WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 06:20 AM EDT

PDB ID	:	6VZA
Title	:	Crystal structure of cytochrome P450 NasF5053 Q65I-A86G mutant variant from Streptomyces sp. NRRL F-5053 in the cyclo-L-Trp-L-Pro-bound state
Authors	:	Luo, Z.; Jia, X.; Sun, C.; Qu, X.; Kobe, B.
Deposited on	:	2020-02-28
Resolution	:	1.47 Å(reported)

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 1.47 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 (i)

There are 8 unique types of molecules in this entry. The entry contains 6635 atoms, of which 3067 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 cytochrome P450 NasF5053.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	393	Total 6045	C 1922	H 2995	N 552	O 563	S 13	0	4	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Na 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

HEM

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
5	A	1	73	34	1	30	4	4	0	0

- Molecule 6 is (3S,8aS)-3-(1H-indol-3-ylmethyl)hexahydropyrrolo[1,2-a]pyrazine-1,4-d ione (three-letter code: QRP) (formula: $C_{16}H_{17}N_3O_2$) (labeled as "Ligand of Interest" by depositor).

QRP
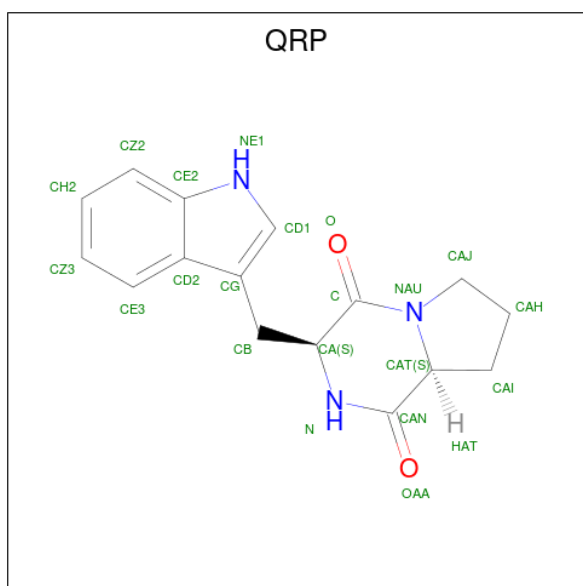
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
6	A	1	38	16	17	3	2	0	0
6	A	1	Total	C	H	N	O	0	0
			38	16	17	3	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	423	Total	O	0	0
			423	423		

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

3 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.23Å 91.31Å 93.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.23 – 1.47	Depositor
% Data completeness (in resolution range)	98.4 (42.23-1.47)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.20 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.154 , 0.180	Depositor
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.413	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
Total number of atoms	6635	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	QRP	A	406	-	23,24,24	2.36	9 (39%)	31,35,35	2.37	11 (35%)
6	QRP	A	407	-	23,24,24	2.77	11 (47%)	31,35,35	2.97	10 (32%)
7	GOL	A	408	-	5,5,5	0.65	0	5,5,5	1.37	1 (20%)
5	HEM	A	405	1	41,50,50	1.43	4 (9%)	45,82,82	1.72	9 (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
6	QRP	A	406	-	-	0/3/30/30	0/4/4/4
6	QRP	A	407	-	-	0/3/30/30	0/4/4/4
7	GOL	A	408	-	-	0/4/4/4	-
5	HEM	A	405	1	-	3/12/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	QRP	CAT-NAU	-5.52	1.35	1.47
6	A	407	QRP	CAJ-NAU	5.41	1.58	1.47
6	A	407	QRP	C-NAU	5.07	1.45	1.34
6	A	406	QRP	CAN-N	4.92	1.41	1.33
6	A	406	QRP	CAJ-NAU	4.90	1.57	1.47
6	A	407	QRP	CAN-N	4.47	1.40	1.33
6	A	407	QRP	CB-CA	3.97	1.63	1.54
6	A	407	QRP	CA-N	-3.79	1.40	1.46
5	A	405	HEM	C3C-C2C	-3.79	1.35	1.40
6	A	406	QRP	CAT-NAU	-3.62	1.39	1.47
6	A	406	QRP	C-NAU	3.62	1.42	1.34
6	A	407	QRP	CAH-CAJ	-3.23	1.40	1.51
5	A	405	HEM	C3C-CAC	3.07	1.54	1.47
6	A	406	QRP	CA-C	-2.99	1.48	1.52
6	A	406	QRP	CAH-CAJ	-2.91	1.41	1.51
5	A	405	HEM	CAA-C2A	2.78	1.56	1.52
5	A	405	HEM	CAB-C3B	2.74	1.54	1.47
6	A	406	QRP	CB-CA	2.69	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	QRP	CAI-CAT	2.60	1.60	1.53
6	A	406	QRP	CAI-CAT	2.54	1.60	1.53
6	A	406	QRP	CA-N	-2.54	1.42	1.46
6	A	407	QRP	CB-CG	2.37	1.57	1.51
6	A	407	QRP	CA-C	-2.16	1.49	1.52
6	A	407	QRP	CAH-CAI	2.00	1.60	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	407	QRP	CB-CG-CD1	-9.12	116.69	127.97
6	A	406	QRP	CB-CG-CD1	-7.33	118.91	127.97
6	A	407	QRP	CAJ-NAU-C	5.73	133.11	123.10
6	A	407	QRP	CB-CG-CD2	5.69	135.10	126.25
6	A	407	QRP	CAJ-NAU-CAT	-5.18	103.79	112.00
6	A	407	QRP	C-CA-N	5.08	122.05	112.60
6	A	406	QRP	CB-CG-CD2	5.02	134.06	126.25
6	A	407	QRP	CB-CA-C	-4.76	100.55	109.91
6	A	406	QRP	CG-CB-CA	-4.12	105.38	113.45
5	A	405	HEM	C4A-C3A-C2A	4.05	109.82	107.00
5	A	405	HEM	C2C-C3C-C4C	4.03	109.71	106.90
6	A	406	QRP	CAI-CAT-CAN	-3.87	108.26	116.23
5	A	405	HEM	C4B-CHC-C1C	3.79	127.56	122.56
6	A	407	QRP	CAN-CAT-NAU	3.59	121.32	112.33
6	A	407	QRP	O-C-NAU	-3.42	118.09	123.03
5	A	405	HEM	CMA-C3A-C4A	-3.39	123.26	128.46
6	A	406	QRP	O-C-CA	3.14	127.34	120.58
6	A	406	QRP	CB-CA-N	-2.97	107.51	111.33
6	A	407	QRP	O-C-CA	2.84	126.71	120.58
5	A	405	HEM	CMC-C2C-C3C	2.82	129.95	124.68
5	A	405	HEM	C3B-C2B-C1B	2.81	108.57	106.49
5	A	405	HEM	C4C-CHD-C1D	2.76	126.19	122.56
5	A	405	HEM	O1D-CGD-CBD	-2.68	114.47	123.08
7	A	408	GOL	C3-C2-C1	-2.53	101.88	111.70
6	A	406	QRP	CA-C-NAU	-2.34	111.24	116.91
5	A	405	HEM	C4D-ND-C1D	2.31	107.46	105.07
6	A	406	QRP	C-CA-N	2.25	116.79	112.60
6	A	406	QRP	CAT-CAN-N	-2.21	112.68	117.16
6	A	407	QRP	CAI-CAT-NAU	-2.17	99.81	103.03
6	A	406	QRP	CE3-CD2-CG	-2.15	130.48	134.42
6	A	406	QRP	CA-N-CAN	-2.02	121.34	125.81

There are no chirality outliers.
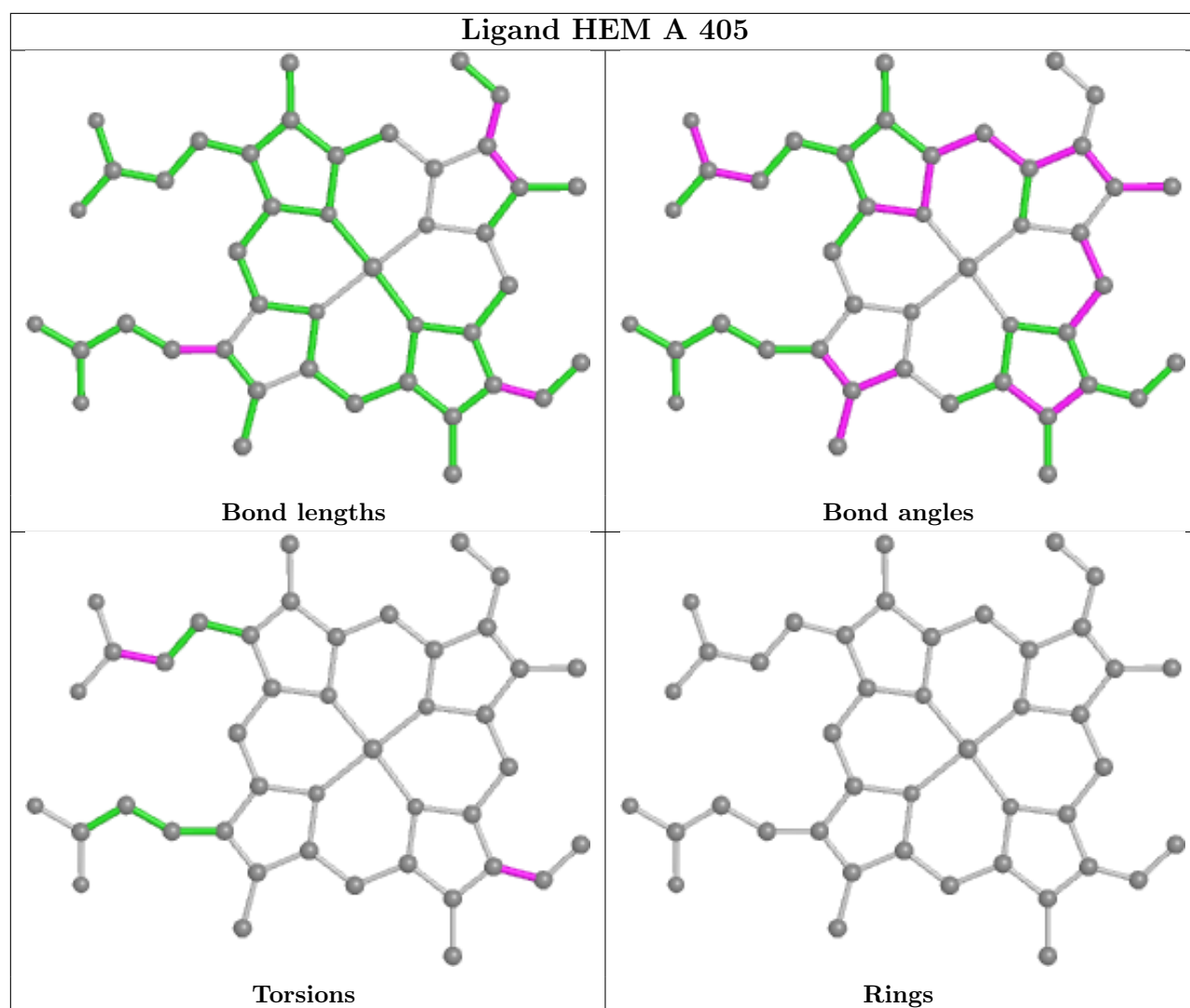
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	HEM	C4B-C3B-CAB-CBB
5	A	405	HEM	CAD-CBD-CGD-O2D
5	A	405	HEM	CAD-CBD-CGD-O1D

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 QRP A 406

Bond lengths

Bond angles

Torsions

Rings

Ligand QRP A 407

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 405

Bond lengths

Bond angles

Torsions

Rings
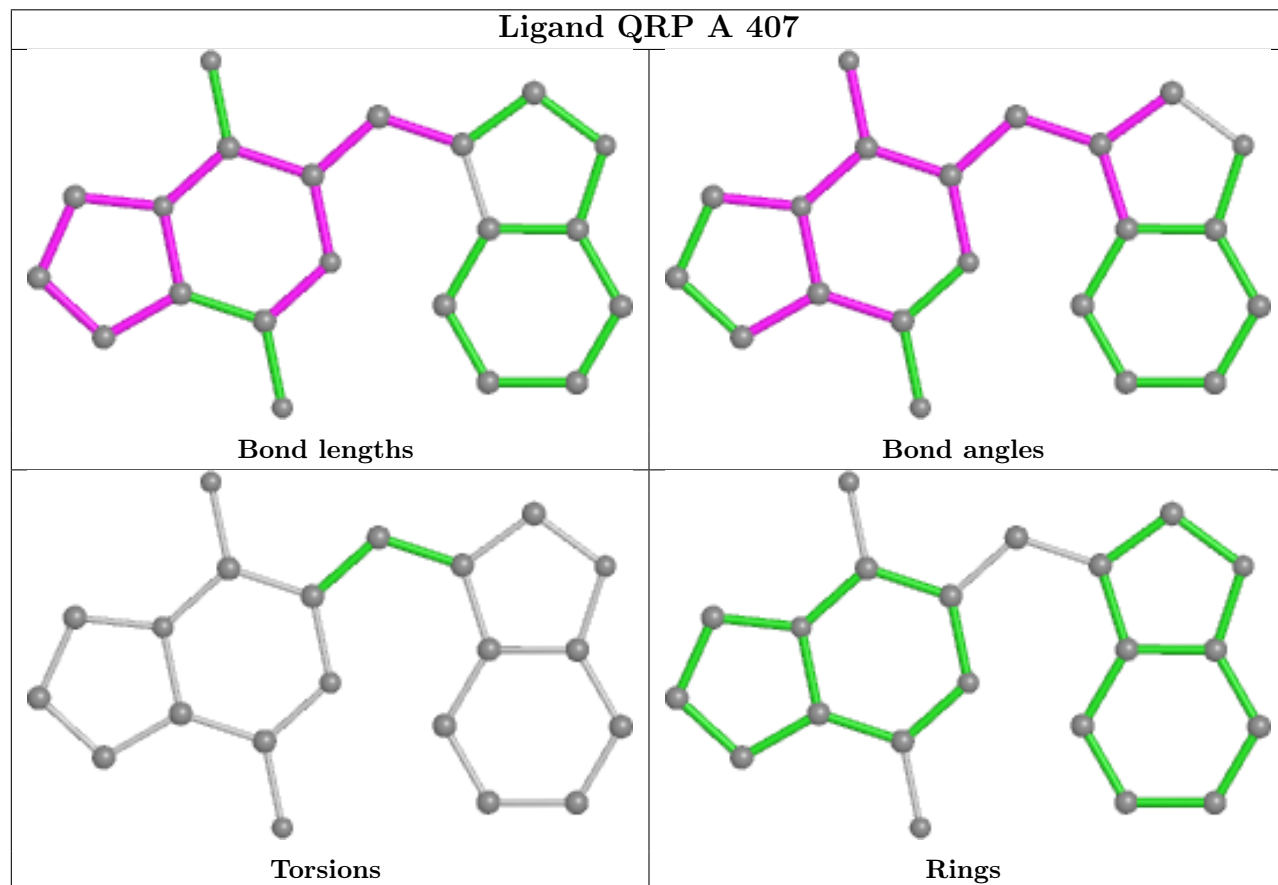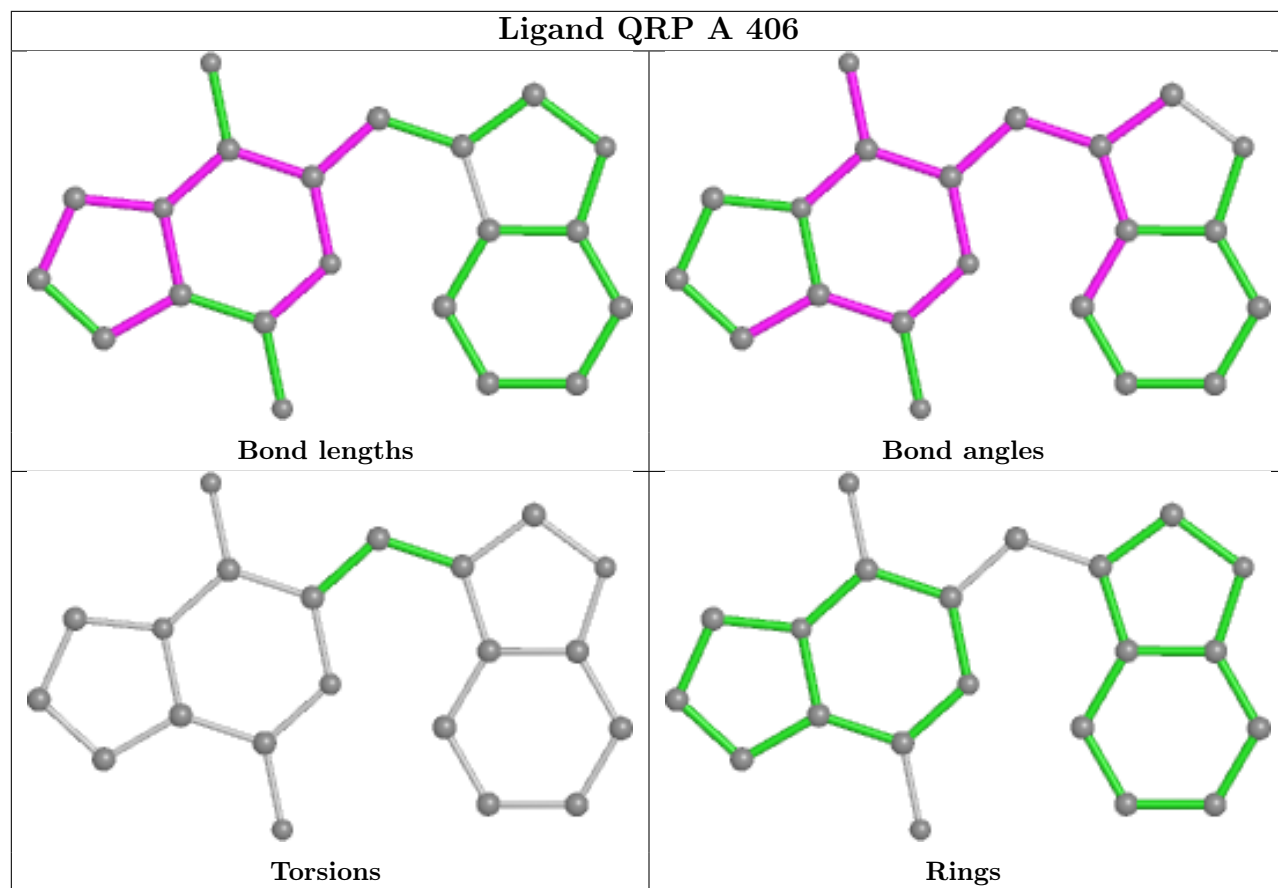
4.7 Other polymers ⓘ

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.