Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 02:53 AM EDT

PDB ID	:	6PN9
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 7-(3-(Aminomethyl)-4-(thiazol-5-ylmethoxy)phenyl)-4-methylquinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2019-07-02
Resolution	:	1.84 Å(reported)

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 1.84 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 7283 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, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	3	0
			3357	2149	573	613	22			
1	B	411	Total	C	N	O	S	0	4	0
			3362	2153	574	613	22			

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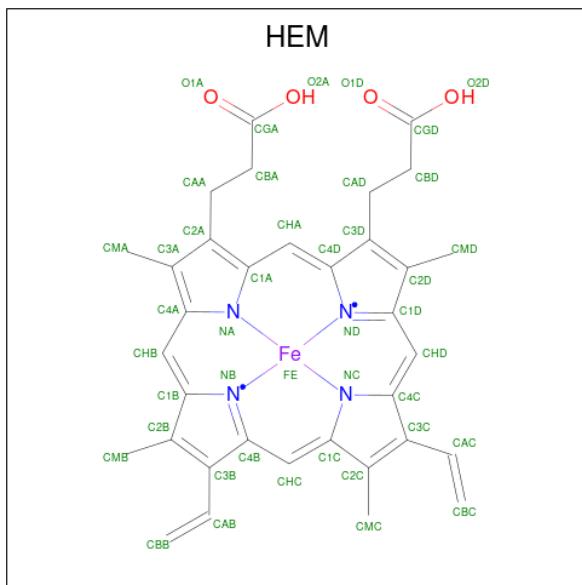
HEM

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
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: $C_9H_{15}N_5O_3$).
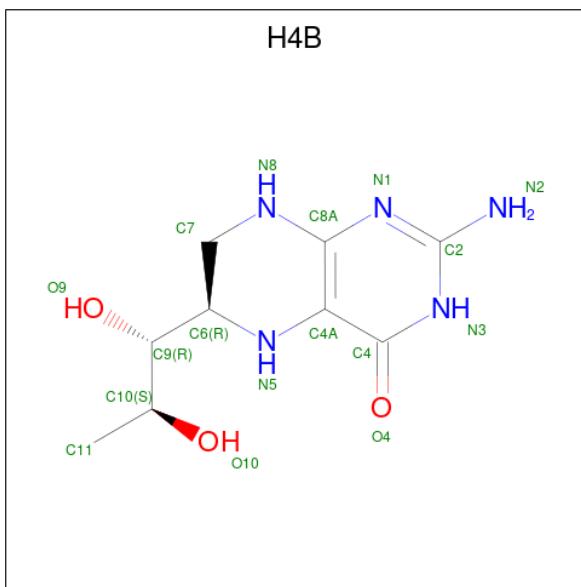
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 17	C 9	N 5	O 3	0	0
3	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is 7-{3-(aminomethyl)-4-[(1,3-thiazol-5-yl)methoxy]phenyl}-4-methylquinolin-2-amine (three-letter code: OU7) (formula: $C_{21}H_{20}N_4OS$) (labeled as "Ligand of Interest" by depositor).
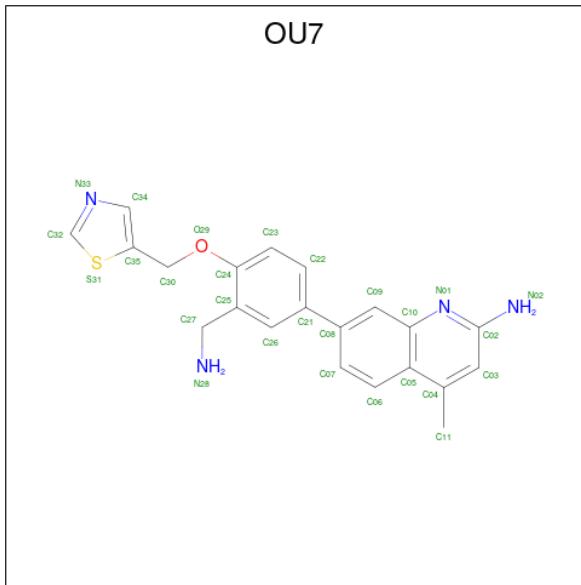
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 21	N 4	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 27	C 21	N 4	O 1	S 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
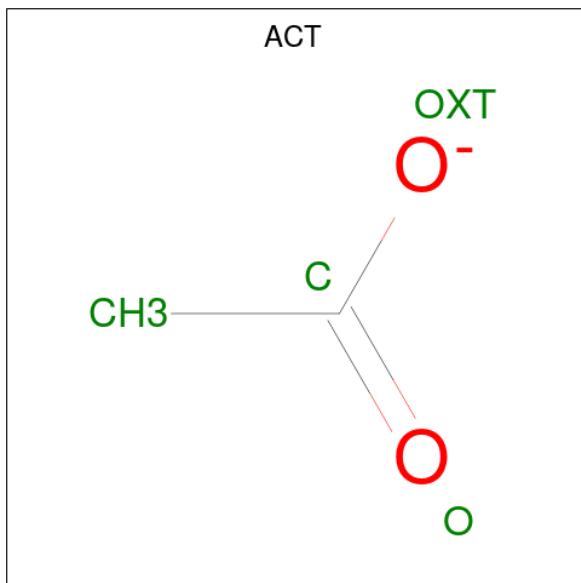
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Zn 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	156	Total 156	O 156	0	0
7	B	225	Total 225	O 225	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.87Å 111.69Å 164.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.14 – 1.84	Depositor
% Data completeness (in resolution range)	98.8 (66.14-1.84)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, R_{free}	0.210 , 0.253	Depositor
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.864	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7283	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 5.79% 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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA ⓘ

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#|Z| > 2$
4	OU7	B	803	-	28,30,30	0.84	0	35,42,42	1.81	6 (17%)
2	HEM	B	801	1	41,50,50	1.45	5 (12%)	45,82,82	1.43	5 (11%)
2	HEM	A	801	1	41,50,50	1.42	5 (12%)	45,82,82	1.53	10 (22%)
3	H4B	B	802	-	16,18,18	0.88	0	11,26,26	2.35	5 (45%)
4	OU7	A	803	-	28,30,30	0.96	1 (3%)	35,42,42	2.61	14 (40%)
5	ACT	B	804	-	3,3,3	0.80	0	3,3,3	0.59	0
3	H4B	A	802	-	16,18,18	0.97	0	11,26,26	2.59	6 (54%)
5	ACT	A	804	-	3,3,3	0.79	0	3,3,3	0.73	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
4	OU7	B	803	-	-	3/9/20/20	0/4/4/4
2	HEM	B	801	1	-	5/12/54/54	-
2	HEM	A	801	1	-	6/12/54/54	-
3	H4B	B	802	-	-	1/8/17/17	0/2/2/2
4	OU7	A	803	-	-	4/9/20/20	0/4/4/4
3	H4B	A	802	-	-	2/8/17/17	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3C-C2C	-3.73	1.35	1.40
2	A	801	HEM	C3C-CAC	3.58	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.25	1.35	1.40
2	A	801	HEM	CAB-C3B	3.08	1.55	1.47
2	B	801	HEM	C3C-CAC	3.07	1.54	1.47
2	B	801	HEM	CAB-C3B	3.02	1.55	1.47
4	A	803	OU7	C02-N01	2.76	1.36	1.33
2	A	801	HEM	CMD-C2D	2.25	1.55	1.50
2	A	801	HEM	CMC-C2C	2.23	1.56	1.51
2	B	801	HEM	CMD-C2D	2.15	1.55	1.50
2	B	801	HEM	C2C-C1C	2.01	1.47	1.42

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	OU7	O29-C24-C25	7.86	126.06	115.78
4	B	803	OU7	C34-N33-C32	7.02	116.73	105.78
4	A	803	OU7	C34-N33-C32	6.81	116.40	105.78
3	B	802	H4B	C8A-C4A-C4	4.27	118.36	114.57
3	A	802	H4B	C8A-C4A-C4	4.24	118.34	114.57
4	A	803	OU7	C30-O29-C24	4.21	126.05	117.76
4	A	803	OU7	C27-C25-C26	-3.75	113.71	120.38
3	A	802	H4B	N1-C2-N3	-3.71	119.59	125.42
2	B	801	HEM	C4B-CHC-C1C	3.68	127.41	122.56
4	B	803	OU7	C26-C21-C08	-3.39	115.25	120.86
2	A	801	HEM	CBA-CAA-C2A	-3.38	106.86	112.62
3	B	802	H4B	N1-C2-N3	-3.23	120.35	125.42
3	A	802	H4B	C2-N3-C4	3.19	121.00	115.93
3	A	802	H4B	N2-C2-N3	3.19	122.21	117.25
2	A	801	HEM	C4B-CHC-C1C	3.15	126.71	122.56
4	A	803	OU7	C27-C25-C24	3.14	126.25	120.12
4	A	803	OU7	O29-C24-C23	-3.12	117.23	123.97
4	A	803	OU7	N02-C02-N01	3.03	120.77	118.26
4	A	803	OU7	C05-C10-N01	-3.02	119.61	122.81
4	A	803	OU7	O29-C30-C35	2.99	117.22	109.76
3	B	802	H4B	C2-N3-C4	2.91	120.55	115.93
4	A	803	OU7	C26-C21-C08	-2.86	116.13	120.86
4	A	803	OU7	C04-C05-C10	2.84	119.55	118.01
3	A	802	H4B	C2-N1-C8A	2.84	120.91	114.54
3	A	802	H4B	C4-C4A-N5	2.75	121.43	119.12
3	B	802	H4B	C2-N1-C8A	2.75	120.69	114.54
2	B	801	HEM	CHD-C1D-ND	2.74	127.41	124.43
2	A	801	HEM	CMC-C2C-C3C	2.72	129.77	124.68
4	B	803	OU7	C04-C05-C10	2.71	119.47	118.01
2	A	801	HEM	C2C-C3C-C4C	2.70	108.79	106.90
4	A	803	OU7	C22-C21-C08	2.64	125.94	121.36
2	A	801	HEM	C3C-C4C-NC	-2.61	106.02	110.94
2	A	801	HEM	CHD-C1D-ND	2.36	126.99	124.43
3	B	802	H4B	C4-C4A-N5	2.33	121.08	119.12
4	B	803	OU7	C05-C10-N01	-2.29	120.38	122.81
2	B	801	HEM	CMC-C2C-C3C	2.21	128.81	124.68
2	B	801	HEM	C3B-C2B-C1B	2.16	108.09	106.49
4	B	803	OU7	C22-C21-C08	2.12	125.03	121.36
4	A	803	OU7	C03-C04-C05	2.12	119.87	117.78
4	B	803	OU7	O29-C24-C25	2.11	118.54	115.78
2	A	801	HEM	CHC-C4B-C3B	2.10	127.78	124.57
2	A	801	HEM	CHB-C1B-NB	2.09	126.96	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	C3B-C2B-C1B	2.09	108.04	106.49
4	A	803	OU7	C23-C24-C25	-2.08	116.70	120.21
2	A	801	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
2	B	801	HEM	CHA-C4D-ND	2.03	126.88	124.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
4	A	803	OU7	C25-C24-O29-C30
4	A	803	OU7	C23-C24-O29-C30
2	B	801	HEM	C2D-C3D-CAD-CBD
2	B	801	HEM	C4D-C3D-CAD-CBD
4	A	803	OU7	C24-C25-C27-N28
4	B	803	OU7	C24-C25-C27-N28
2	A	801	HEM	C2A-CAA-CBA-CGA
2	B	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	C4D-C3D-CAD-CBD
2	A	801	HEM	C2D-C3D-CAD-CBD
4	A	803	OU7	C35-C30-O29-C24
3	A	802	H4B	C7-C6-C9-C10
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAD-CBD-CGD-O2D
4	B	803	OU7	C07-C08-C21-C26
2	B	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	C4B-C3B-CAB-CBB
3	B	802	H4B	C7-C6-C9-C10
4	B	803	OU7	C23-C24-O29-C30
2	A	801	HEM	CAD-CBD-CGD-O1D
3	A	802	H4B	N5-C6-C9-O9

There are no ring outliers.

No monomer is involved in short contacts.

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 OU7 B 803

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 801

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand OU7 A 803

Bond lengths

Bond angles

Torsions

Rings
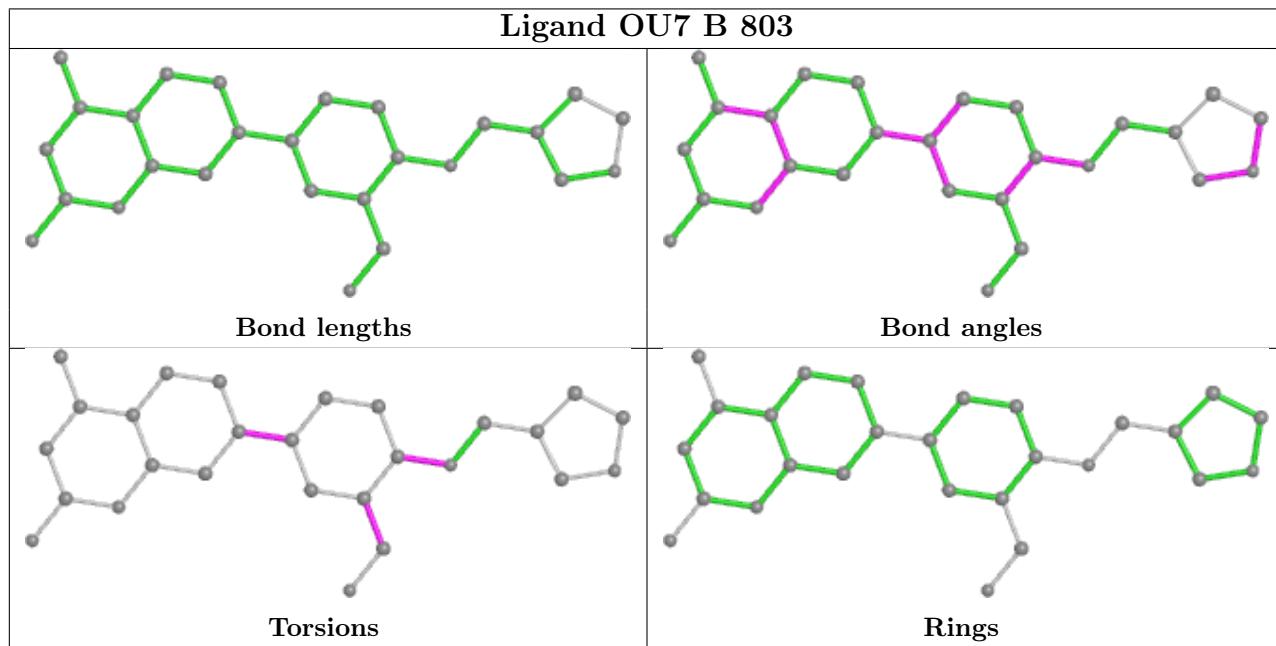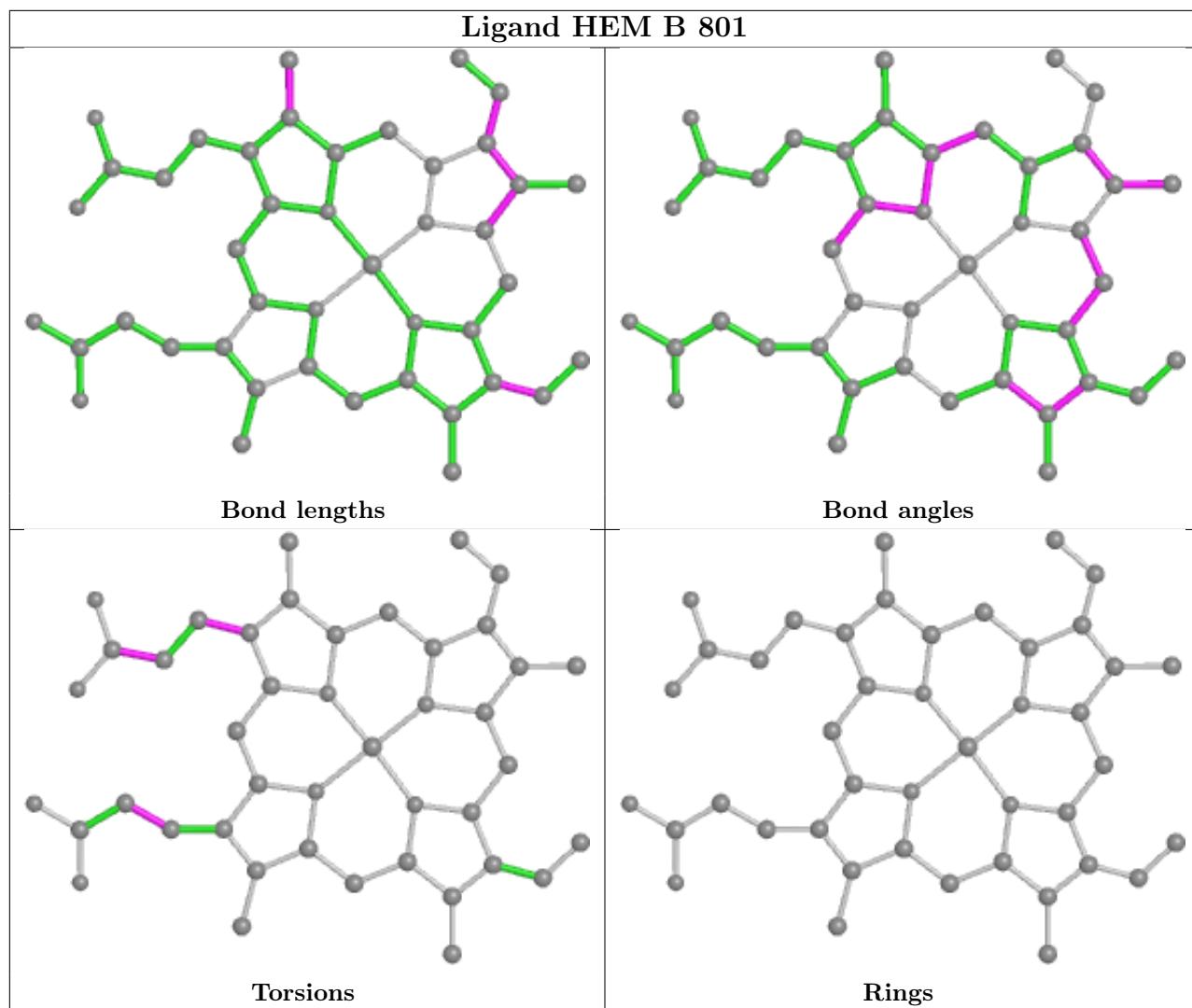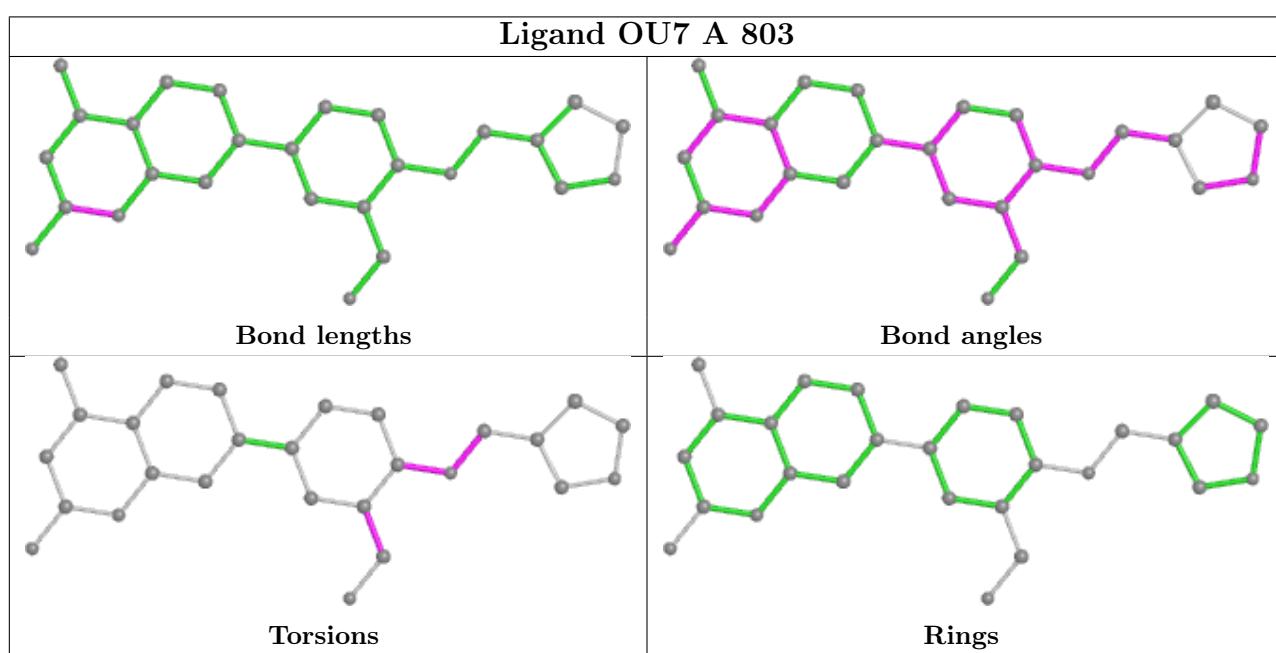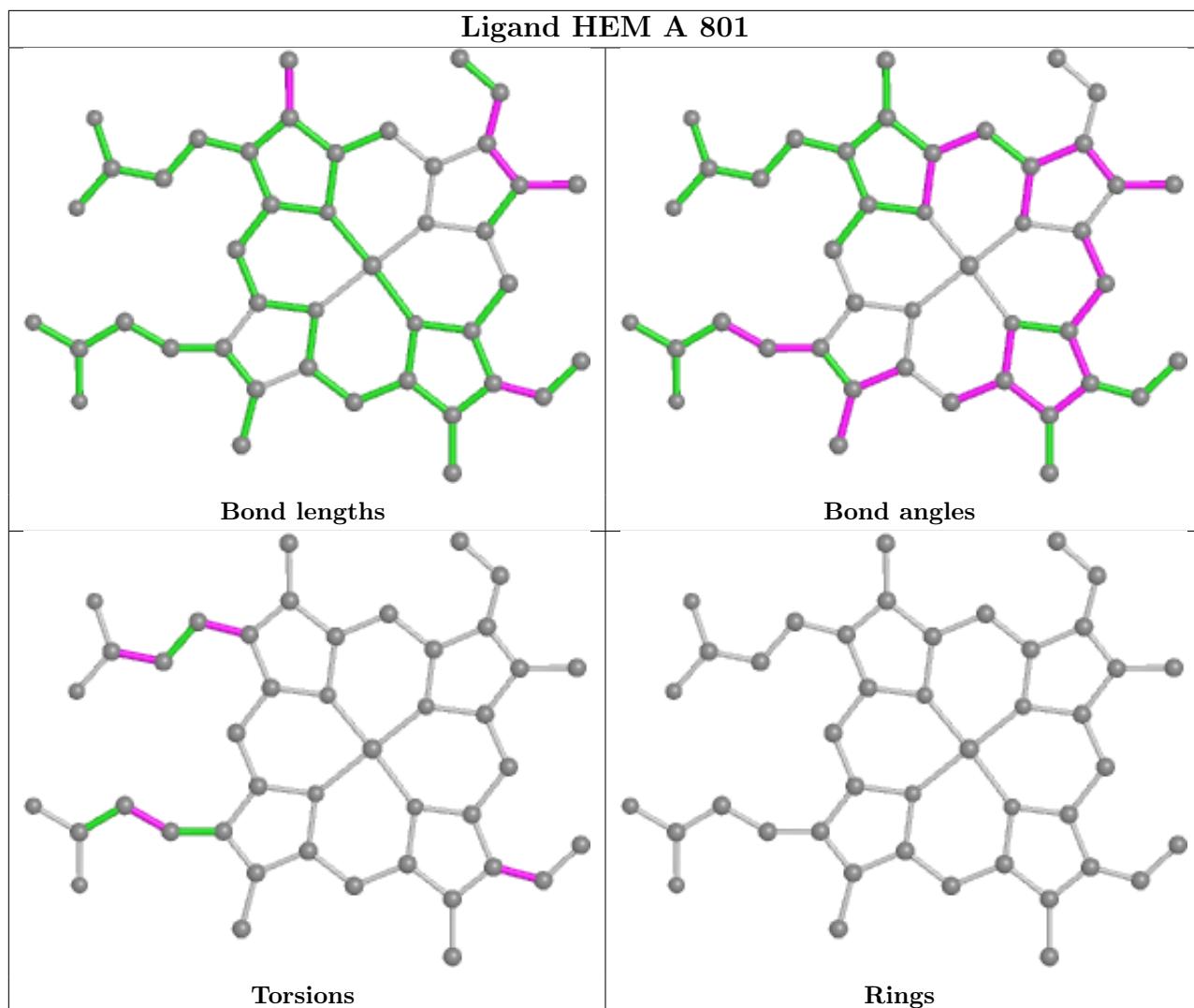
4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.