WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 10:40 AM EDT

PDB ID : 5VVN
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 4-(2-(((2-Aminoquinolin-7-yl)methyl)amino)ethyl)benzonitrile
Authors : Li, H.; Poulos, T.L.
Deposited on : 2017-05-19
Resolution : 2.40 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

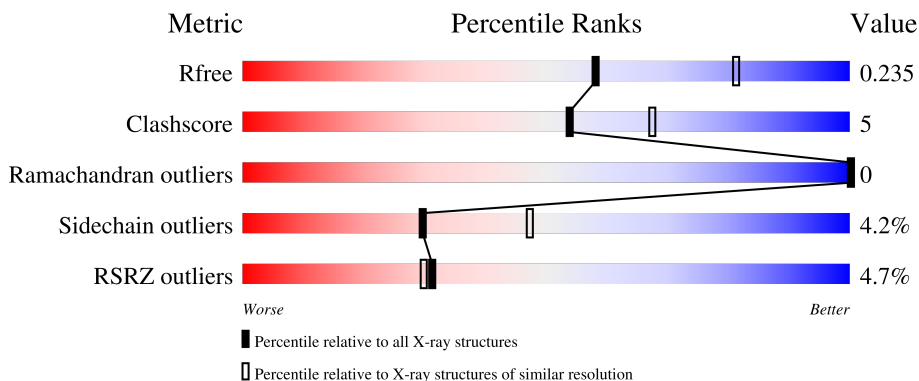|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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		0.235
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		4.2%
RSRZ outliers		4.7%

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	5% / 79% 12% 8%
1	B	443	4% / 77% 14% • 9%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 6739 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	406	Total	As	C	N	O	S	0	0	0
			3230	1	2054	569	590	16			
1	B	404	Total	As	C	N	O	S	0	0	0
			3221	1	2048	568	588	16			

There are 2 discrepancies between the modelled and reference sequences:

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

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 4 is 4-(2-{[(2-aminoquinolin-7-yl)methyl]amino}ethyl)benzonitrile (three-letter code: P94) (formula: $C_{19}H_{18}N_4$).
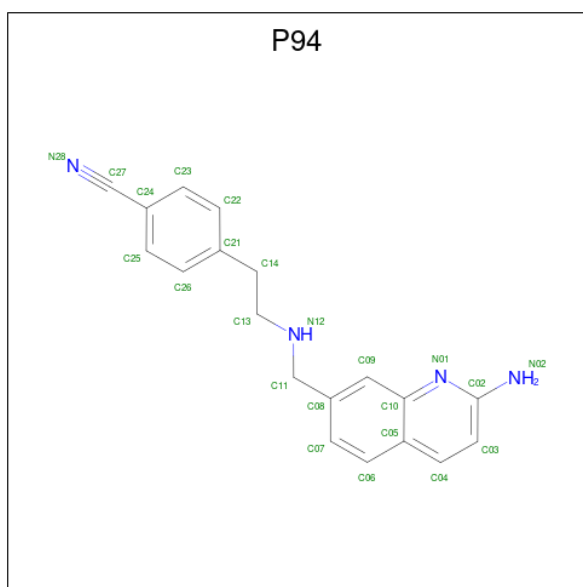
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 23	C 19	N 4	0	0
4	B	1	Total 23	C 19	N 4	0	0

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

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

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

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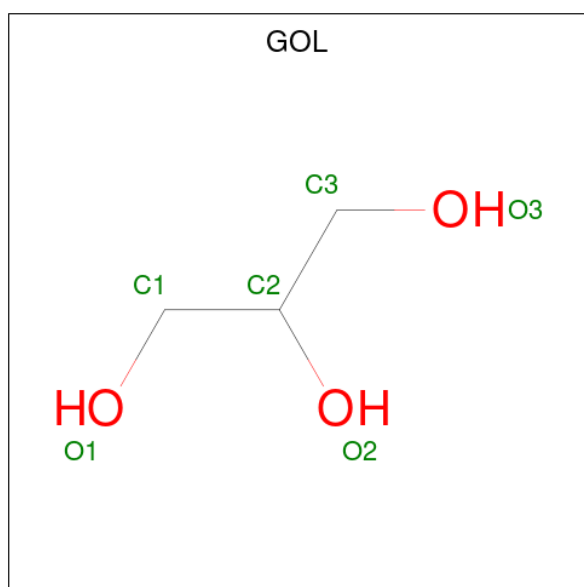
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0

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

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

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	57	Total 57	O 57	0	0
8	B	36	Total 36	O 36	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: Nitric oxide synthase, endothelial

Chain A:

• Molecule 1: Nitric oxide synthase, endothelial

Chain B:
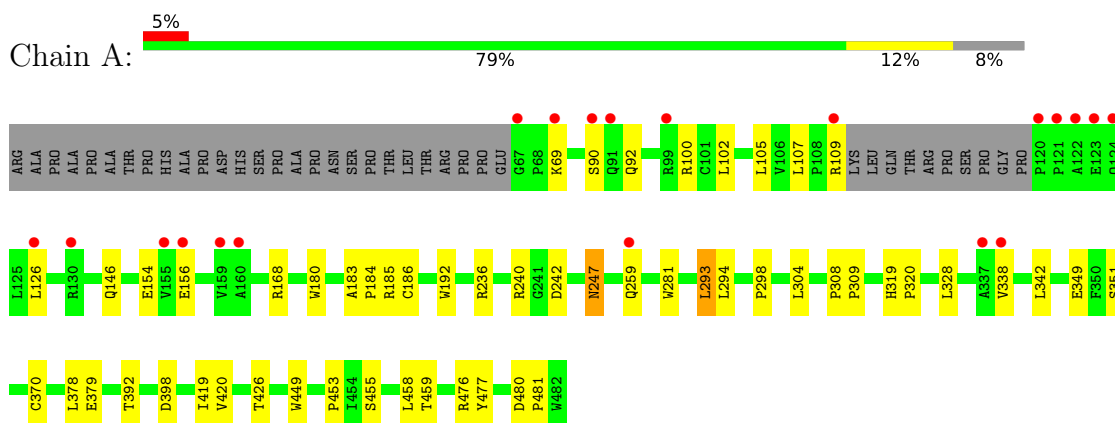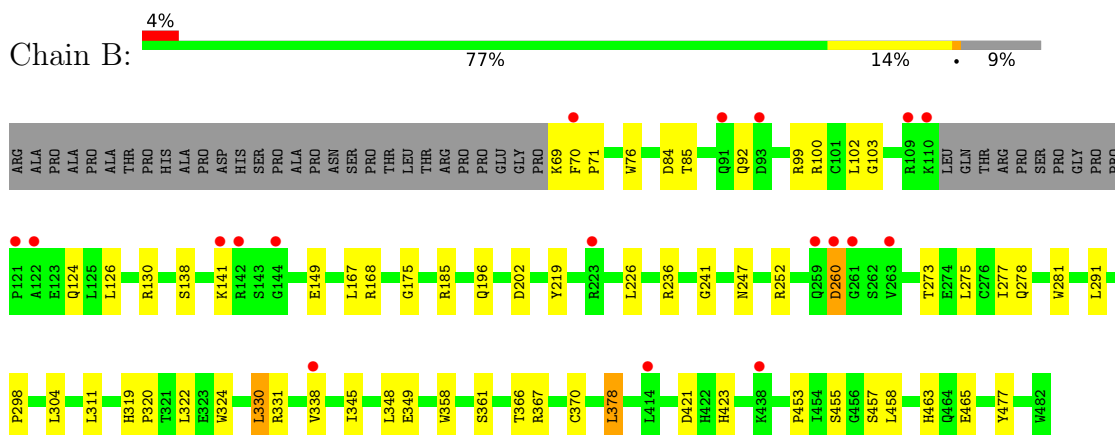
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.09Å 106.39Å 156.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.23 – 2.40 39.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.23-2.40) 99.5 (39.23-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.180 , 0.234 0.180 , 0.235	Depositor DCC
R_{free} test set	1924 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	59.1	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6739	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, P94, GOL, CAS, HEM, ACT, 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	0.41	0/3311	0.55	0/4509
1	B	0.38	0/3300	0.52	0/4491
All	All	0.39	0/6611	0.54	0/9000

There are no bond length outliers.

There are no bond angle outliers.

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	3230	0	3134	32	0
1	B	3221	0	3130	38	0
2	A	43	0	30	6	0
2	B	43	0	30	6	0
3	A	17	0	15	2	0
3	B	17	0	15	1	0
4	A	23	0	0	1	0
4	B	23	0	0	1	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	57	0	0	0	0
8	B	36	0	0	4	0
All	All	6739	0	6382	69	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 5.

All (69) 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)
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.78	0.66
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.78	0.65
1:A:338:VAL:HG21	4:A:503:P94:C07	2.28	0.64
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.80	0.64
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.84	0.58
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.85	0.58
1:B:370:CYS:HB3	1:B:378:LEU:HD22	1.87	0.56
1:A:90:SER:O	1:B:99:ARG:NH1	2.39	0.56
1:B:477:TYR:OH	2:B:501:HEM:O1D	2.15	0.55
1:B:463:HIS:ND1	8:B:602:HOH:O	2.33	0.55
1:A:458:LEU:HD22	1:B:378:LEU:HD21	1.89	0.54
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.90	0.53
1:A:398:ASP:OD2	1:B:455:SER:OG	2.18	0.53
1:B:366:THR:O	1:B:370:CYS:HB2	2.09	0.53
1:B:338:VAL:HG21	4:B:503:P94:C07	2.39	0.52
1:A:342:LEU:HD12	1:A:351:SER:HA	1.92	0.51
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.95	0.49
1:B:358:TRP:NE1	2:B:501:HEM:HAB	2.29	0.48
1:A:185:ARG:HB2	2:A:501:HEM:HAD2	1.96	0.48
1:B:367:ARG:HH12	3:B:502:H4B:C4	2.26	0.48
1:A:154:GLU:OE1	1:A:168:ARG:NH2	2.46	0.48
2:A:501:HEM:HHC	2:A:501:HEM:CBB	2.44	0.48
1:B:103:GLY:O	8:B:601:HOH:O	2.20	0.48
1:A:186:CYS:HB2	2:A:501:HEM:C4D	2.49	0.47
1:B:70:PHE:CD1	1:B:85:THR:HG22	2.49	0.47
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.55	0.47
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.49	0.47
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.96	0.47
1:B:241:GLY:O	1:B:298:PRO:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.50	0.47
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.50	0.47
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.97	0.46
1:B:175:GLY:HA3	1:B:345:ILE:HD13	1.97	0.46
3:A:502:H4B:O4	6:A:506:GOL:O2	2.33	0.46
1:B:358:TRP:CD1	2:B:501:HEM:HAB	2.51	0.46
1:B:366:THR:HG21	1:B:453:PRO:HB2	1.98	0.45
1:B:126:LEU:O	1:B:130:ARG:HG3	2.17	0.45
6:A:506:GOL:H2	8:B:602:HOH:O	2.17	0.45
1:A:419:ILE:HG13	1:A:420:VAL:N	2.32	0.45
1:A:426:THR:OG1	1:A:459:THR:HB	2.17	0.44
2:A:501:HEM:HBB2	2:A:501:HEM:CHC	2.47	0.44
1:A:92:GLN:OE1	1:A:476:ARG:NH1	2.50	0.44
1:B:260:ASP:OD1	1:B:260:ASP:N	2.51	0.44
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.99	0.44
1:B:196:GLN:HG2	1:B:219:TYR:CZ	2.53	0.43
1:A:247:ASN:OD1	1:A:247:ASN:N	2.52	0.43
1:A:453:PRO:HB2	1:B:457:SER:OG	2.18	0.43
1:B:273:THR:O	1:B:277:ILE:HG13	2.18	0.43
1:A:392:THR:HB	1:B:423:HIS:HB2	2.01	0.43
1:A:477:TYR:OH	2:A:501:HEM:O1D	2.33	0.43
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.54	0.42
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.84	0.42
1:B:252:ARG:HB2	1:B:291:LEU:HD12	2.01	0.42
1:A:236:ARG:HG2	1:A:242:ASP:OD1	2.19	0.42
1:B:236:ARG:NH1	1:B:349:GLU:OE1	2.52	0.42
1:A:480:ASP:HA	1:A:481:PRO:HD3	1.90	0.42
1:B:330:LEU:HD12	1:B:330:LEU:HA	1.81	0.42
1:B:185:ARG:HB2	2:B:501:HEM:HAD2	2.00	0.42
1:B:361:SER:OG	1:B:421:ASP:HA	2.20	0.42
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.86	0.41
1:A:449:TRP:HA	3:A:502:H4B:N1	2.36	0.41
1:A:107:LEU:HD12	1:B:76:TRP:HH2	1.85	0.41
1:B:358:TRP:CE2	2:B:501:HEM:HAB	2.55	0.41
1:A:342:LEU:HD11	1:A:349:GLU:HB3	2.03	0.41
1:B:453:PRO:HG3	8:B:629:HOH:O	2.20	0.41
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.85	0.40
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.87	0.40
1:B:247:ASN:OD1	1:B:247:ASN:N	2.54	0.40
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.49	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	401/443 (90%)	390 (97%)	11 (3%)	0	100	100
1	B	399/443 (90%)	379 (95%)	20 (5%)	0	100	100
All	All	800/886 (90%)	769 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	344/375 (92%)	333 (97%)	11 (3%)	39	59
1	B	343/375 (92%)	325 (95%)	18 (5%)	23	38
All	All	687/750 (92%)	658 (96%)	29 (4%)	30	47

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	100	ARG
1	A	102	LEU
1	A	109	ARG
1	A	146	GLN
1	A	247	ASN
1	A	259	GLN
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	294	LEU
1	A	328	LEU
1	A	379	GLU
1	B	69	LYS
1	B	92	GLN
1	B	100	ARG
1	B	102	LEU
1	B	124	GLN
1	B	138	SER
1	B	141	LYS
1	B	149	GLU
1	B	168	ARG
1	B	202	ASP
1	B	226	LEU
1	B	260	ASP
1	B	278	GLN
1	B	311	LEU
1	B	330	LEU
1	B	331	ARG
1	B	378	LEU
1	B	458	LEU

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

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	A	384	1	5,8,9	0.95	0	1,9,11	0.18	0
1	CAS	B	384	1	5,8,9	1.11	0	1,9,11	0.05	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	-
1	CAS	B	384	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#|Z| > 2$
5	ACT	B	504	-	3,3,3	0.73	0	3,3,3	0.78	0
6	GOL	B	506	-	5,5,5	0.30	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	H4B	B	502	-	16,18,18	1.07	1 (6%)	11,26,26	2.54	4 (36%)
4	P94	A	503	-	25,25,25	1.65	1 (4%)	31,33,33	0.95	0
5	ACT	A	504	-	3,3,3	0.71	0	3,3,3	0.84	0
5	ACT	A	505	-	3,3,3	0.75	0	3,3,3	0.75	0
2	HEM	A	501	1	41,50,50	1.90	6 (14%)	45,82,82	1.54	7 (15%)
6	GOL	A	506	-	5,5,5	0.36	0	5,5,5	0.51	0
4	P94	B	503	-	25,25,25	1.63	1 (4%)	31,33,33	1.09	2 (6%)
5	ACT	B	505	-	3,3,3	0.77	0	3,3,3	0.80	0
2	HEM	B	501	1	41,50,50	1.97	6 (14%)	45,82,82	1.99	8 (17%)
3	H4B	A	502	-	16,18,18	1.00	0	11,26,26	2.70	5 (45%)

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
6	GOL	B	506	-	-	4/4/4/4	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	P94	A	503	-	-	0/9/9/9	0/3/3/3
2	HEM	A	501	1	-	3/12/54/54	-
6	GOL	A	506	-	-	2/4/4/4	-
4	P94	B	503	-	-	2/9/9/9	0/3/3/3
2	HEM	B	501	1	-	2/12/54/54	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3D-C2D	7.86	1.53	1.36
2	A	501	HEM	C3D-C2D	7.65	1.53	1.36
4	A	503	P94	C24-C27	-7.08	1.28	1.44
4	B	503	P94	C24-C27	-6.89	1.29	1.44
2	A	501	HEM	C3C-C2C	-4.20	1.34	1.40
2	B	501	HEM	C3C-C2C	-3.69	1.35	1.40
2	B	501	HEM	C3C-CAC	3.65	1.55	1.47
2	A	501	HEM	C3C-CAC	3.52	1.55	1.47
2	B	501	HEM	FE-NB	3.11	2.12	1.96
2	B	501	HEM	CAB-C3B	3.07	1.55	1.47
2	B	501	HEM	FE-ND	2.82	2.10	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CAB-C3B	2.71	1.54	1.47
2	A	501	HEM	CAA-C2A	2.68	1.56	1.52
3	B	502	H4B	C4A-C4	-2.66	1.37	1.41
2	A	501	HEM	CMD-C2D	2.30	1.55	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4D-ND-C1D	6.67	111.97	105.07
3	B	502	H4B	C8A-C4A-C4	6.08	119.97	114.57
3	A	502	H4B	C8A-C4A-C4	5.99	119.89	114.57
2	B	501	HEM	CBA-CAA-C2A	-4.69	104.61	112.62
2	B	501	HEM	C4C-CHD-C1D	4.68	128.74	122.56
2	A	501	HEM	C4D-ND-C1D	4.34	109.55	105.07
3	A	502	H4B	N1-C2-N3	-3.35	120.16	125.42
2	B	501	HEM	CBD-CAD-C3D	-3.24	103.63	112.63
2	A	501	HEM	C4B-CHC-C1C	3.23	126.82	122.56
2	B	501	HEM	C1B-NB-C4B	3.14	108.32	105.07
3	A	502	H4B	C2-N3-C4	3.14	120.91	115.93
2	B	501	HEM	C3B-C2B-C1B	3.08	108.77	106.49
3	B	502	H4B	N1-C2-N3	-2.98	120.75	125.42
3	A	502	H4B	C2-N1-C8A	2.76	120.72	114.54
3	B	502	H4B	C2-N3-C4	2.68	120.18	115.93
3	B	502	H4B	C2-N1-C8A	2.66	120.51	114.54
2	A	501	HEM	CHB-C1B-NB	2.61	127.60	124.38
4	B	503	P94	C13-C14-C21	-2.52	107.04	112.87
2	A	501	HEM	CBD-CAD-C3D	-2.51	105.65	112.63
2	B	501	HEM	C4B-CHC-C1C	2.50	125.86	122.56
2	A	501	HEM	C1D-C2D-C3D	-2.33	104.50	106.96
2	A	501	HEM	CMA-C3A-C4A	-2.29	124.94	128.46
4	B	503	P94	C03-C02-N01	-2.22	119.41	122.08
2	B	501	HEM	CAD-C3D-C4D	2.14	128.39	124.66
3	A	502	H4B	N2-C2-N1	2.09	120.51	117.25
2	A	501	HEM	CAD-C3D-C4D	2.03	128.20	124.66

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	506	GOL	O1-C1-C2-C3
6	B	506	GOL	C1-C2-C3-O3
4	B	503	P94	C14-C13-N12-C11

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Mol	Chain	Res	Type	Atoms
6	A	506	GOL	O1-C1-C2-C3
6	B	506	GOL	O2-C2-C3-O3
2	B	501	HEM	C4B-C3B-CAB-CBB
6	A	506	GOL	O1-C1-C2-O2
6	B	506	GOL	O1-C1-C2-O2
2	A	501	HEM	C3D-CAD-CBD-CGD
2	A	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C3D-CAD-CBD-CGD
2	A	501	HEM	C2A-CAA-CBA-CGA
4	B	503	P94	C25-C24-C27-N28

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	H4B	1	0
4	A	503	P94	1	0
2	A	501	HEM	6	0
6	A	506	GOL	2	0
4	B	503	P94	1	0
2	B	501	HEM	6	0
3	A	502	H4B	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 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 P94 A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand P94 B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings
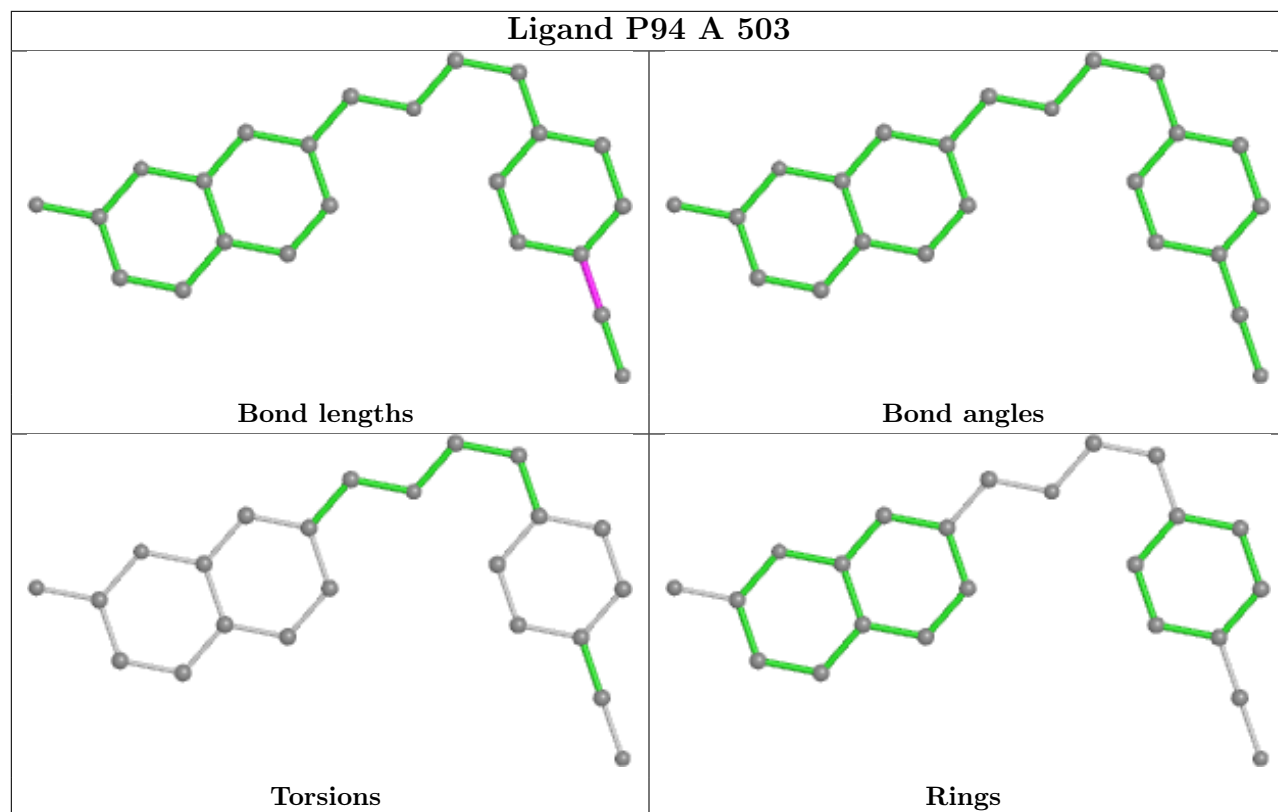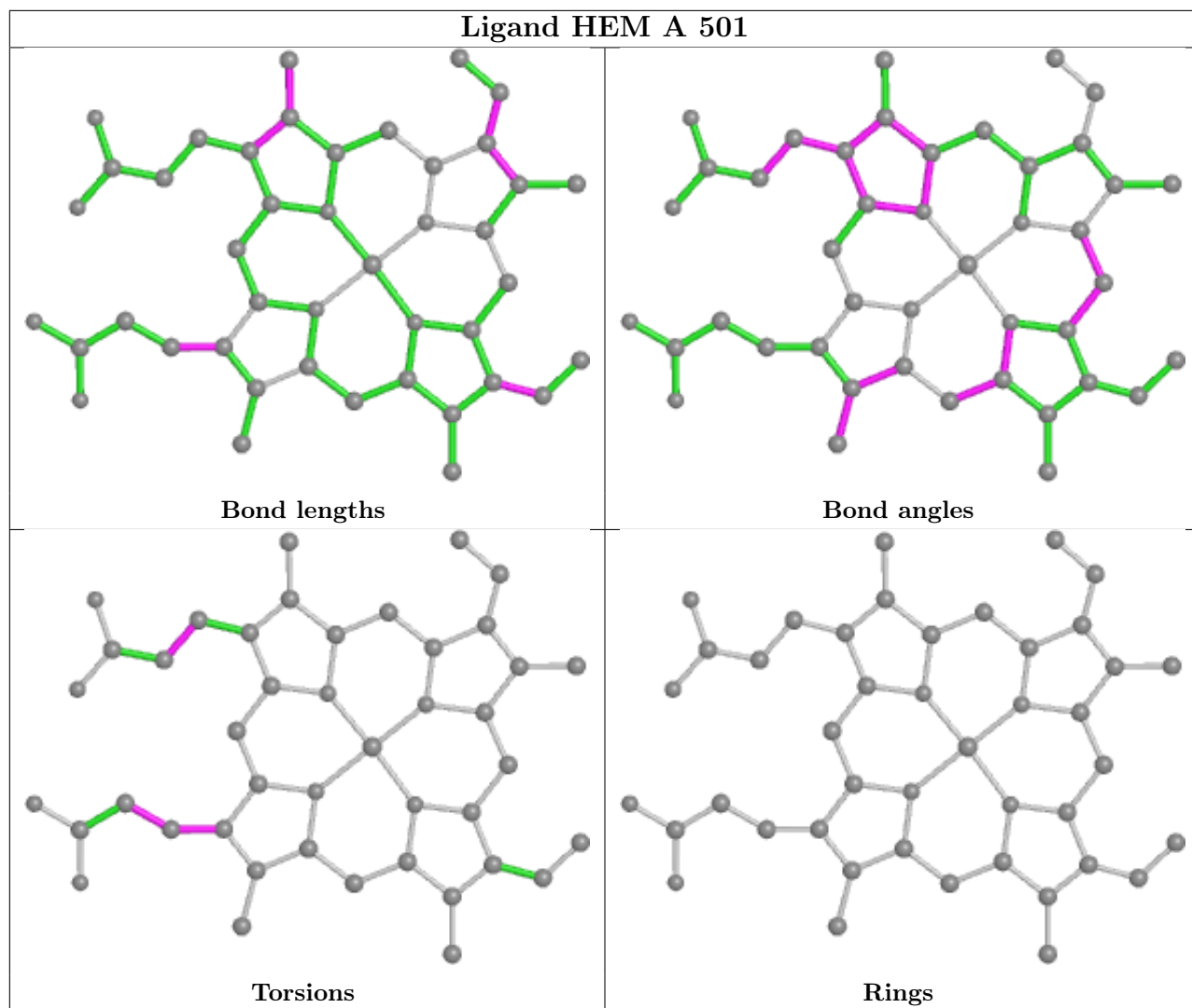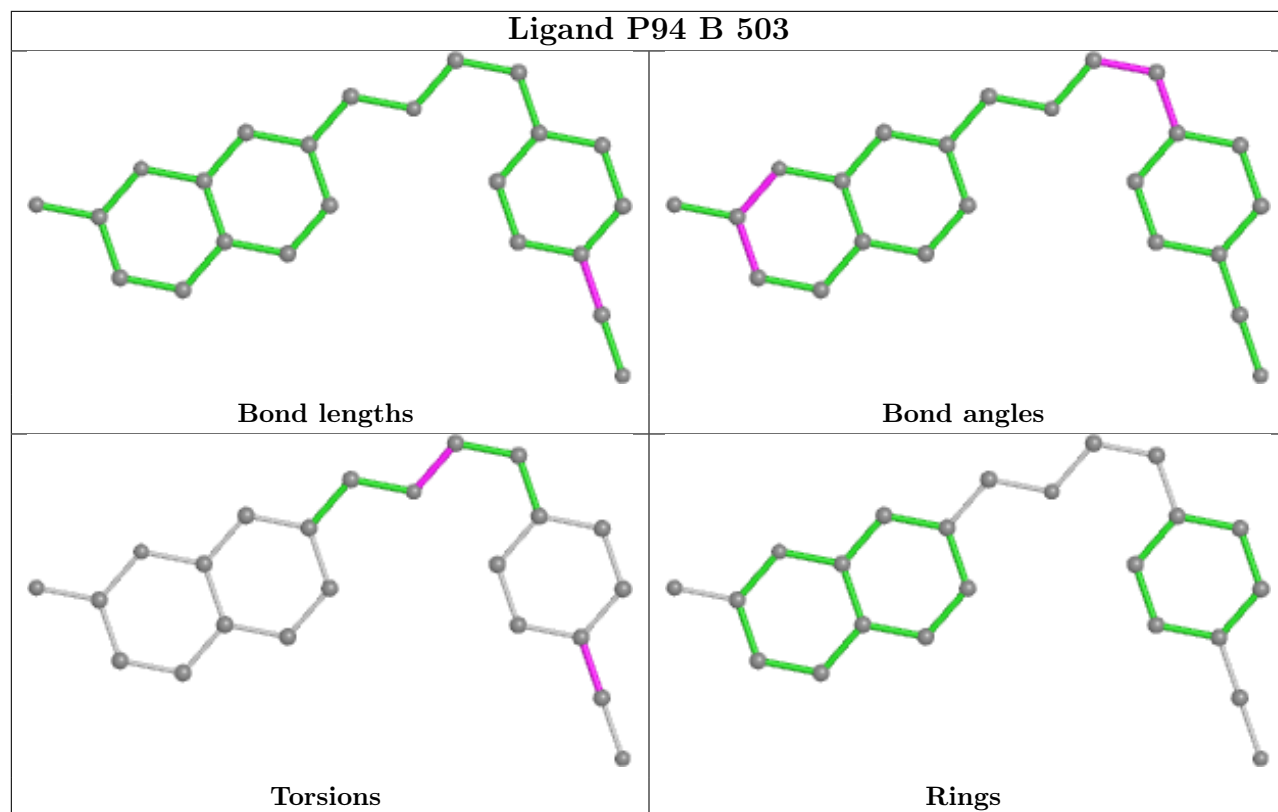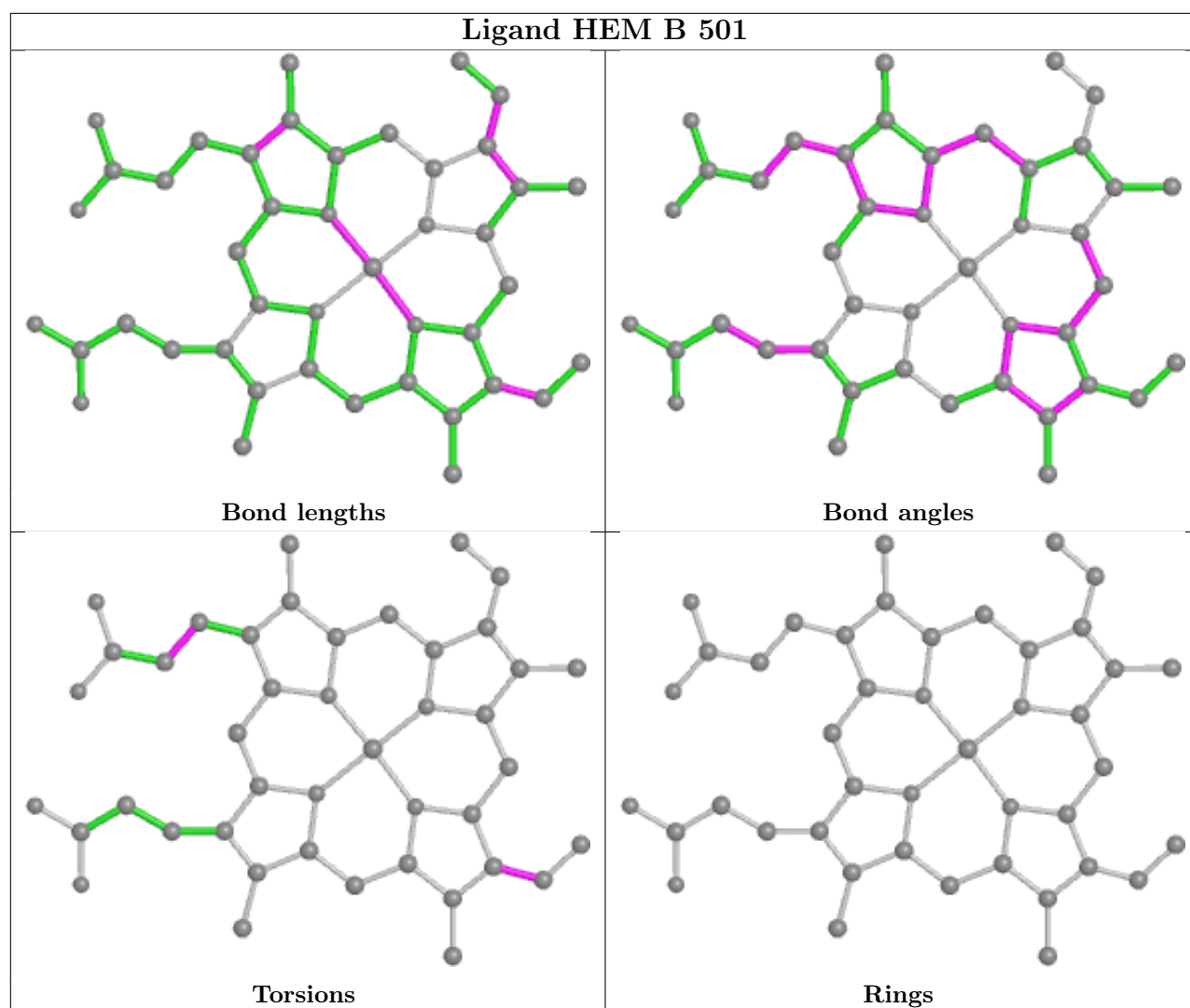
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	405/443 (91%)	0.09	20 (4%)	29	28	37, 55, 91, 120	0
1	B	403/443 (90%)	0.11	18 (4%)	33	31	39, 59, 92, 130	0
All	All	808/886 (91%)	0.10	38 (4%)	31	30	37, 57, 92, 130	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	LYS	4.7
1	A	69	LYS	4.5
1	A	120	PRO	4.5
1	A	259	GLN	4.4
1	A	159	VAL	4.2
1	A	160	ALA	4.2
1	B	260	ASP	3.8
1	A	91	GLN	3.8
1	A	123	GLU	3.8
1	B	142	ARG	3.7
1	A	126	LEU	3.4
1	A	121	PRO	3.4
1	A	109	ARG	3.3
1	B	70	PHE	3.3
1	A	67	GLY	3.2
1	A	99	ARG	3.0
1	A	122	ALA	3.0
1	A	130	ARG	3.0
1	B	122	ALA	3.0
1	B	144	GLY	2.9
1	A	155	VAL	2.8
1	A	156	GLU	2.6
1	B	338	VAL	2.5
1	A	124	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	141	LYS	2.4
1	A	90	SER	2.4
1	B	414	LEU	2.4
1	B	121	PRO	2.3
1	B	261	GLY	2.3
1	B	438	LYS	2.3
1	A	338	VAL	2.3
1	B	93	ASP	2.2
1	B	223	ARG	2.1
1	B	91	GLN	2.1
1	B	259	GLN	2.1
1	B	109	ARG	2.1
1	A	337	ALA	2.0
1	B	263	VAL	2.0

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

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.
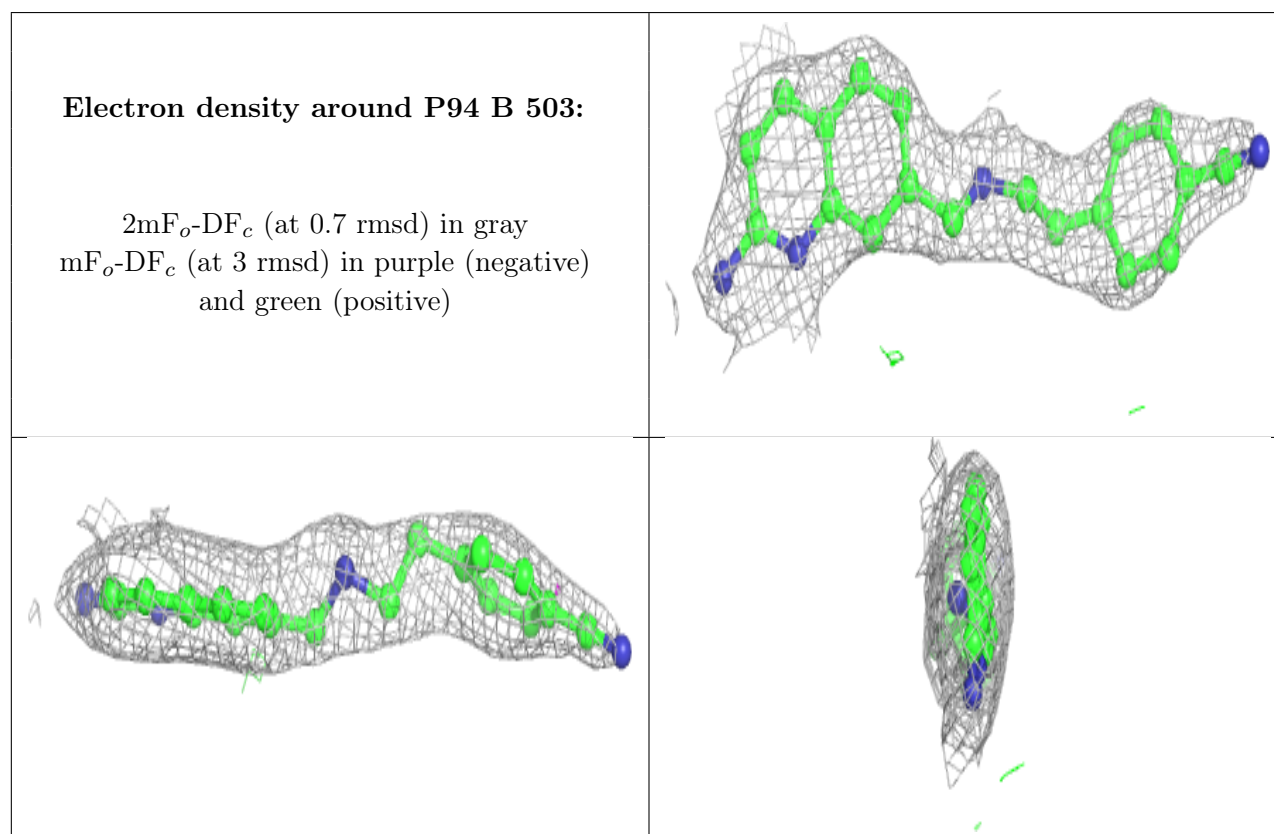
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	CAS	A	384	9/10	0.95	0.10	49,55,97,111	0
1	CAS	B	384	9/10	0.95	0.12	81,82,114,164	0

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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	B	506	6/6	0.91	0.22	68,72,73,74	0
6	GOL	A	506	6/6	0.92	0.34	84,89,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	A	504	4/4	0.93	0.15	55,60,60,62	0
4	P94	B	503	23/23	0.94	0.20	44,50,65,66	0
3	H4B	A	502	17/17	0.95	0.22	56,65,78,79	0
4	P94	A	503	23/23	0.95	0.24	34,50,79,92	0
3	H4B	B	502	17/17	0.96	0.25	58,68,75,75	0
5	ACT	B	505	4/4	0.96	0.14	70,74,76,76	0
5	ACT	B	504	4/4	0.97	0.24	57,60,60,62	0
2	HEM	A	501	43/43	0.98	0.20	21,36,60,71	0
5	ACT	A	505	4/4	0.98	0.25	56,56,57,58	0
2	HEM	B	501	43/43	0.98	0.20	38,45,68,75	0
7	ZN	A	507	1/1	0.99	0.08	53,53,53,53	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.
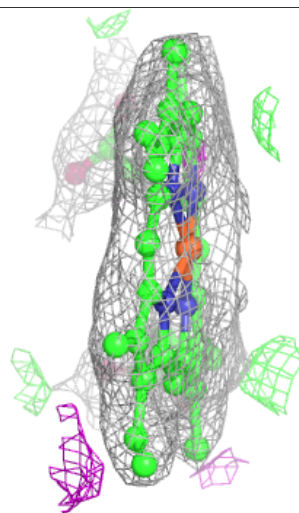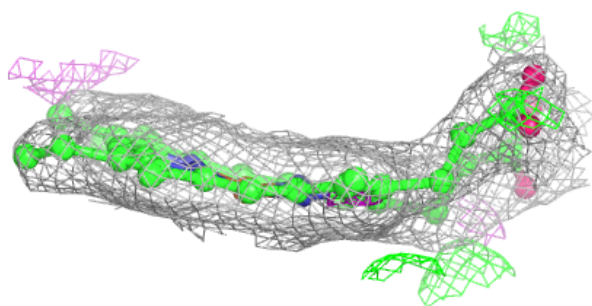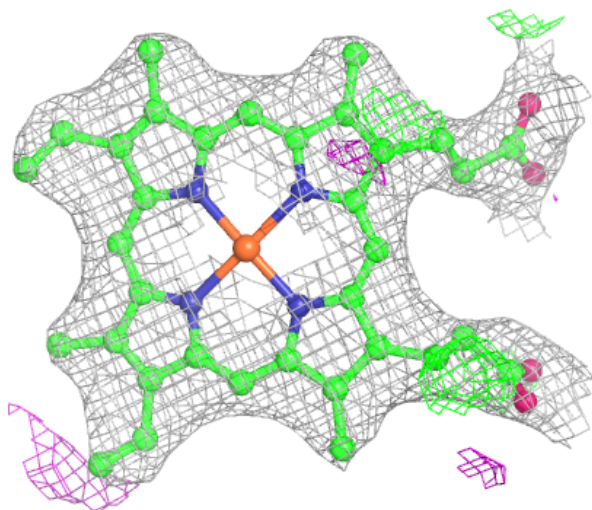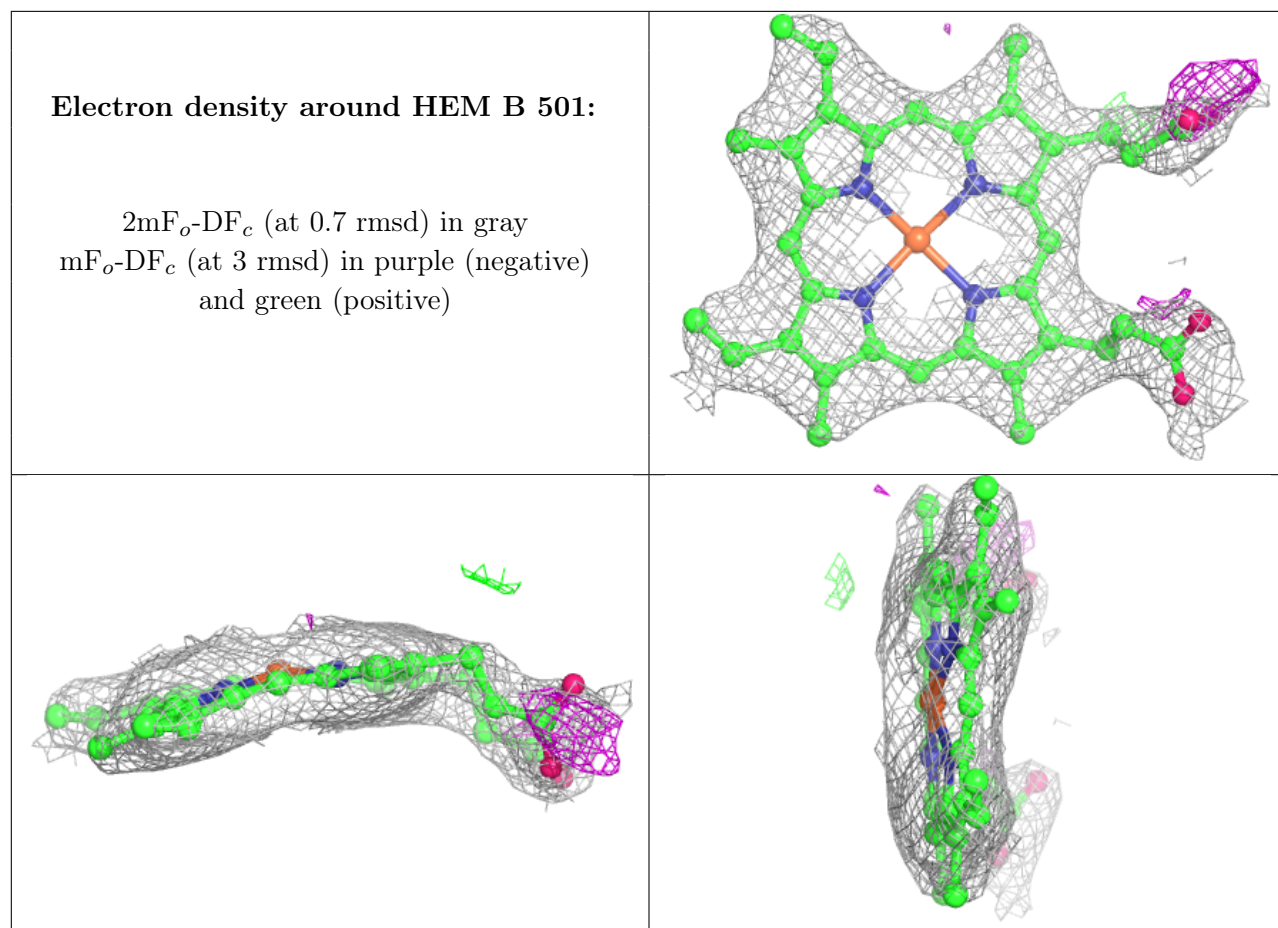

Electron density around P94 B 503:

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 P94 A 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
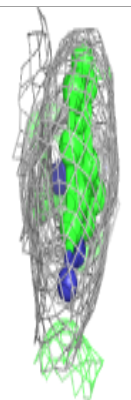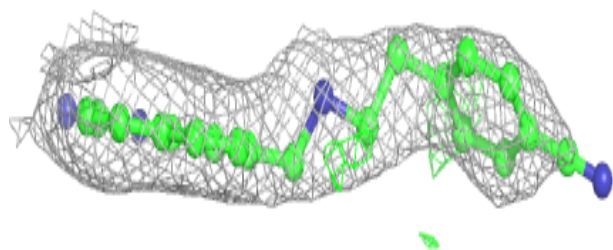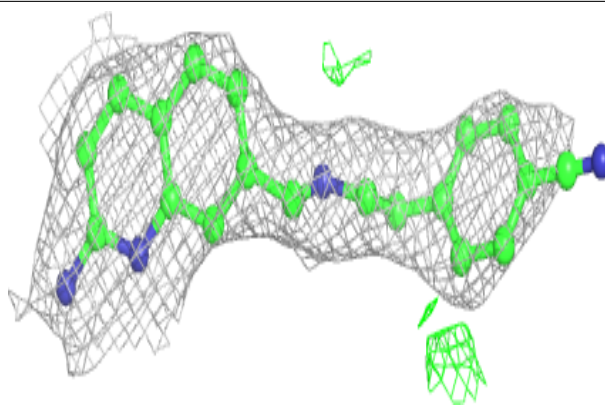
Electron density around HEM A 501:

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

Electron density around HEM B 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.