Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 05:45 AM EDT

PDB ID	:	6VXV
Title	:	Crystal structure of cyclo-L-Trp-L-Pro-bound cytochrome P450 NasF5053 from Streptomyces sp. NRRL F-5053
Authors	:	Luo, Z.; Jia, X.; Sun, C.; Qu, X.; Kobe, B.
Deposited on	:	2020-02-24
Resolution	:	1.60 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	:	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 (i)

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

The reported resolution of this entry is 1.60 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 6 unique types of molecules in this entry. The entry contains 3570 atoms, of which 64 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.

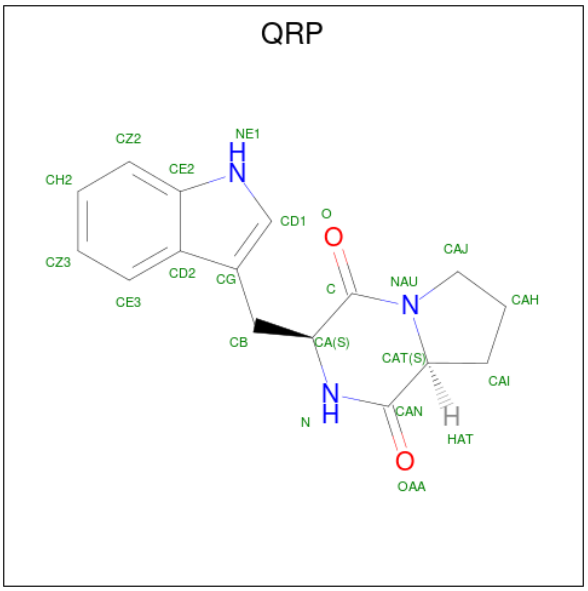
- Molecule 1 is a protein called cytochrome P450 NasF5053.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	3	0
			3068	1928	561	567	12			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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



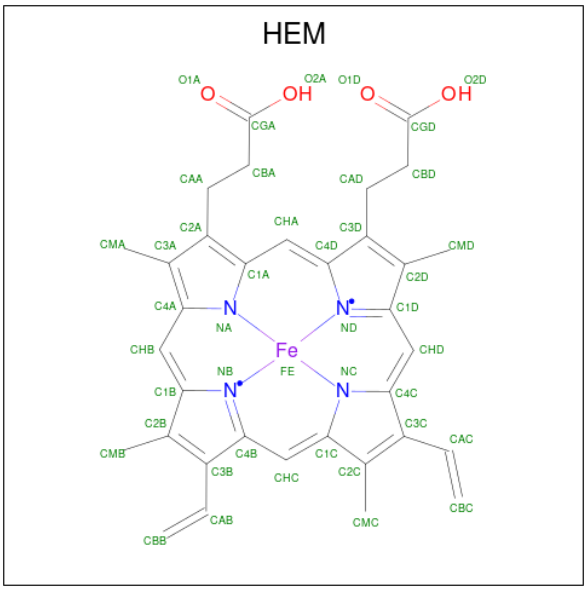
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			38	16	17	3	2		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	351	Total	O	0	0
			351	351		

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 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.31Å 91.84Å 93.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 1.60	Depositor
% Data completeness (in resolution range)	99.7 (46.80-1.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.170 , 0.203	Depositor
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.451	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
Total number of atoms	3570	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	HEM	A	404	1	41,50,50	1.44	5 (12%)	45,82,82	1.54	9 (20%)
3	QRP	A	403	-	23,24,24	2.99	10 (43%)	31,35,35	3.13	11 (35%)
3	QRP	A	402	-	23,24,24	2.82	9 (39%)	31,35,35	2.77	14 (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
4	HEM	A	404	1	-	2/12/54/54	-
3	QRP	A	403	-	-	0/3/30/30	0/4/4/4
3	QRP	A	402	-	-	0/3/30/30	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	QRP	CAJ-NAU	7.09	1.61	1.47
3	A	402	QRP	CAJ-NAU	6.72	1.60	1.47
3	A	402	QRP	CAN-N	6.15	1.43	1.33
3	A	403	QRP	CAT-NAU	-5.75	1.35	1.47
3	A	403	QRP	CAN-N	5.07	1.41	1.33
3	A	402	QRP	C-NAU	5.01	1.45	1.34
3	A	403	QRP	C-NAU	4.82	1.44	1.34
4	A	404	HEM	C3C-C2C	-4.55	1.34	1.40
3	A	402	QRP	CAT-NAU	-4.13	1.38	1.47
3	A	402	QRP	CAH-CAJ	-3.70	1.38	1.51
3	A	403	QRP	CAH-CAJ	-3.65	1.39	1.51
3	A	403	QRP	CB-CA	3.44	1.62	1.54
3	A	403	QRP	CA-N	-3.35	1.41	1.46
4	A	404	HEM	C3C-CAC	3.24	1.54	1.47
3	A	403	QRP	CAI-CAT	3.08	1.61	1.53
3	A	402	QRP	CB-CA	2.89	1.61	1.54
3	A	403	QRP	CB-CG	2.75	1.59	1.51
3	A	402	QRP	CAI-CAT	2.66	1.60	1.53
4	A	404	HEM	CAB-C3B	2.48	1.54	1.47
4	A	404	HEM	CAA-C2A	2.35	1.55	1.52
3	A	402	QRP	CB-CG	2.25	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	QRP	CAT-CAN	2.24	1.56	1.51
4	A	404	HEM	CMB-C2B	2.05	1.55	1.50
3	A	403	QRP	CAT-CAN	2.03	1.56	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	QRP	CB-CG-CD1	-8.45	117.53	127.97
3	A	403	QRP	CB-CG-CD1	-8.38	117.62	127.97
3	A	403	QRP	C-CA-N	6.97	125.57	112.60
3	A	403	QRP	CAJ-NAU-C	6.39	134.27	123.10
3	A	403	QRP	CB-CG-CD2	6.36	136.15	126.25
3	A	402	QRP	CB-CG-CD2	5.83	135.32	126.25
3	A	403	QRP	CAN-CAT-NAU	4.92	124.66	112.33
3	A	403	QRP	CAJ-NAU-CAT	-4.58	104.74	112.00
3	A	402	QRP	CAI-CAT-CAN	-4.45	107.05	116.23
3	A	402	QRP	CG-CB-CA	-4.43	104.77	113.45
3	A	403	QRP	CB-CA-C	-3.61	102.81	109.91
3	A	402	QRP	CAT-CAN-N	-3.54	109.98	117.16
4	A	404	HEM	CMA-C3A-C4A	-3.54	123.02	128.46
3	A	403	QRP	CB-CA-N	-3.19	107.23	111.33
3	A	402	QRP	CB-CA-N	-3.16	107.27	111.33
4	A	404	HEM	C1B-NB-C4B	3.04	108.21	105.07
3	A	402	QRP	CA-N-CAN	-2.99	119.18	125.81
3	A	402	QRP	C-CA-N	2.86	117.92	112.60
3	A	402	QRP	O-C-CA	2.71	126.41	120.58
3	A	403	QRP	CA-N-CAN	-2.67	119.88	125.81
3	A	402	QRP	CAN-CAT-NAU	2.64	118.94	112.33
3	A	402	QRP	CAJ-NAU-C	2.63	127.69	123.10
3	A	402	QRP	OAA-CAN-N	2.46	126.01	122.69
3	A	402	QRP	CA-C-NAU	-2.41	111.06	116.91
4	A	404	HEM	C4C-CHD-C1D	2.39	125.71	122.56
4	A	404	HEM	C4D-ND-C1D	2.32	107.47	105.07
4	A	404	HEM	O2A-CGA-CBA	2.31	121.44	114.03
3	A	402	QRP	CAT-NAU-C	-2.27	119.67	124.30
4	A	404	HEM	CHB-C1B-NB	2.17	127.07	124.38
4	A	404	HEM	C4B-CHC-C1C	2.15	125.39	122.56
3	A	403	QRP	CAI-CAT-NAU	-2.10	99.91	103.03
4	A	404	HEM	O1A-CGA-CBA	-2.10	116.34	123.08
3	A	403	QRP	O-C-CA	2.03	124.95	120.58
4	A	404	HEM	C2C-C3C-C4C	2.02	108.31	106.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

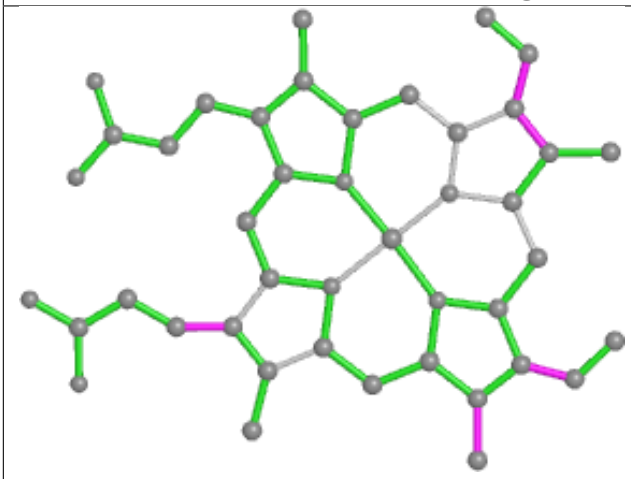
Mol	Chain	Res	Type	Atoms
4	A	404	HEM	CAA-CBA-CGA-O2A
4	A	404	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

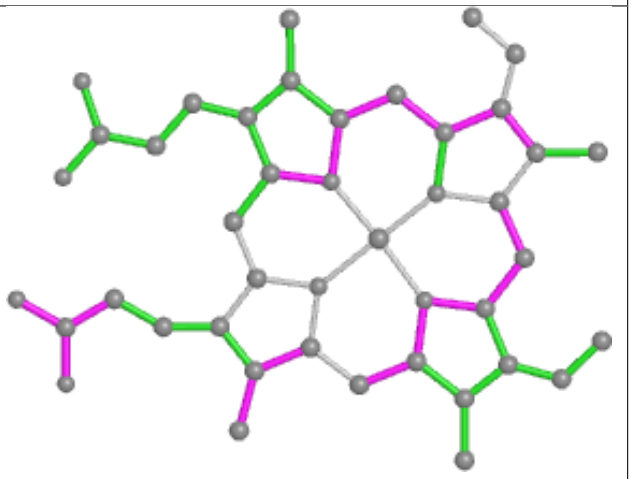
No monomer is involved in short contacts.

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.

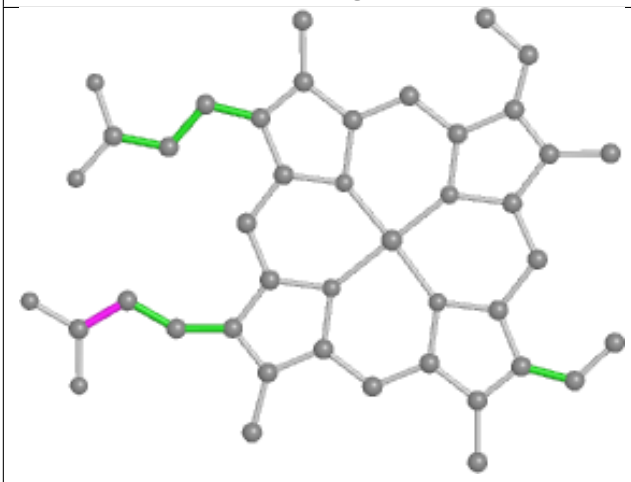
Ligand HEM A 404



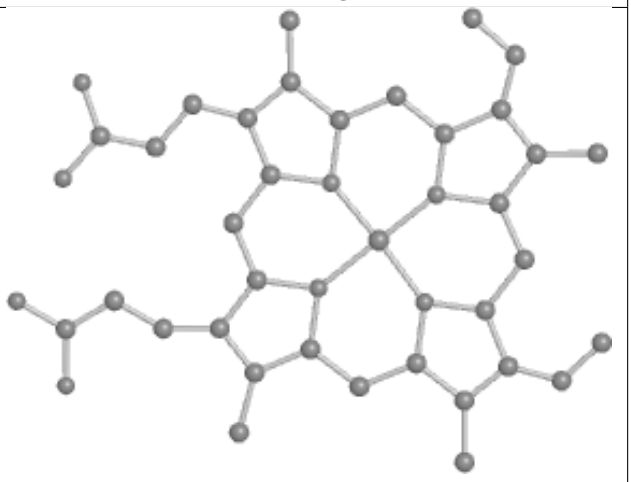
Bond lengths



Bond angles

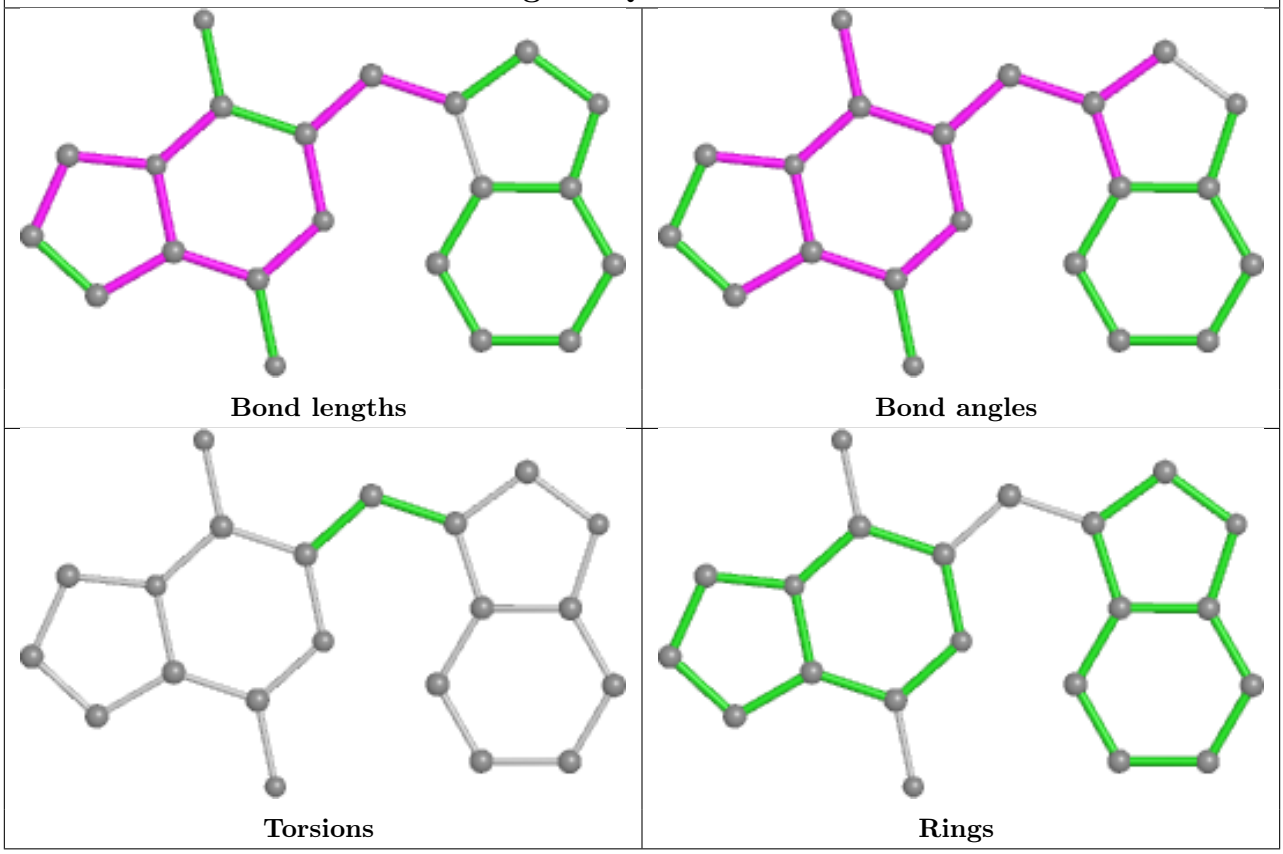


Torsions

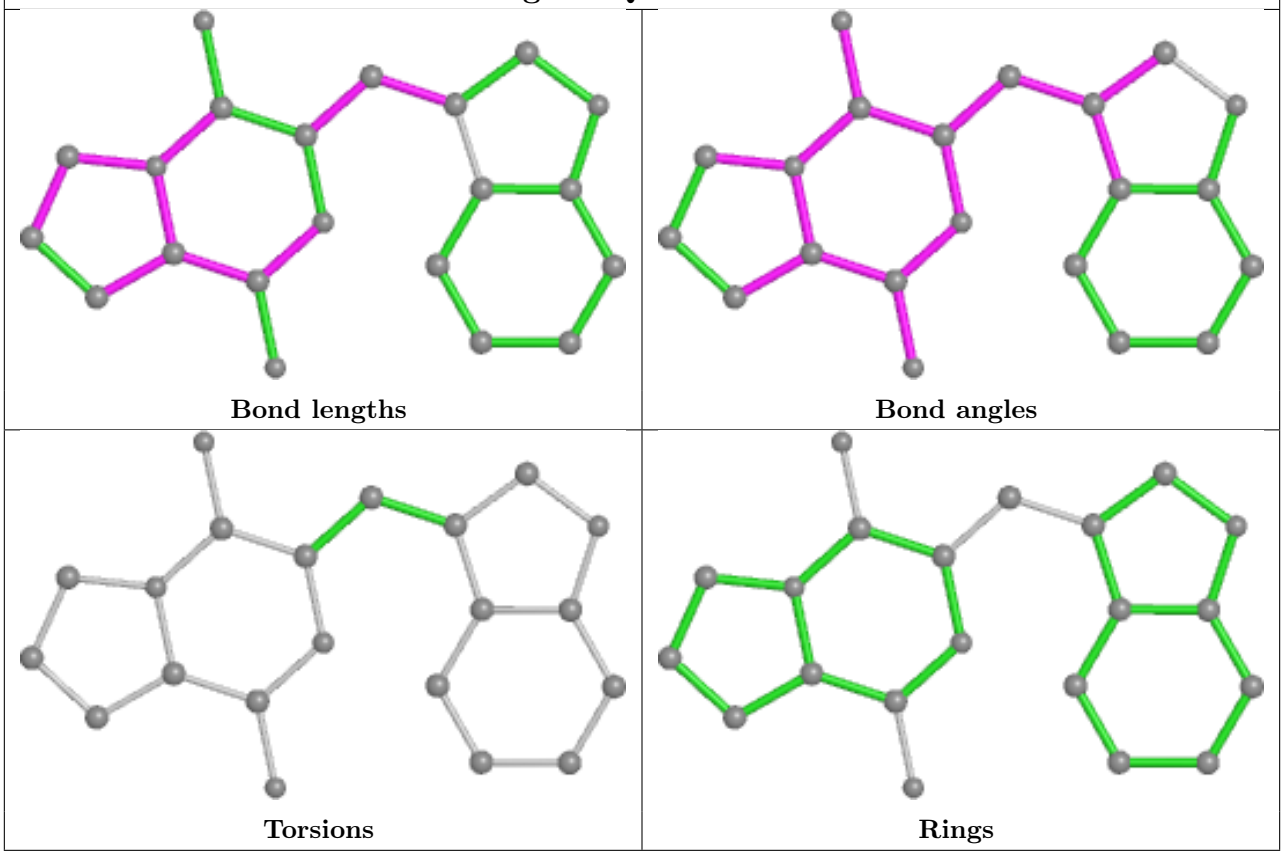


Rings

Ligand QRP A 403



Ligand QRP A 402



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

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.