



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 06:10 PM EDT

PDB ID : 4CAR
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 7-((3-Fluorophenethylamino)methyl)quinolin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-10-08
Resolution : 2.05 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

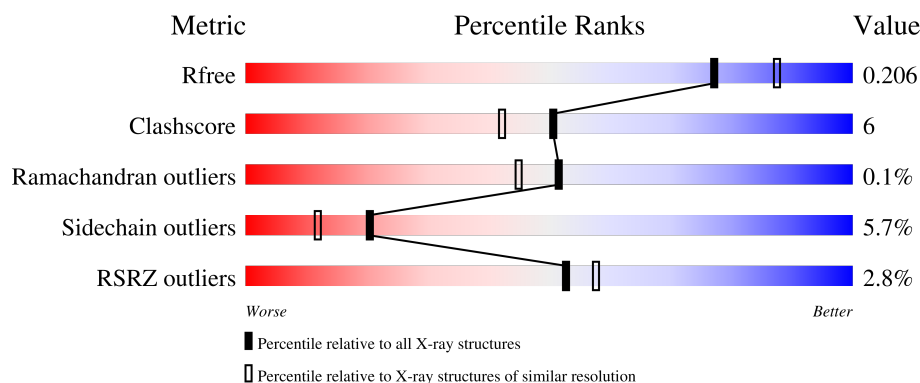
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

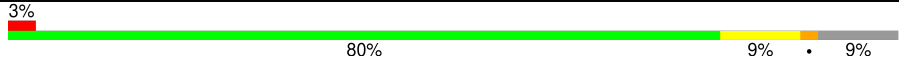

The reported resolution of this entry is 2.05 Å.

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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	443	
1	B	443	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7031 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 NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	405	Total	As	C	N	O	S	0	0	0
			3229	1	2054	569	589	16			

There are 2 discrepancies between the modelled and reference sequences:

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

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



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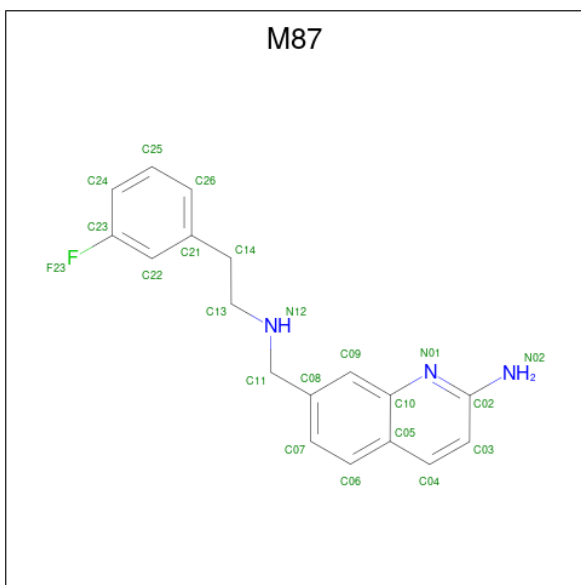
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 4 is 7-[[2-(3-fluorophenyl)ethylamino]methyl]quinolin-2-amine (three-letter code: M87) (formula: $C_{18}H_{18}FN_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			22	18	1	3		
4	B	1	Total	C	F	N	0	0
			22	18	1	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

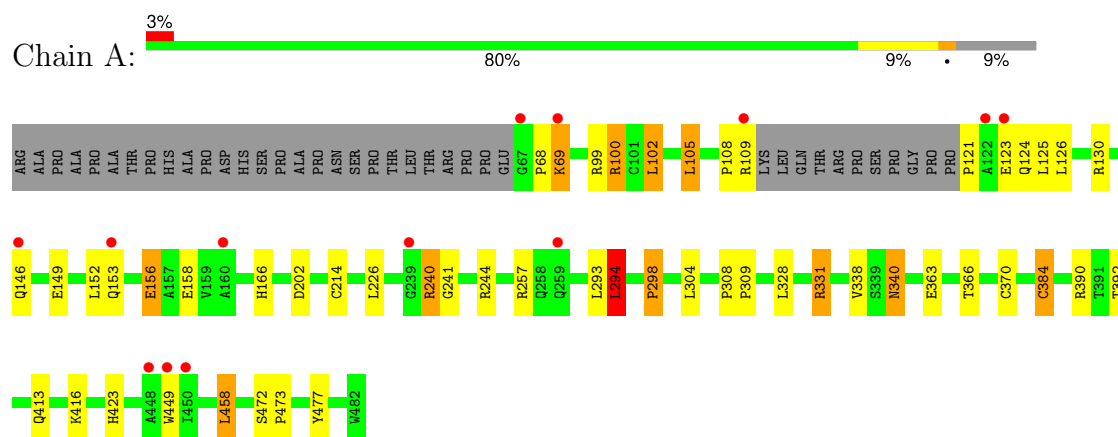
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	211	Total	O	0	0
			211	211		
8	B	175	Total	O	0	0
			175	175		

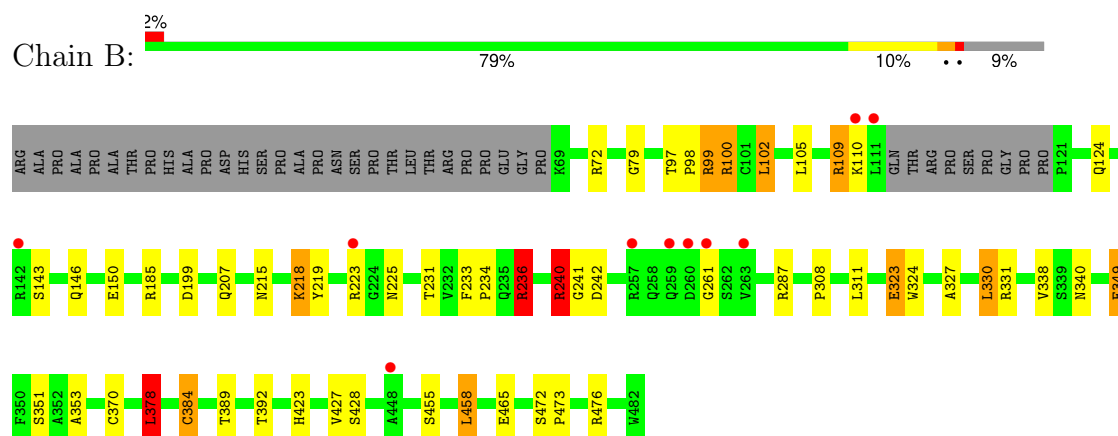
3 Residue-property plots [i](#)

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: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



• Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.76Å 106.30Å 156.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.05 48.28 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.33-2.05) 98.5 (48.28-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.154 , 0.198 0.165 , 0.206	Depositor DCC
R_{free} test set	3010 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7031	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: M87, GOL, CAS, ACT, H4B, HEM, ZN

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	0.99	0/3303	1.01	8/4497 (0.2%)
1	B	0.97	3/3308 (0.1%)	1.00	12/4502 (0.3%)
All	All	0.98	3/6611 (0.0%)	1.01	20/8999 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	GLY	C-O	-5.87	1.14	1.23
1	B	349	GLU	CD-OE2	-5.62	1.19	1.25
1	B	428	SER	CB-OG	5.37	1.49	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	B	240	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	240	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	240	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	B	185	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	331	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	100	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	378	LEU	CB-CG-CD1	6.40	121.89	111.00
1	A	331	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	330	LEU	CB-CG-CD1	6.00	121.21	111.00
1	A	244	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	72	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	294	LEU	CB-CG-CD1	5.73	120.74	111.00
1	B	242	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	199	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	458	LEU	CB-CG-CD1	5.51	120.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	LEU	CB-CG-CD2	5.42	120.21	111.00
1	B	236	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	476	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	202	ASP	CB-CG-OD1	5.05	122.85	118.30

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	3223	0	3127	41	0
1	B	3229	0	3141	31	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	22	0	18	2	0
4	B	22	0	18	1	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	211	0	0	4	0
8	B	175	0	0	3	0
All	All	7031	0	6422	74	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 6.

All (74) 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:SG	1:A:384:CAS:AS	2.46	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:CAS:SG	1:B:384:CAS:AS	2.59	1.21
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.61	0.83
1:A:108:PRO:HD3	8:A:2029:HOH:O	1.89	0.72
1:A:126:LEU:HD23	1:A:130:ARG:NH2	2.08	0.67
1:B:240:ARG:HD2	1:B:241:GLY:O	1.95	0.66
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.27	0.65
1:A:108:PRO:CD	8:A:2029:HOH:O	2.44	0.65
1:A:384:CAS:AS	1:A:384:CAS:CB	3.05	0.64
1:B:384:CAS:SG	1:B:384:CAS:CE1	2.87	0.63
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.65	0.61
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.42	0.60
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.82	0.59
1:A:152:LEU:O	1:A:156:GLU:HG2	2.02	0.59
1:A:69:LYS:HA	1:A:69:LYS:HE2	1.86	0.58
1:A:294:LEU:HD13	1:A:304:LEU:HD12	1.88	0.55
1:B:384:CAS:AS	1:B:384:CAS:CB	3.15	0.55
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.88	0.54
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.38	0.54
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.89	0.53
1:A:240:ARG:HD2	1:A:241:GLY:O	2.08	0.53
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.74	0.53
1:B:323:GLU:H	1:B:323:GLU:CD	2.12	0.53
1:A:240:ARG:CD	1:A:241:GLY:O	2.57	0.52
1:B:427:VAL:HG23	8:B:2145:HOH:O	2.09	0.52
1:B:324:TRP:O	1:B:327:ALA:HB3	2.10	0.52
1:B:378:LEU:HB2	8:B:2134:HOH:O	2.10	0.52
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.93	0.51
2:A:500:HEM:HBC2	2:A:500:HEM:HMC1	1.93	0.51
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.93	0.50
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.94	0.50
1:A:158:GLU:OE2	1:A:166:HIS:HD2	1.95	0.50
1:A:449:TRP:HA	3:A:600:H4B:N1	2.27	0.49
1:A:294:LEU:HD13	1:A:304:LEU:CD1	2.42	0.49
2:A:500:HEM:HBC2	2:A:500:HEM:CMC	2.43	0.49
1:B:97:THR:HB	1:B:98:PRO:HD2	1.95	0.48
1:A:68:PRO:O	1:B:109:ARG:NH2	2.47	0.48
1:A:338:VAL:HG21	4:A:800:M87:C07	2.45	0.47
1:B:146:GLN:O	1:B:150:GLU:HG3	2.14	0.47
1:B:218:LYS:HD3	1:B:219:TYR:N	2.29	0.47
1:A:392:THR:HB	1:B:423:HIS:HB2	1.97	0.47
1:A:472:SER:HA	1:A:473:PRO:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HG3	1:B:349:GLU:HB2	1.98	0.46
1:A:149:GLU:O	1:A:153:GLN:HG3	2.16	0.46
1:A:214:CYS:SG	8:A:2083:HOH:O	2.34	0.46
1:A:366:THR:O	1:A:370:CYS:HB2	2.16	0.46
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.63	0.46
1:A:69:LYS:HA	1:A:69:LYS:CE	2.46	0.46
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.98	0.45
1:A:477:TYR:OH	2:A:500:HEM:O2D	2.27	0.45
1:A:384:CAS:AS	1:A:384:CAS:HB2	2.78	0.44
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.98	0.44
8:A:2001:HOH:O	1:B:109:ARG:HG2	2.17	0.44
1:B:384:CAS:AS	1:B:384:CAS:HB2	2.78	0.43
1:A:413:GLN:O	1:A:416:LYS:HE3	2.17	0.43
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.49	0.43
1:A:423:HIS:HB2	1:B:392:THR:HB	2.00	0.43
1:A:105:LEU:HD23	1:A:105:LEU:N	2.34	0.43
1:A:340:ASN:H	1:A:340:ASN:HD22	1.67	0.43
1:B:231:THR:O	1:B:353:ALA:HA	2.19	0.43
1:A:100:ARG:CZ	1:A:102:LEU:HD22	2.49	0.43
1:B:287:ARG:HD3	8:B:2110:HOH:O	2.18	0.43
1:A:363:GLU:OE1	4:A:800:M87:N01	2.52	0.43
1:B:455:SER:CB	1:B:458:LEU:HD22	2.48	0.42
1:A:100:ARG:NH1	1:A:102:LEU:HD22	2.35	0.42
1:A:240:ARG:HD3	1:A:298:PRO:CG	2.50	0.42
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.95	0.42
2:B:500:HEM:HBC2	2:B:500:HEM:HMC1	2.02	0.42
1:A:126:LEU:HD23	1:A:130:ARG:HH21	1.83	0.41
1:A:121:PRO:O	1:A:124:GLN:HB3	2.20	0.41
1:A:240:ARG:HD3	1:A:241:GLY:O	2.20	0.41
1:B:215:ASN:O	1:B:218:LYS:HD3	2.21	0.41
1:B:338:VAL:HG21	4:B:800:M87:C07	2.51	0.40
1:B:472:SER:HA	1:B:473:PRO:C	2.41	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	400/443 (90%)	387 (97%)	13 (3%)	0	100	100
1	B	400/443 (90%)	387 (97%)	12 (3%)	1 (0%)	41	31
All	All	800/886 (90%)	774 (97%)	25 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	GLY

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	343/375 (92%)	325 (95%)	18 (5%)	23	14
1	B	344/375 (92%)	323 (94%)	21 (6%)	18	10
All	All	687/750 (92%)	648 (94%)	39 (6%)	20	12

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	109	ARG
1	A	123	GLU
1	A	125	LEU
1	A	146	GLN
1	A	156	GLU
1	A	226	LEU

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Mol	Chain	Res	Type
1	A	293	LEU
1	A	294	LEU
1	A	298	PRO
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	458	LEU
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	110	LYS
1	B	124	GLN
1	B	143	SER
1	B	207	GLN
1	B	218	LYS
1	B	223	ARG
1	B	225	ASN
1	B	236	ARG
1	B	240	ARG
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	389	THR
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	178	GLN
1	B	222	ASN
1	B	225	ASN

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Mol	Chain	Res	Type
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	CAS	B	384	1	5,8,9	1.84	2 (40%)	1,9,11	0.66	0
1	CAS	A	384	1	5,8,9	1.40	1 (20%)	1,9,11	0.70	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	B	384	1	-	0/0/7/9	-
1	CAS	A	384	1	-	0/0/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE2	3.19	2.04	1.96
1	A	384	CAS	AS-CE2	2.88	2.03	1.96
1	B	384	CAS	AS-CE1	2.30	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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	384	CAS	4	0
1	A	384	CAS	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	H4B	B	600	-	16,18,18	1.32	3 (18%)	14,26,26	2.41	5 (35%)
5	ACT	A	860	-	3,3,3	0.73	0	3,3,3	1.05	0
2	HEM	A	500	1	42,50,50	1.29	3 (7%)	46,82,82	2.27	14 (30%)
2	HEM	B	500	1	42,50,50	1.66	8 (19%)	46,82,82	2.11	15 (32%)
5	ACT	A	861	-	3,3,3	0.93	0	3,3,3	0.56	0
5	ACT	B	860	-	3,3,3	0.93	0	3,3,3	0.80	0
5	ACT	B	861	-	3,3,3	0.97	0	3,3,3	0.41	0
4	M87	B	800	-	24,24,24	1.17	1 (4%)	30,32,32	1.36	6 (20%)
6	GOL	A	880	-	5,5,5	0.82	0	5,5,5	1.55	2 (40%)
6	GOL	B	880	-	5,5,5	0.71	0	5,5,5	1.06	0
3	H4B	A	600	-	16,18,18	1.24	1 (6%)	14,26,26	2.58	7 (50%)
4	M87	A	800	-	24,24,24	1.32	3 (12%)	30,32,32	1.74	6 (20%)

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	H4B	B	600	-	-	0/8/17/17	0/2/2/2
2	HEM	A	500	1	-	0/12/54/54	-
2	HEM	B	500	1	-	1/12/54/54	-
4	M87	B	800	-	-	0/7/7/7	0/3/3/3
6	GOL	A	880	-	-	0/4/4/4	-
6	GOL	B	880	-	-	0/4/4/4	-
3	H4B	A	600	-	-	2/8/17/17	0/2/2/2
4	M87	A	800	-	-	0/7/7/7	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1B-NB	-5.82	1.30	1.40
3	B	600	H4B	C4A-C8A	-3.60	1.34	1.41
2	B	500	HEM	C3B-C4B	3.58	1.51	1.44
2	A	500	HEM	C1B-NB	-3.53	1.34	1.40
4	B	800	M87	C02-N01	3.28	1.37	1.33
2	B	500	HEM	C1D-ND	-3.07	1.32	1.38
4	A	800	M87	C10-N01	2.70	1.41	1.37
2	A	500	HEM	C3D-C2D	-2.50	1.31	1.36
2	B	500	HEM	C4B-NB	-2.40	1.34	1.38
2	B	500	HEM	C1D-C2D	2.36	1.49	1.44
3	A	600	H4B	C8A-N1	-2.34	1.30	1.34
2	B	500	HEM	CHB-C1B	2.31	1.40	1.34
2	A	500	HEM	CMA-C3A	-2.14	1.47	1.51
4	A	800	M87	C24-C23	2.10	1.41	1.37
4	A	800	M87	C02-N02	-2.08	1.29	1.35
2	B	500	HEM	C4D-C3D	2.07	1.48	1.45
3	B	600	H4B	C7-C6	2.06	1.54	1.52
3	B	600	H4B	C6-N5	-2.02	1.42	1.45
2	B	500	HEM	C3C-C4C	2.00	1.44	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	H4B	C8A-C4A-C4	6.79	120.68	114.50
2	A	500	HEM	C4D-ND-C1D	-5.29	98.94	105.21
3	B	600	H4B	C8A-C4A-C4	5.12	119.16	114.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	M87	F23-C23-C22	-4.47	111.93	118.28
2	A	500	HEM	C3D-C4D-ND	4.34	114.94	110.17
2	A	500	HEM	CAD-C3D-C4D	4.32	132.23	124.70
2	A	500	HEM	CHD-C1D-C2D	-4.21	118.37	125.03
3	B	600	H4B	C11-C10-C9	-4.12	107.06	112.11
2	B	500	HEM	CHC-C4B-NB	4.03	128.77	124.44
2	A	500	HEM	C2D-C1D-ND	4.02	114.55	109.90
4	A	800	M87	F23-C23-C24	3.85	124.72	118.55
2	B	500	HEM	CAD-C3D-C4D	3.76	131.26	124.70
2	B	500	HEM	CBA-CAA-C2A	-3.71	106.29	112.54
2	B	500	HEM	C1B-NB-C4B	3.65	109.53	105.21
2	A	500	HEM	CHC-C4B-NB	3.62	128.33	124.44
2	B	500	HEM	C4B-C3B-C2B	-3.59	103.98	107.28
2	B	500	HEM	CHA-C4D-C3D	-3.58	118.62	125.23
4	A	800	M87	C14-C21-C22	-3.54	114.60	120.54
3	B	600	H4B	C2-N1-C8A	3.49	122.88	114.59
2	B	500	HEM	CHD-C1D-C2D	-3.47	119.55	125.03
2	A	500	HEM	CMA-C3A-C4A	-3.47	123.38	128.46
3	A	600	H4B	N2-C2-N3	3.38	122.29	117.22
3	B	600	H4B	N2-C2-N3	3.15	121.95	117.22
2	A	500	HEM	CBA-CAA-C2A	-3.13	107.28	112.54
4	B	800	M87	C11-C08-C09	-3.13	115.90	121.46
2	B	500	HEM	CHD-C1D-ND	2.98	127.64	124.44
2	A	500	HEM	CHA-C4D-C3D	-2.96	119.78	125.23
3	B	600	H4B	N1-C2-N3	-2.93	121.00	125.48
2	B	500	HEM	CHA-C4D-ND	2.92	127.99	124.37
2	A	500	HEM	C4C-CHD-C1D	-2.90	118.73	122.56
2	A	500	HEM	CMD-C2D-C1D	2.86	129.51	125.03
2	B	500	HEM	C3B-C4B-NB	-2.80	107.46	109.47
2	A	500	HEM	CAD-C3D-C2D	-2.78	122.66	127.87
2	B	500	HEM	CMD-C2D-C1D	2.73	129.31	125.03
3	A	600	H4B	O9-C9-C10	2.68	114.24	109.14
2	A	500	HEM	O2D-CGD-CBD	2.65	122.36	114.00
4	B	800	M87	C13-C14-C21	-2.55	107.07	112.83
4	A	800	M87	N02-C02-N01	-2.51	116.16	118.24
2	A	500	HEM	C4A-C3A-C2A	2.48	108.72	107.00
4	A	800	M87	C04-C03-C02	-2.46	117.57	119.49
6	A	880	GOL	C3-C2-C1	2.38	120.51	111.80
3	A	600	H4B	C4A-C4-N3	-2.36	117.94	123.91
2	B	500	HEM	CMB-C2B-C1B	2.36	128.72	125.03
4	B	800	M87	C03-C04-C05	-2.30	117.40	120.84
3	A	600	H4B	C2-N3-C4	2.29	119.15	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	C2D-C1D-ND	2.28	112.53	109.90
4	B	800	M87	F23-C23-C22	-2.24	115.10	118.28
4	B	800	M87	F23-C23-C24	2.20	122.08	118.55
2	B	500	HEM	CMC-C2C-C3C	2.20	129.08	124.68
2	B	500	HEM	O2A-CGA-CBA	2.19	120.92	114.00
6	A	880	GOL	O1-C1-C2	-2.17	100.61	110.38
4	A	800	M87	C13-C14-C21	-2.14	108.01	112.83
4	B	800	M87	C09-C10-C05	2.11	121.41	119.20
3	A	600	H4B	C11-C10-C9	2.04	114.61	112.11
3	A	600	H4B	N2-C2-N1	-2.02	114.20	117.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

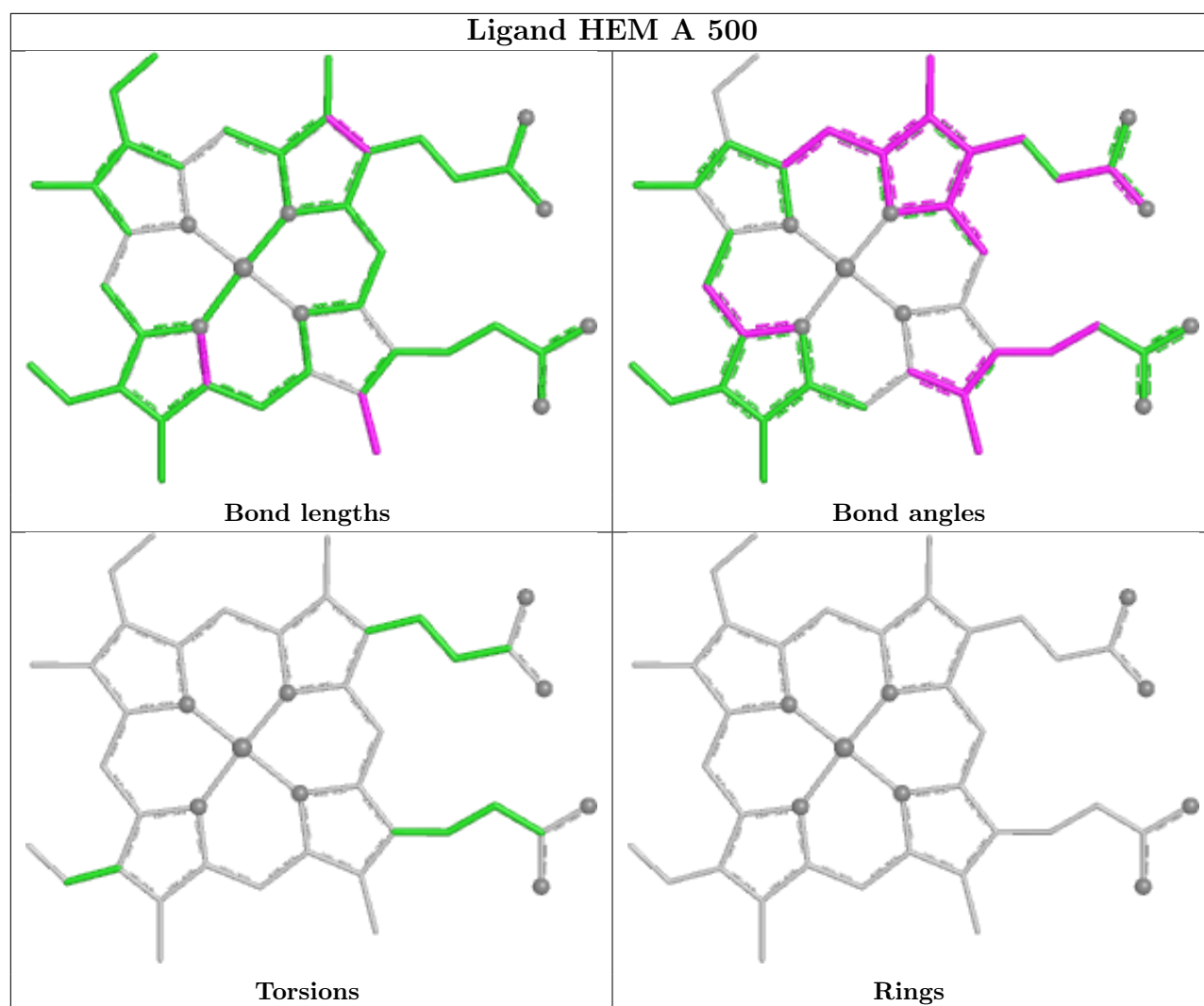
Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C4B-C3B-CAB-CBB
3	A	600	H4B	C7-C6-C9-O9
3	A	600	H4B	N5-C6-C9-O9

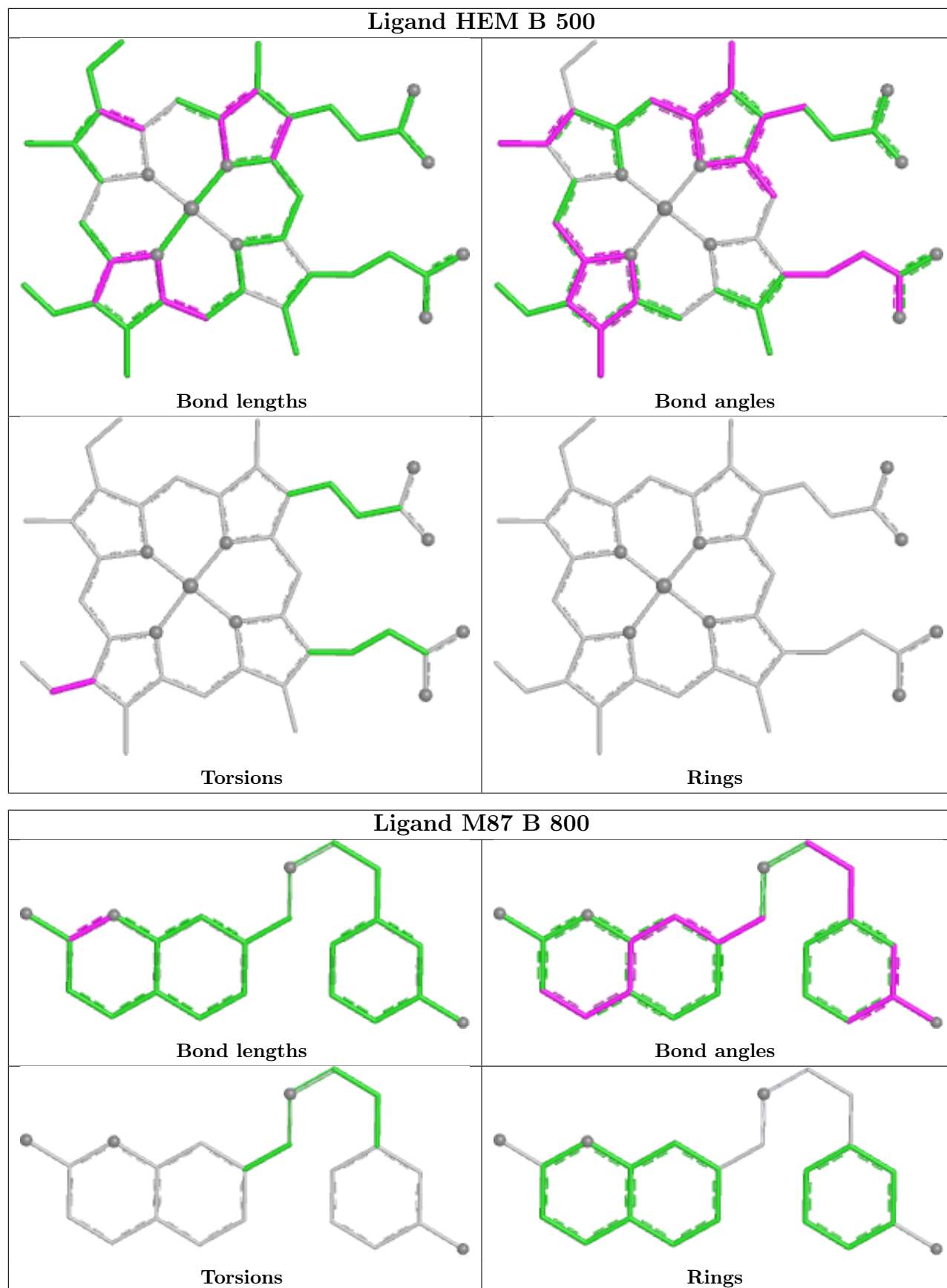
There are no ring outliers.

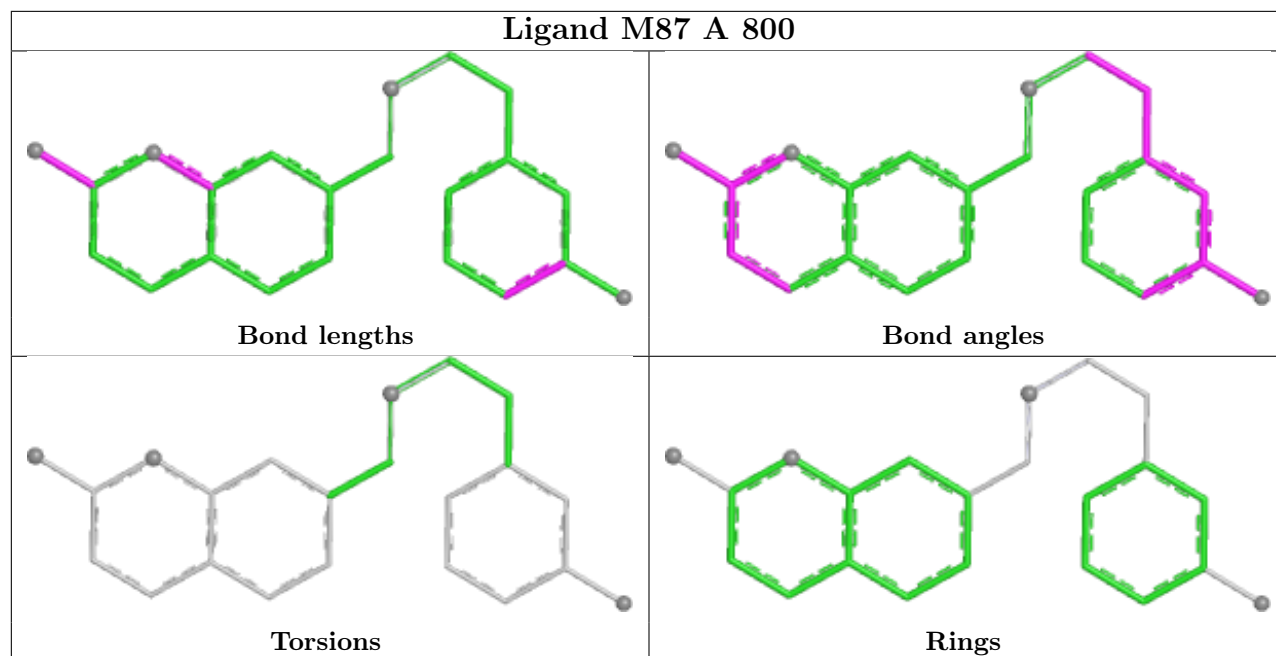
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	4	0
2	B	500	HEM	3	0
4	B	800	M87	1	0
3	A	600	H4B	1	0
4	A	800	M87	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/443 (91%)	-0.15	13 (3%) 47 52	24, 34, 62, 102	0
1	B	404/443 (91%)	-0.25	10 (2%) 57 61	24, 38, 67, 100	0
All	All	808/886 (91%)	-0.20	23 (2%) 53 58	24, 37, 66, 102	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	6.6
1	A	123	GLU	4.1
1	B	261	GLY	3.8
1	A	259	GLN	3.8
1	A	160	ALA	3.2
1	A	239	GLY	2.9
1	B	110	LYS	2.8
1	B	111	LEU	2.7
1	B	260	ASP	2.6
1	A	109	ARG	2.5
1	A	146	GLN	2.5
1	A	69	LYS	2.4
1	B	142	ARG	2.4
1	A	122	ALA	2.4
1	A	450	ILE	2.3
1	A	67	GLY	2.3
1	A	448	ALA	2.2
1	A	449	TRP	2.2
1	B	223	ARG	2.2
1	B	263	VAL	2.1
1	A	153	GLN	2.1
1	B	448	ALA	2.1
1	B	257	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	B	384	9/10	0.96	0.08	46,48,58,69	0
1	CAS	A	384	9/10	0.97	0.08	34,35,61,65	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

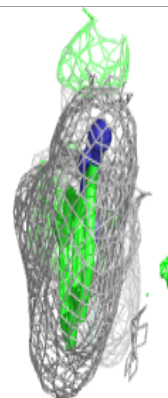
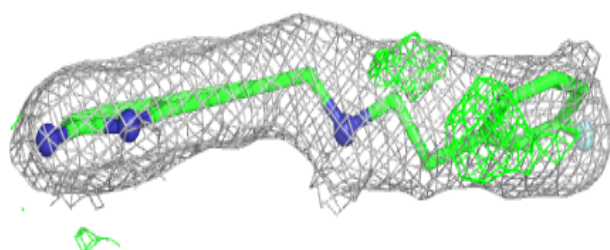
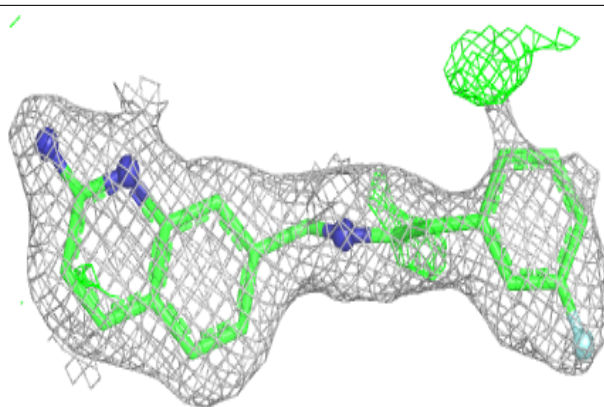
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	880	6/6	0.90	0.15	43,49,54,56	0
6	GOL	B	880	6/6	0.92	0.17	45,50,57,57	0
5	ACT	B	860	4/4	0.95	0.19	45,47,50,50	0
4	M87	A	800	22/22	0.95	0.15	23,27,69,74	0
4	M87	B	800	22/22	0.95	0.12	26,31,70,71	0
5	ACT	A	860	4/4	0.96	0.12	36,45,46,47	0
3	H4B	B	600	17/17	0.97	0.13	23,27,35,39	0
5	ACT	B	861	4/4	0.97	0.11	32,35,37,43	0
2	HEM	A	500	43/43	0.97	0.16	23,26,35,42	0
5	ACT	A	861	4/4	0.97	0.08	32,33,35,37	0
3	H4B	A	600	17/17	0.98	0.16	25,28,35,35	0
2	HEM	B	500	43/43	0.98	0.10	25,28,35,45	0
7	ZN	A	1483	1/1	1.00	0.05	34,34,34,34	0

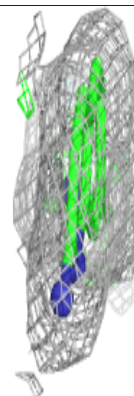
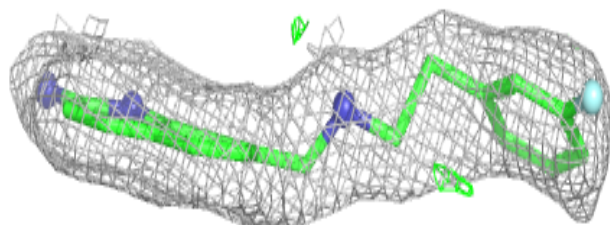
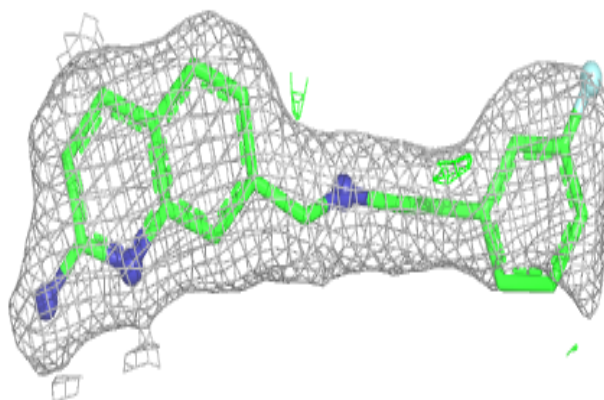
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M87 A 800:

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

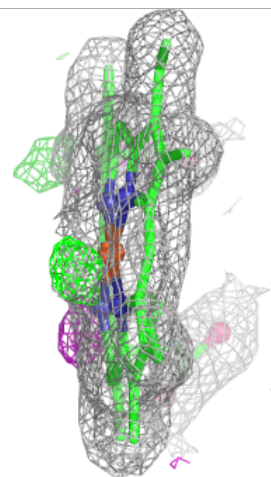
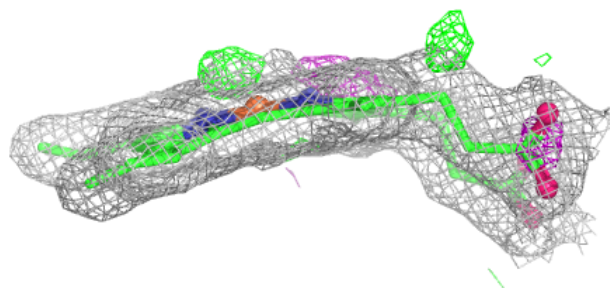
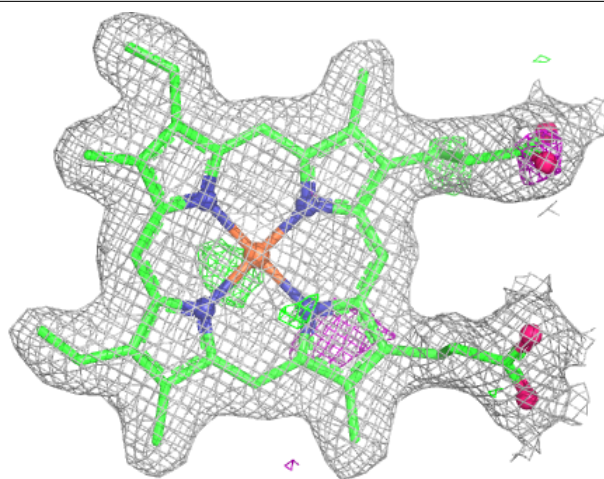
**Electron density around M87 B 800:**

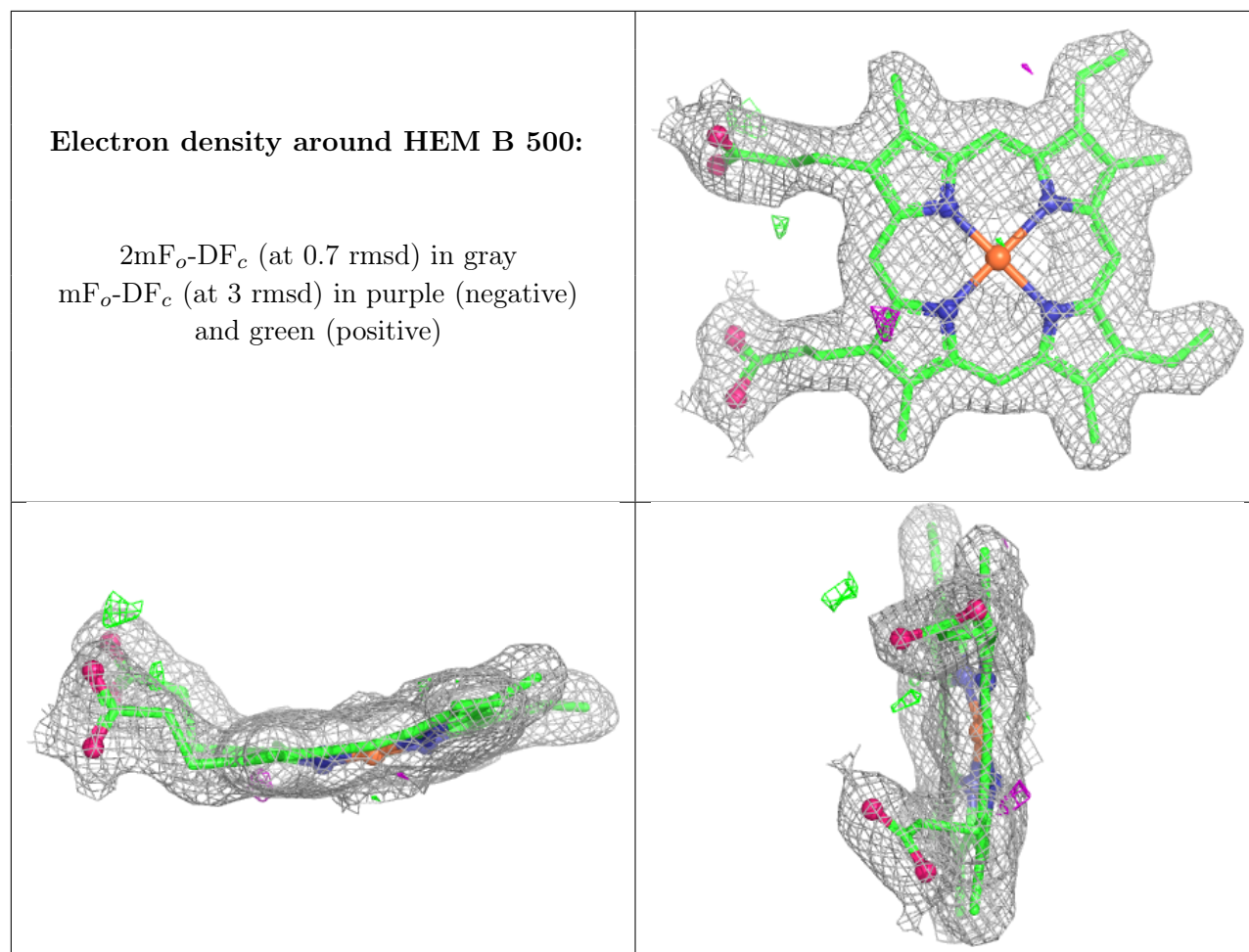
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 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 [i](#)

There are no such residues in this entry.