Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 12:36 AM BST

PDB ID	:	4CFT
Title	:	Structure of bovine endothelial nitric oxide synthase heme domain in complex with 7-((3-Fluorophenethylamino)ethyl)quinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2013-11-19
Resolution	:	1.79 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:
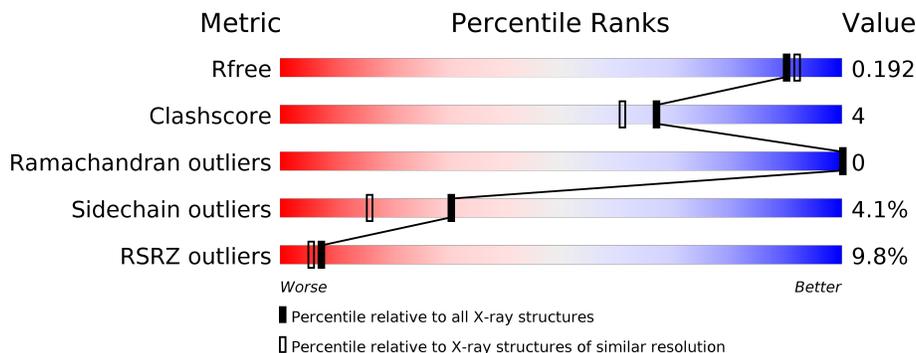
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.192
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		4.1%
RSRZ outliers		9.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	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 <=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	443	11% 82% 8% · 9%
2	B	443	7% 84% 5% · 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6952 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 ENDOTHELIAL NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
1	A	405	3223	1	2049	568	589	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473

- Molecule 2 is a protein called ENDOTHELIAL NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	403	3209	2040	566	587	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ARG	CYS	conflict	UNP P29473

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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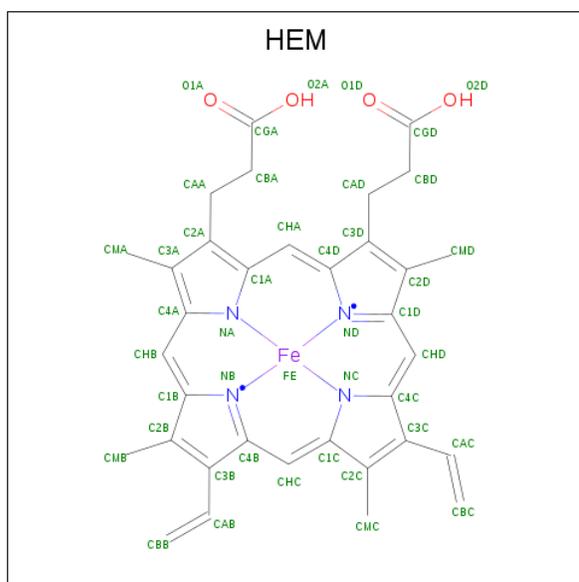
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).

H4B
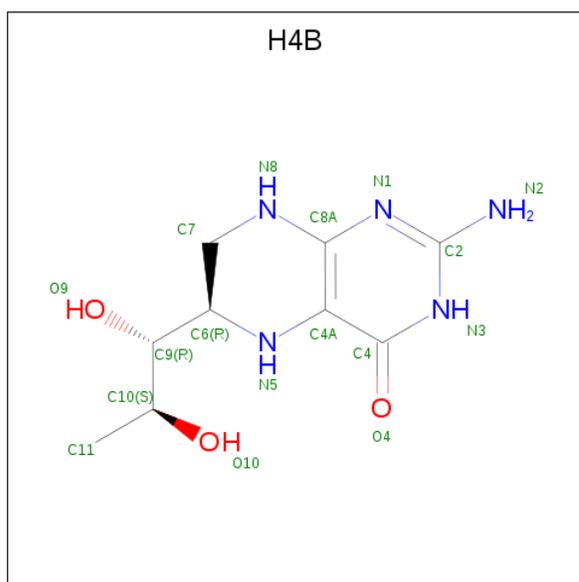
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 5 is 7-[2-[2-(3-fluorophenyl)ethylamino]ethyl]quinolin-2-amine (three-letter code: M48) (formula: $C_{19}H_{20}FN_3$).
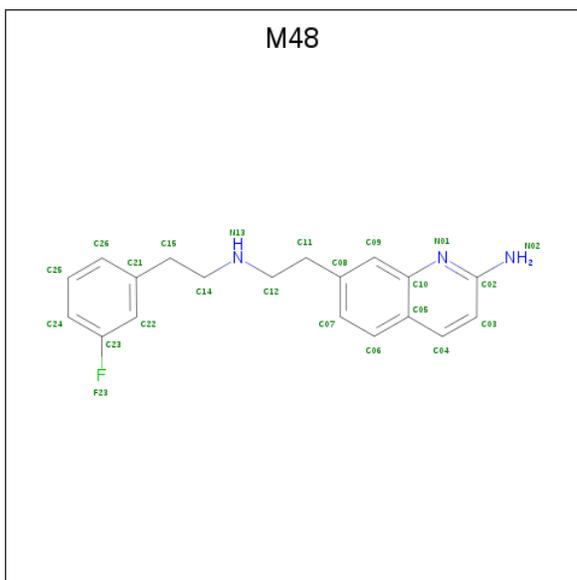
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 23	C 19	F 1	N 3	0	0
5	B	1	Total 23	C 19	F 1	N 3	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
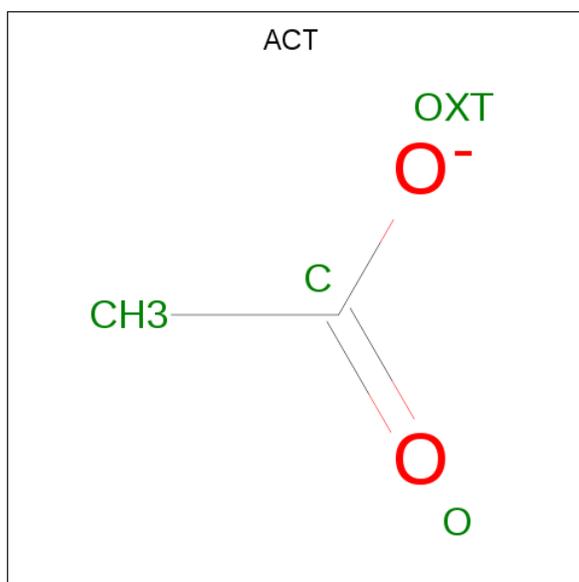
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
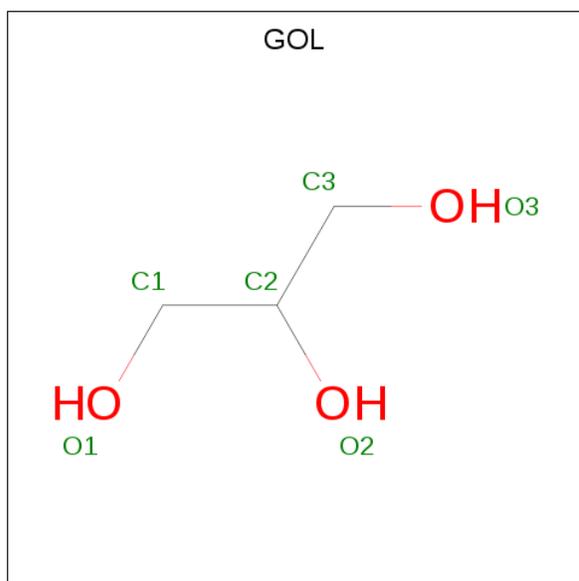
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Zn 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	177	Total 177	O 177	0	0
9	B	148	Total 148	O 148	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: ENDOTHELIAL NITRIC OXIDE SYNTHASE
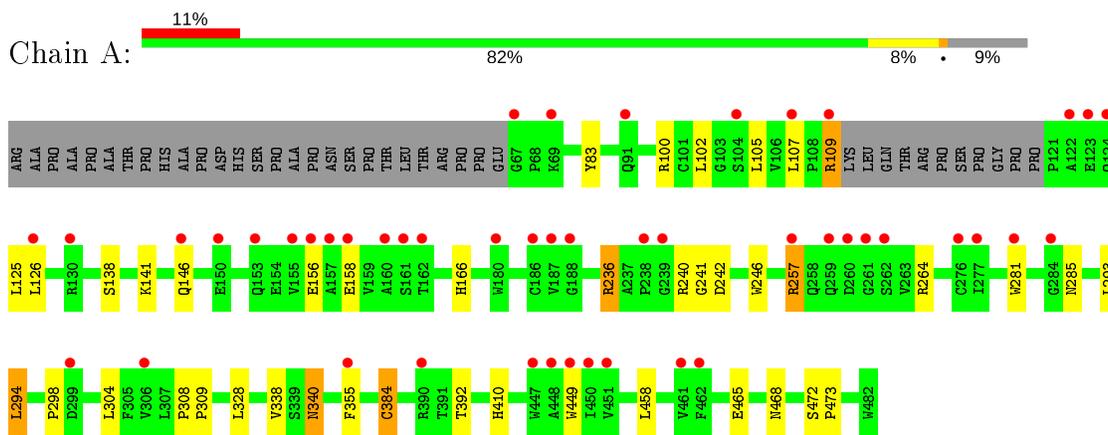
- Molecule 2: ENDOTHELIAL NITRIC OXIDE SYNTHASE
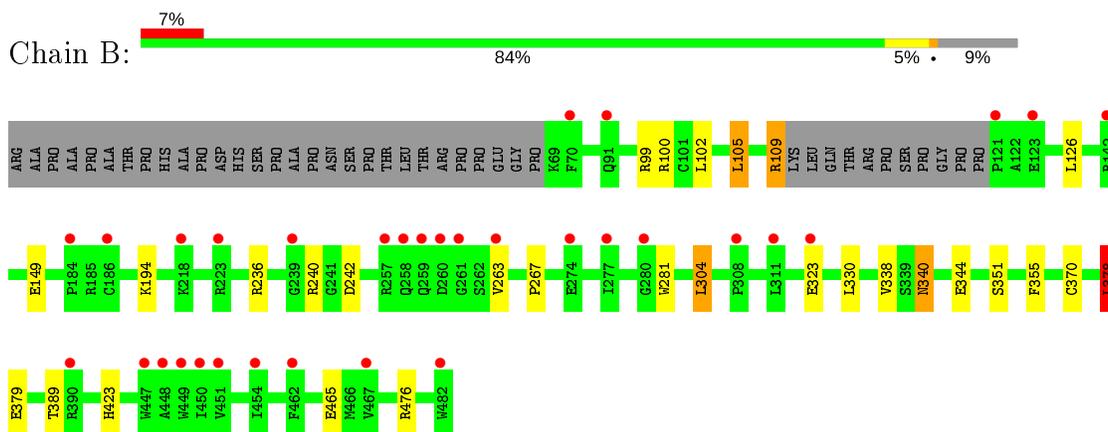
4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.81Å　　106.51Å　　156.95Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	88.13　–　1.79 48.34　–　1.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (88.13-1.79) 98.7 (48.34-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.34 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.165　,　0.192 0.165　,　0.192	Depositor DCC
R_{free} test set	4577 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.6	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6952	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, CAS, M48, ACT, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.53	0/3303	0.64	0/4497
2	B	0.51	0/3298	0.64	2/4491 (0.0%)
All	All	0.52	0/6601	0.64	2/8988 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	378	LEU	CA-CB-CG	5.17	127.20	115.30
2	B	304	LEU	CB-CG-CD2	-5.10	102.32	111.00

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	3223	0	3127	37	0
2	B	3209	0	3118	15	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
4	A	17	0	15	1	0
4	B	17	0	15	0	0
5	A	23	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	23	0	20	4	0
6	A	8	0	6	0	0
6	B	8	0	6	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	1	0	0	0	0
9	A	177	0	0	2	0
9	B	148	0	0	2	0
All	All	6952	0	6403	51	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 4.

All (51) 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:384:CAS:AS	1:A:384:CAS:SG	2.51	1.27
1:A:236:ARG:HG3	1:A:236:ARG:HH11	1.09	1.16
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.27	0.96
1:A:236:ARG:HG3	1:A:236:ARG:NH1	1.82	0.84
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.70	0.74
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.01	0.73
1:A:236:ARG:CG	1:A:236:ARG:HH11	1.95	0.71
2:B:236:ARG:HD2	2:B:242:ASP:OD1	1.91	0.70
1:A:109:ARG:HH11	1:A:109:ARG:HA	1.57	0.69
9:A:2001:HOH:O	2:B:109:ARG:HG3	1.94	0.68
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.28	0.63
1:A:294:LEU:HD13	1:A:304:LEU:HD13	1.79	0.62
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.58	0.59
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.85	0.58
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.84	0.58
1:A:338:VAL:HG21	5:A:801:M48:C07	2.34	0.57
2:B:338:VAL:HG21	5:B:801:M48:C07	2.36	0.56
2:B:281:TRP:HB2	2:B:304:LEU:HD21	1.87	0.55
1:A:107:LEU:HD21	5:A:801:M48:H25	1.88	0.55
1:A:109:ARG:NH1	1:A:109:ARG:HA	2.20	0.54
1:A:410:HIS:ND1	9:A:2143:HOH:O	2.33	0.53
1:A:294:LEU:HD13	1:A:304:LEU:CD1	2.38	0.52
1:A:355:PHE:HE1	5:A:801:M48:H06	1.74	0.52
2:B:378:LEU:HB2	9:B:2118:HOH:O	2.09	0.52
2:B:355:PHE:HE1	5:B:801:M48:H06	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD22	2:B:465:GLU:HB3	1.91	0.51
1:A:240:ARG:HD2	1:A:241:GLY:O	2.10	0.51
1:A:384:CAS:CB	1:A:384:CAS:AS	3.19	0.51
1:A:257:ARG:CG	1:A:257:ARG:NH1	2.74	0.50
1:A:138:SER:O	1:A:141:LYS:HE3	2.10	0.50
5:B:801:M48:H151	9:B:2147:HOH:O	2.12	0.50
1:A:83:TYR:HE2	2:B:109:ARG:HH21	1.60	0.49
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.94	0.49
1:A:384:CAS:CE2	1:A:384:CAS:SG	3.01	0.48
1:A:236:ARG:HG2	1:A:242:ASP:OD1	2.13	0.48
1:A:340:ASN:HD22	1:A:340:ASN:H	1.62	0.48
1:A:240:ARG:HD3	1:A:298:PRO:CG	2.44	0.47
2:B:344:GLU:OE1	2:B:476:ARG:NH2	2.49	0.46
3:B:500:HEM:HBA2	5:B:801:M48:C09	2.45	0.46
1:A:392:THR:HB	2:B:423:HIS:HB2	1.97	0.45
2:B:263:VAL:HG11	2:B:267:PRO:HA	1.99	0.45
1:A:465:GLU:HB3	2:B:105:LEU:HD22	1.99	0.44
2:B:370:CYS:SG	2:B:378:LEU:HD13	2.56	0.44
2:B:236:ARG:HD3	2:B:351:SER:HB3	1.99	0.44
1:A:264:ARG:HD3	1:A:285:ASN:O	2.18	0.43
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.93	0.43
1:A:472:SER:HA	1:A:473:PRO:C	2.38	0.43
3:B:500:HEM:HBC2	3:B:500:HEM:CMC	2.48	0.42
2:B:340:ASN:HD22	2:B:340:ASN:H	1.67	0.42
1:A:158:GLU:OE2	1:A:166:HIS:HD2	2.02	0.42
1:A:449:TRP:HA	4:A:600:H4B:N1	2.35	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	400/443 (90%)	393 (98%)	7 (2%)	0	100	100
2	B	399/443 (90%)	389 (98%)	10 (2%)	0	100	100
All	All	799/886 (90%)	782 (98%)	17 (2%)	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	343/375 (92%)	330 (96%)	13 (4%)	33	18
2	B	343/376 (91%)	328 (96%)	15 (4%)	28	14
All	All	686/751 (91%)	658 (96%)	28 (4%)	30	16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	102	LEU
1	A	109	ARG
1	A	125	LEU
1	A	146	GLN
1	A	236	ARG
1	A	257	ARG
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	458	LEU
1	A	468	ASN
2	B	99	ARG
2	B	100	ARG
2	B	102	LEU
2	B	105	LEU
2	B	109	ARG

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Mol	Chain	Res	Type
2	B	126	LEU
2	B	149	GLU
2	B	194	LYS
2	B	240	ARG
2	B	323	GLU
2	B	330	LEU
2	B	340	ASN
2	B	378	LEU
2	B	379	GLU
2	B	389	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	153	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
2	B	191	GLN
2	B	222	ASN
2	B	225	ASN
2	B	340	ASN
2	B	376	ASN
2	B	405	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	#$|Z| > 2$
1	CAS	A	384	1	5,8,9	1.26	1 (20%)	1,9,11	0.14	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
1	CAS	A	384	1	-	0/0/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	CAS	AS-CE1	2.36	2.02	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	#$|Z| > 2$
3	HEM	A	500	1	27,50,50	1.05	3 (11%)	17,82,82	1.51	3 (17%)
3	HEM	B	500	2	27,50,50	1.04	2 (7%)	17,82,82	1.86	3 (17%)
4	H4B	B	600	-	16,18,18	1.01	1 (6%)	11,26,26	2.51	6 (54%)
7	GOL	A	880	-	5,5,5	0.22	0	5,5,5	0.57	0
5	M48	B	801	-	25,25,25	0.97	0	30,33,33	1.02	1 (3%)
5	M48	A	801	-	25,25,25	0.99	1 (4%)	30,33,33	1.26	3 (10%)
6	ACT	B	861	-	1,3,3	1.97	0	0,3,3	0.00	-
6	ACT	A	861	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
7	GOL	B	880	-	5,5,5	0.20	0	5,5,5	0.75	0
4	H4B	A	600	-	16,18,18	1.01	0	11,26,26	2.80	6 (54%)
6	ACT	B	860	-	1,3,3	1.10	0	0,3,3	0.00	-
6	ACT	A	860	-	1,3,3	0.89	0	0,3,3	0.00	-

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
3	HEM	A	500	1	-	0/6/54/54	-
3	HEM	B	500	2	-	0/6/54/54	-
4	H4B	B	600	-	-	0/8/17/17	0/2/2/2
7	GOL	A	880	-	-	0/4/4/4	-
5	M48	B	801	-	-	3/8/8/8	0/3/3/3
5	M48	A	801	-	-	5/8/8/8	0/3/3/3
7	GOL	B	880	-	-	0/4/4/4	-
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C4A-NA	2.96	1.42	1.36
3	B	500	HEM	C4D-C3D	2.79	1.48	1.42
3	B	500	HEM	C4A-NA	2.65	1.41	1.36
5	A	801	M48	C02-N01	2.28	1.36	1.33
6	A	861	ACT	CH3-C	2.06	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C4D-C3D	2.05	1.47	1.42
3	A	500	HEM	C1D-ND	2.04	1.40	1.36
4	B	600	H4B	C4-C4A	-2.00	1.38	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	HEM	CBA-CAA-C2A	-5.38	102.56	112.49
4	A	600	H4B	C4-C4A-C8A	4.77	118.81	114.57
4	B	600	H4B	C4-C4A-C8A	3.75	117.90	114.57
4	A	600	H4B	C4-N3-C2	3.74	121.88	115.93
4	A	600	H4B	N3-C2-N1	-3.68	119.64	125.42
4	B	600	H4B	N3-C2-N1	-3.64	119.71	125.42
4	A	600	H4B	C4-C4A-N5	3.42	121.99	119.12
4	B	600	H4B	C4-C4A-N5	3.39	121.96	119.12
4	B	600	H4B	C4-N3-C2	3.22	121.04	115.93
4	A	600	H4B	N2-C2-N3	3.07	122.03	117.25
3	A	500	HEM	CBA-CAA-C2A	-3.00	106.96	112.49
4	A	600	H4B	C2-N1-C8A	2.96	121.17	114.54
3	A	500	HEM	CAA-CBA-CGA	2.94	117.61	112.67
3	B	500	HEM	C1D-C2D-C3D	-2.72	105.11	107.00
4	B	600	H4B	C2-N1-C8A	2.71	120.61	114.54
5	B	801	M48	C24-C23-C22	-2.71	119.77	123.29
5	A	801	M48	C24-C23-C22	-2.55	119.97	123.29
3	A	500	HEM	CMC-C2C-C3C	2.48	129.32	124.68
3	B	500	HEM	CMC-C2C-C3C	2.38	129.13	124.68
5	A	801	M48	C05-C10-N01	-2.33	118.80	122.26
4	B	600	H4B	N2-C2-N3	2.12	120.55	117.25
5	A	801	M48	C12-N13-C14	2.06	123.15	113.45

There are no chirality outliers.
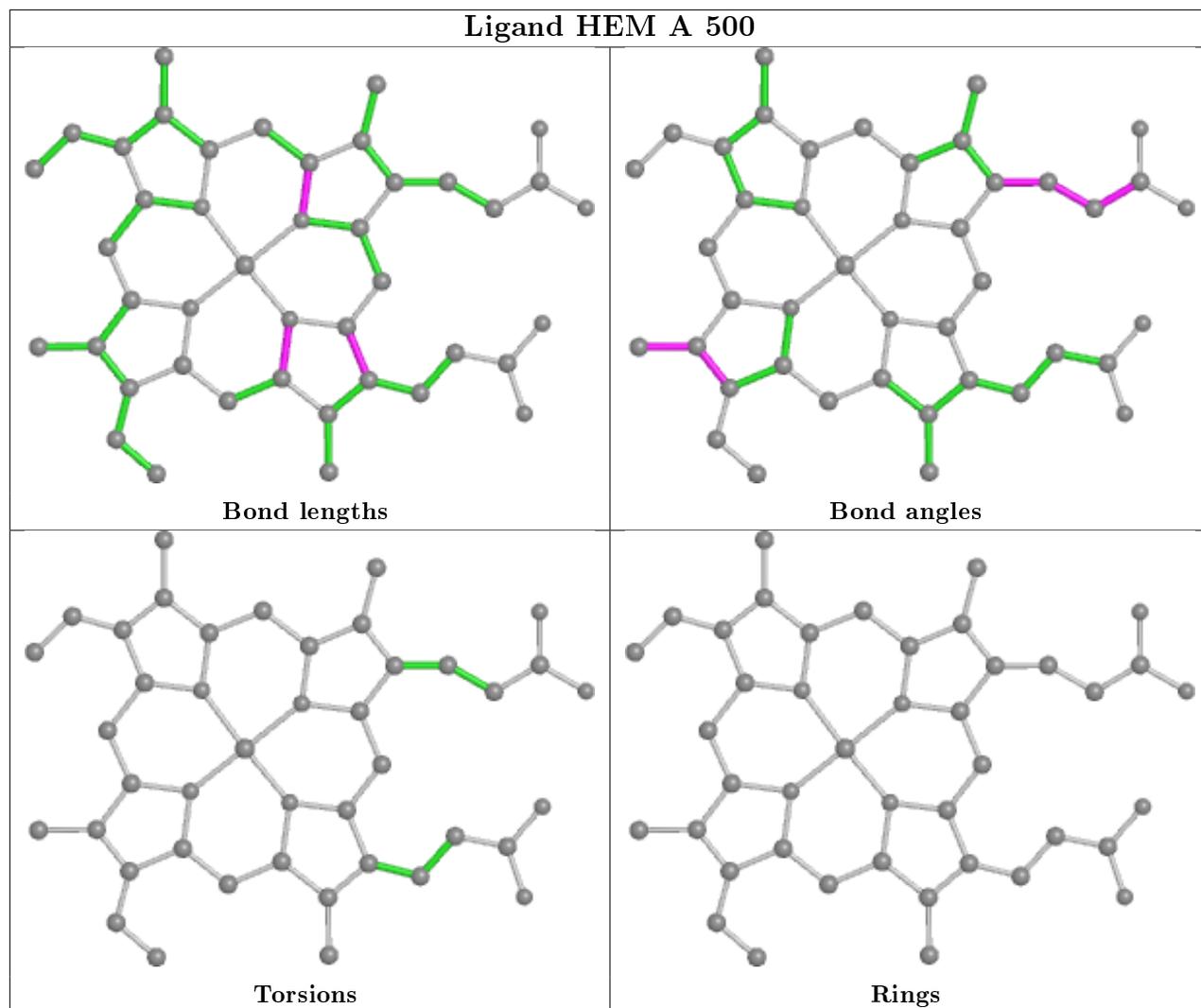
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	M48	N13-C14-C15-C21
5	A	801	M48	N13-C14-C15-C21
5	A	801	M48	C11-C12-N13-C14
5	B	801	M48	C11-C12-N13-C14
5	A	801	M48	C15-C14-N13-C12
5	B	801	M48	C15-C14-N13-C12
5	A	801	M48	C07-C08-C11-C12
5	A	801	M48	C09-C08-C11-C12

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	HEM	2	0
5	B	801	M48	4	0
5	A	801	M48	3	0
4	A	600	H4B	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand M48 B 801

Bond lengths

Bond angles

Torsions

Rings

Ligand M48 A 801

Bond lengths

Bond angles

Torsions

Rings
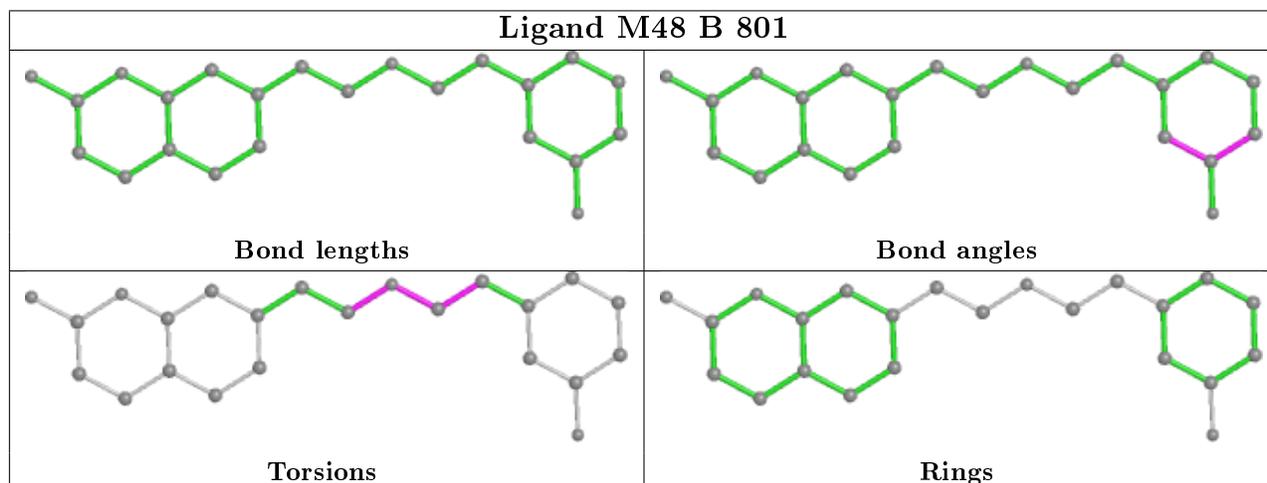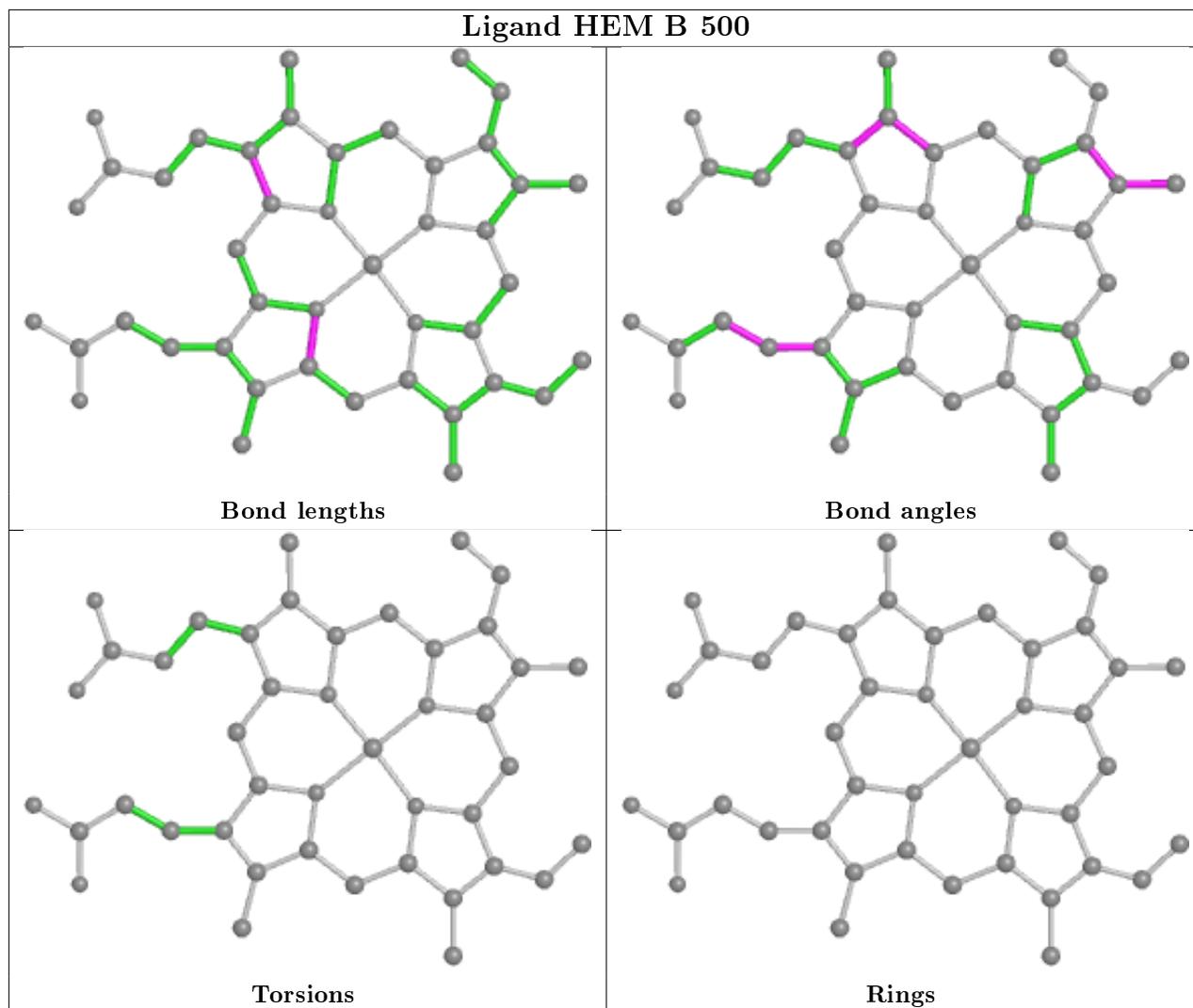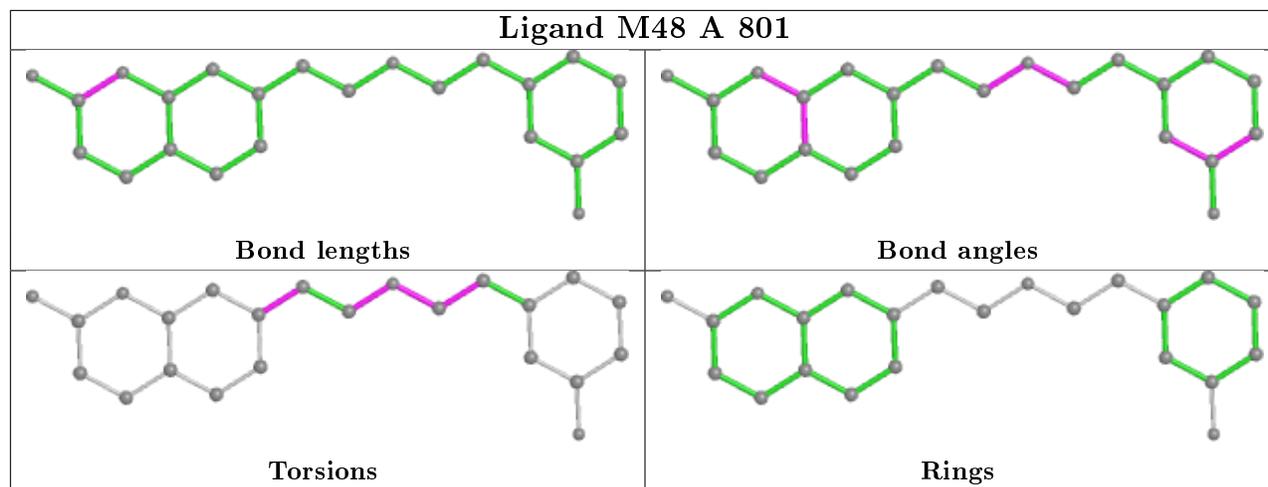
5.7 Other polymers (i)

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	404/443 (91%)	0.75	47 (11%)	4	3	31, 42, 68, 91	0
2	B	403/443 (90%)	0.49	32 (7%)	12	9	31, 44, 69, 99	0
All	All	807/886 (91%)	0.62	79 (9%)	7	5	31, 43, 69, 99	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	GLY	11.0
1	A	160	ALA	8.1
2	B	259	GLN	7.4
1	A	239	GLY	6.9
1	A	123	GLU	5.2
1	A	259	GLN	5.0
2	B	261	GLY	4.9
2	B	70	PHE	4.6
1	A	450	ILE	4.3
1	A	157	ALA	4.1
2	B	223	ARG	4.1
1	A	448	ALA	4.1
1	A	126	LEU	4.0
1	A	238	PRO	4.0
1	A	122	ALA	4.0
1	A	69	LYS	3.9
2	B	447	TRP	3.8
1	A	146	GLN	3.8
1	A	91	GLN	3.7
1	A	447	TRP	3.7
2	B	239	GLY	3.7
1	A	156	GLU	3.7
1	A	449	TRP	3.6
1	A	187	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	448	ALA	3.2
1	A	153	GLN	3.2
2	B	123	GLU	3.2
2	B	449	TRP	3.2
2	B	451	VAL	3.2
2	B	260	ASP	3.1
1	A	260	ASP	3.1
1	A	451	VAL	3.1
1	A	161	SER	3.0
2	B	323	GLU	3.0
1	A	461	VAL	3.0
1	A	462	PHE	2.9
1	A	257	ARG	2.9
2	B	462	PHE	2.9
2	B	257	ARG	2.8
1	A	281	TRP	2.8
2	B	121	PRO	2.8
1	A	155	VAL	2.7
2	B	467	VAL	2.7
1	A	186	CYS	2.6
1	A	284	GLY	2.6
1	A	180	TRP	2.6
2	B	184	PRO	2.6
1	A	299	ASP	2.5
2	B	311	LEU	2.5
2	B	277	ILE	2.5
1	A	261	GLY	2.5
2	B	274	GLU	2.4
2	B	450	ILE	2.4
1	A	355	PHE	2.4
1	A	109	ARG	2.3
2	B	258	GLN	2.4
2	B	91	GLN	2.3
2	B	142	ARG	2.3
2	B	263	VAL	2.3
1	A	104	SER	2.3
1	A	124	GLN	2.2
2	B	186	CYS	2.2
1	A	162	THR	2.2
1	A	276	CYS	2.2
2	B	390	ARG	2.2
2	B	482	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	280	GLY	2.1
1	A	188	GLY	2.1
1	A	130	ARG	2.1
1	A	306	VAL	2.1
1	A	277	ILE	2.1
2	B	308	PRO	2.1
1	A	107	LEU	2.1
2	B	218	LYS	2.1
1	A	262	SER	2.1
2	B	454	ILE	2.1
1	A	150	GLU	2.0
1	A	158	GLU	2.0
1	A	390	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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.
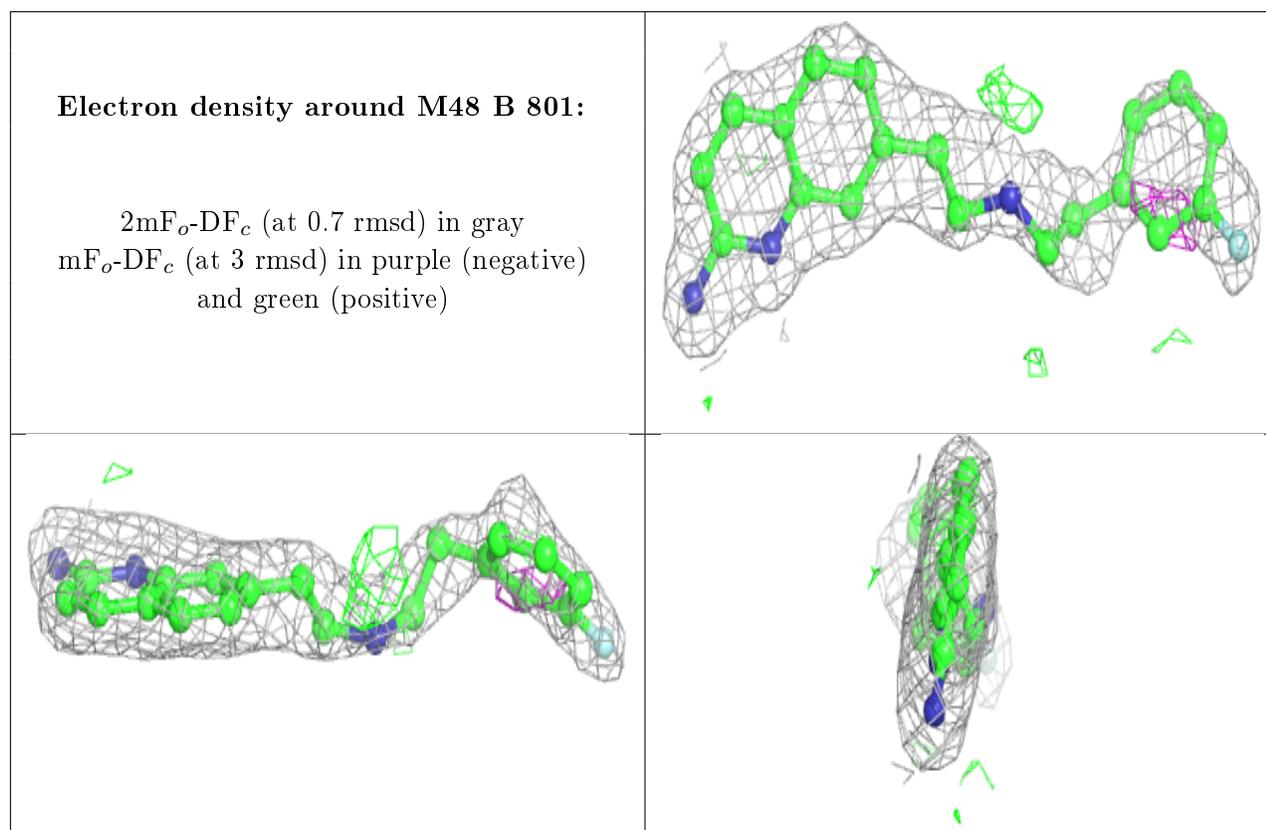
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CAS	A	384	9/10	0.89	0.14	40,41,81,87	0

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
6	ACT	B	861	4/4	0.84	0.20	48,52,55,55	0
7	GOL	A	880	6/6	0.89	0.19	54,62,66,69	0
7	GOL	B	880	6/6	0.93	0.17	52,59,62,64	0
5	M48	B	801	23/23	0.94	0.15	39,47,89,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	M48	A	801	23/23	0.94	0.16	34,47,94,95	0
4	H4B	B	600	17/17	0.95	0.13	35,38,41,41	0
4	H4B	A	600	17/17	0.95	0.15	33,38,40,42	0
6	ACT	B	860	4/4	0.96	0.11	45,52,53,57	0
6	ACT	A	860	4/4	0.96	0.12	46,50,52,56	0
3	HEM	A	500	43/43	0.97	0.18	30,34,42,44	0
6	ACT	A	861	4/4	0.97	0.11	44,46,46,46	0
3	HEM	B	500	43/43	0.97	0.12	33,36,43,48	0
8	ZN	A	1483	1/1	0.99	0.06	40,40,40,40	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.
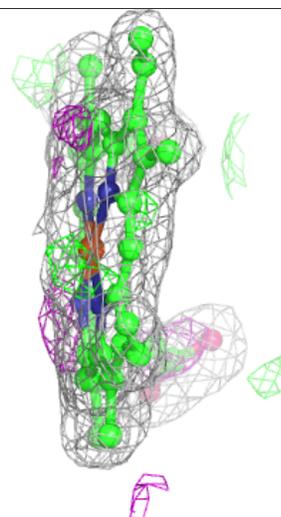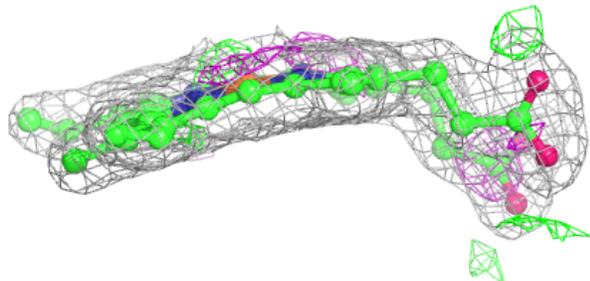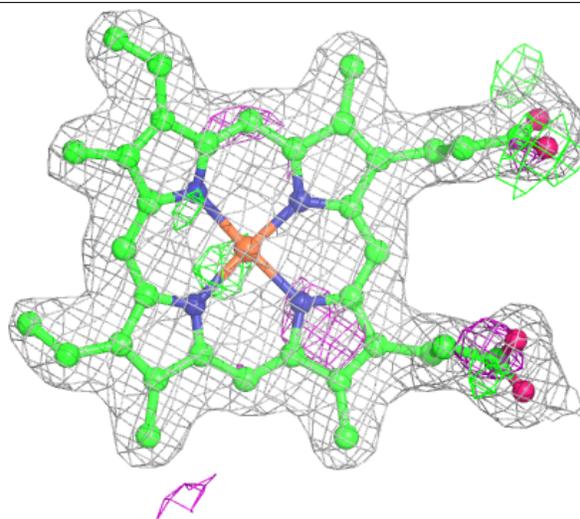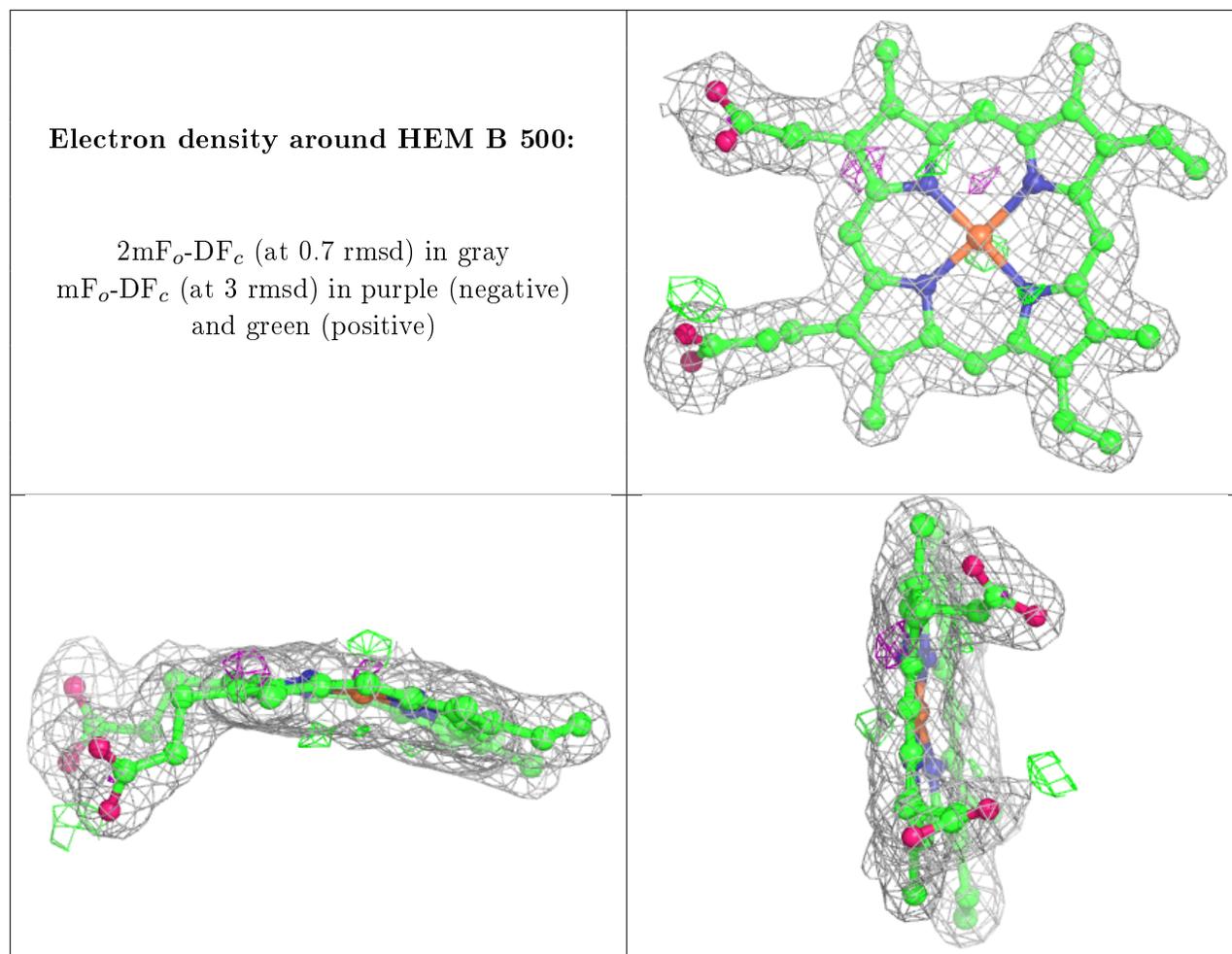

Electron density around M48 B 801:

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

Electron density around M48 A 801:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
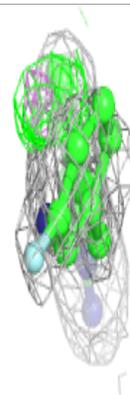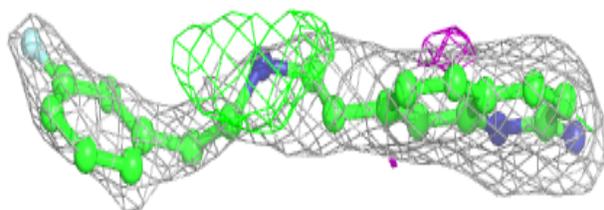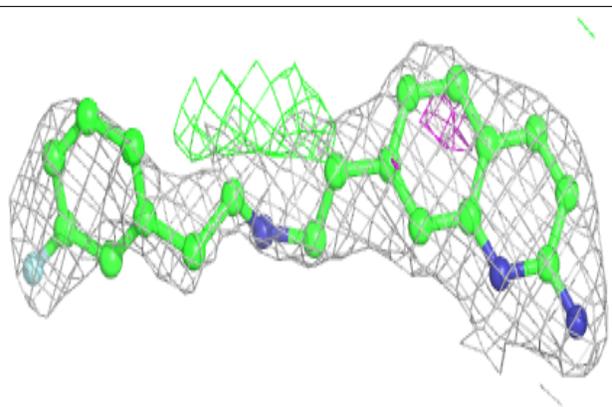
Electron density around HEM A 500:

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

Electron density around HEM B 500:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.