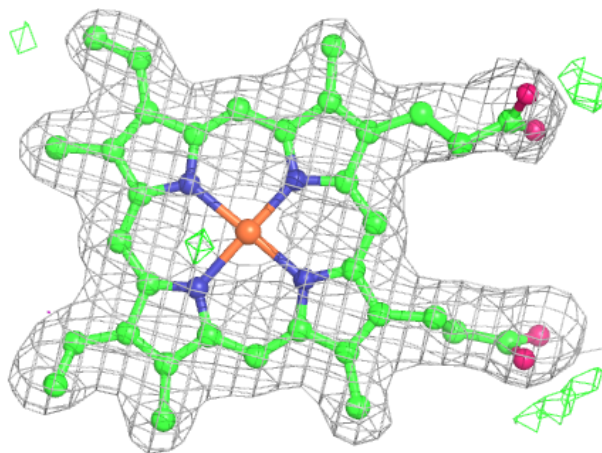
Electron density around HEM A 501 (A):

$2mF_o-DF_c$ (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 (B):

$2mF_o-DF_c$ (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.