

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 5, 2023 – 09:17 AM EDT

PDB ID	:	6VVV
Title	:	Crystal structure of a Mycobacterium smegmatis transcription initiation com-
		plex with Rifampicin-resistant RNA polymerase
Authors	:	Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2020-02-18
Resolution	:	3.20 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 (i) 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 (1)) 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:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 3.20 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.



#### 6VVV

# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 22970 atoms, of which 16 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 RNA polymerase-binding protein RbpA.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	J	88	Total 678	C 425	N 122	0 129	${ m S} { m 2}$	0	0	0

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	А	223	Total C N 1645 1038 28	O S 320 3	0	0	0
2	В	235	Total         C         N           1643         1037         29	O S 312 1	0	0	0
2	Т	53	Total         C         N           374         236         65	0 0	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
3	С	790	Total 5774	C 3620	N 1008	0 1121	S 25	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	447	LEU	SER	conflict	UNP P60281

• Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues		А	toms			ZeroOcc	AltConf	Trace
4	D	1174	Total 8679	C 5438	N 1548	O 1654	S 39	0	0	0

• Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.



Mol	Chain	Residues		Ato	$\mathbf{ms}$		ZeroOcc	AltConf	Trace
5	Ε	77	Total 586	C 372	N 100	0 114	0	0	0

• Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	F	302	Total 2349	C 1474	N 423	O 445	${ m S} 7$	0	0	0

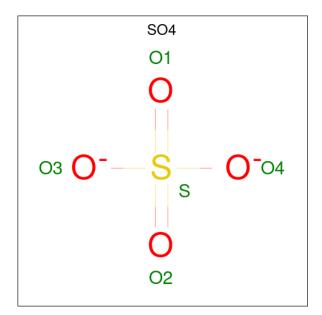
• Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
7	0	31	Total 635		N 114	O 185	Р 30	0	0	0

• Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
8	Р	26	Total 526	C 254	N 94	0 153	Р 25	0	0	0

• Molecule 9 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 2 & 1 & 1 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
9	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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• Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	С	1	$\begin{array}{ccc} \text{Total} & \text{H} & \text{O} \\ 3 & 2 & 1 \end{array}$	0	0
11	D	3	Total         H         O           9         6         3	0	0
11	F	3	Total         H         O           9         6         3	0	0
11	Р	1	$\begin{array}{ccc} \text{Total} & \text{H} & \text{O} \\ 3 & 2 & 1 \end{array}$	0	0

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



# 3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	129.75Å 162.34Å 137.16Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $111.27^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	49.83 - 3.20	Depositor	
% Data completeness	95.5 (49.83-3.20)	Depositor	
(in resolution range)	55.5 (45.05-5.20)	Depositor	
R <sub>merge</sub>	0.15	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.03 (at 3.19 \text{\AA})$	Xtriage	
Refinement program	PHENIX v0	Depositor	
$R, R_{free}$	0.234 , $0.262$	Depositor	
Wilson B-factor $(Å^2)$	119.1	Xtriage	
Anisotropy	0.081	Xtriage	
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	22970	wwPDB-VP	
Average B, all atoms $(Å^2)$	117.0	wwPDB-VP	

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 4 Model quality (i)

## 4.1 Standard geometry (i)

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

### 4.2 Too-close contacts (i)

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

### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

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

#### 4.3.2 Protein sidechains (i)

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

### 4.3.3 RNA (i)

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

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

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

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 4.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are 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



			-				- · ·	<i></i> ,		
Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
9	SO4	D	1408	-	4,4,4	0.14	0	$6,\!6,\!6$	0.07	0
9	SO4	D	1403	-	4,4,4	0.15	0	$6,\!6,\!6$	0.07	0
9	SO4	F	1202	-	4,4,4	0.14	0	$6,\!6,\!6$	0.04	0
9	SO4	D	1405	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
9	SO4	D	1407	-	4,4,4	0.15	0	$6,\!6,\!6$	0.05	0
9	SO4	D	1406	-	4,4,4	0.14	0	$6,\!6,\!6$	0.04	0
9	SO4	F	1204	-	4,4,4	0.13	0	$6,\!6,\!6$	0.09	0
9	SO4	D	1402	-	0,1,4	-	-	-		
9	SO4	F	1203	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
9	SO4	F	1201	-	4,4,4	0.15	0	$6,\!6,\!6$	0.06	0
9	SO4	D	1404	-	4,4,4	0.14	0	$6,\!6,\!6$	0.04	0

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).

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

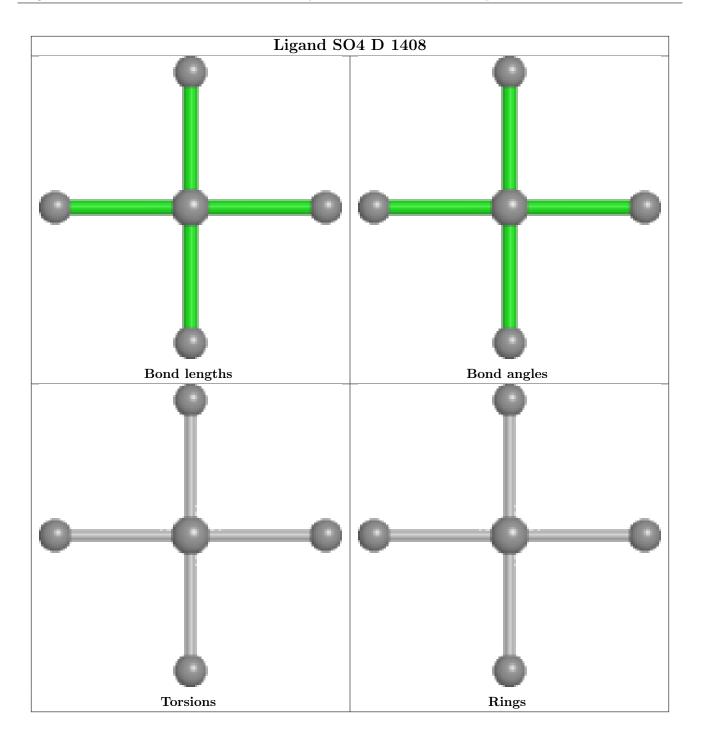
There are no ring outliers.

1 monomer is involved in 1 short contact:

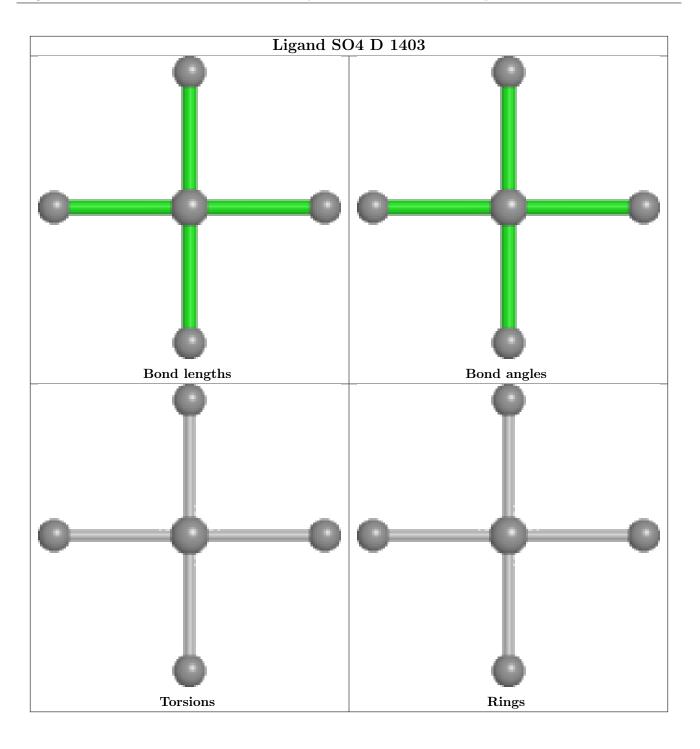
Mol	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
9	F	1201	SO4	0	1

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 sup 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.

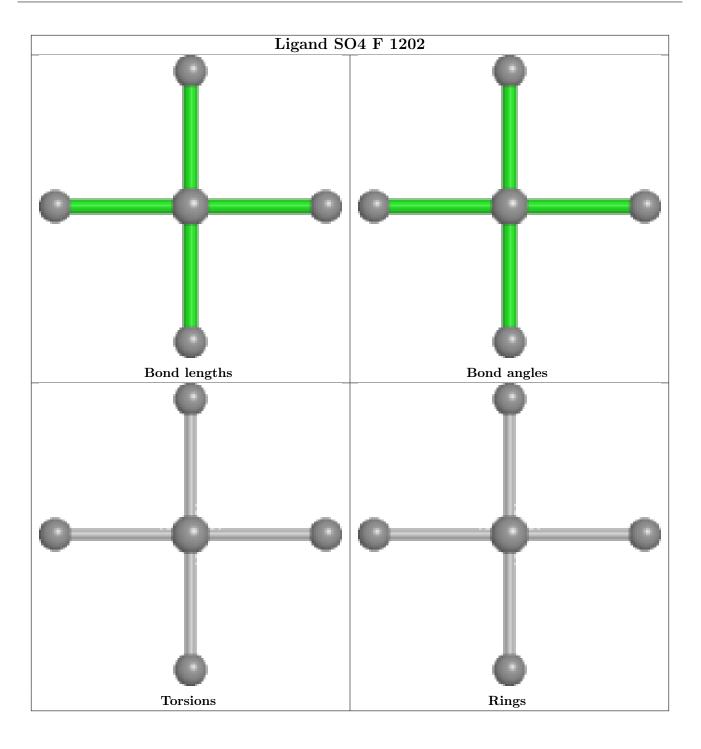




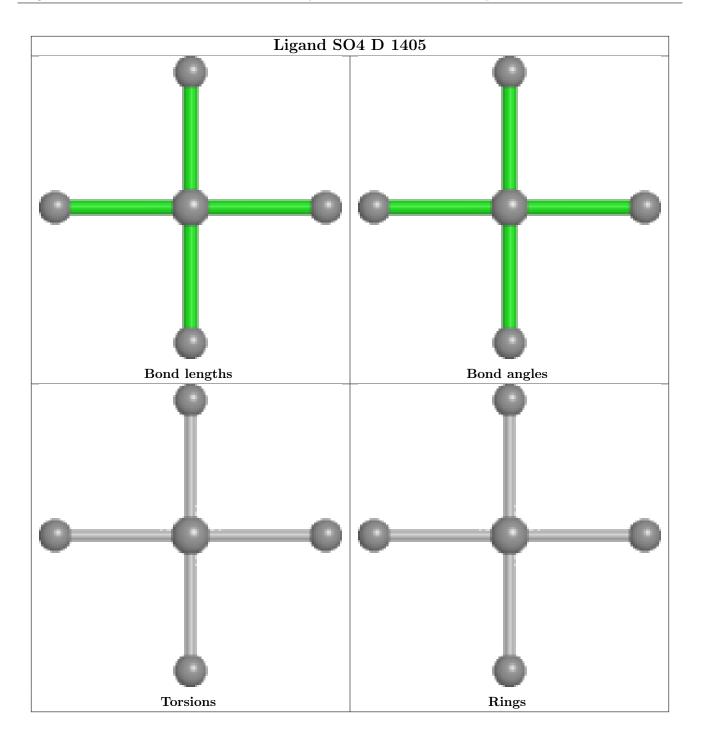




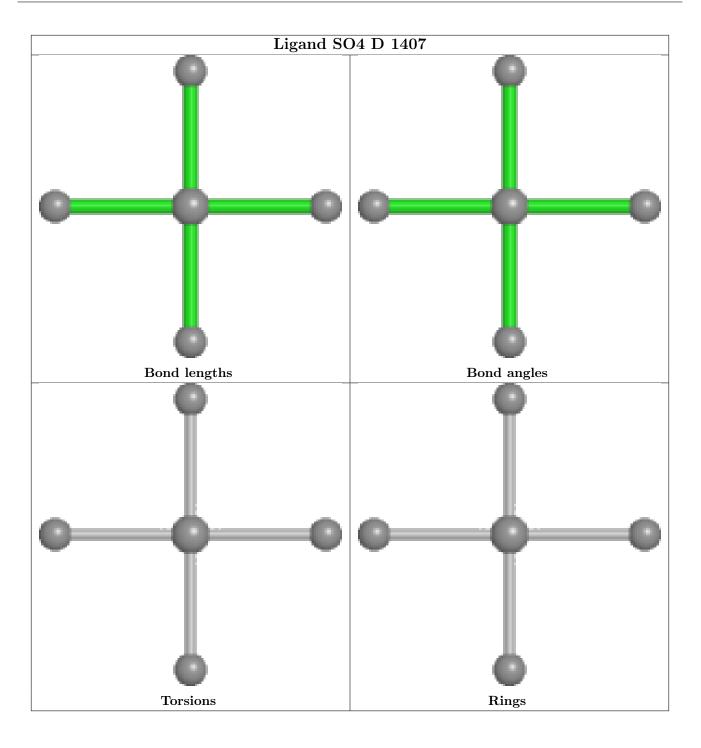




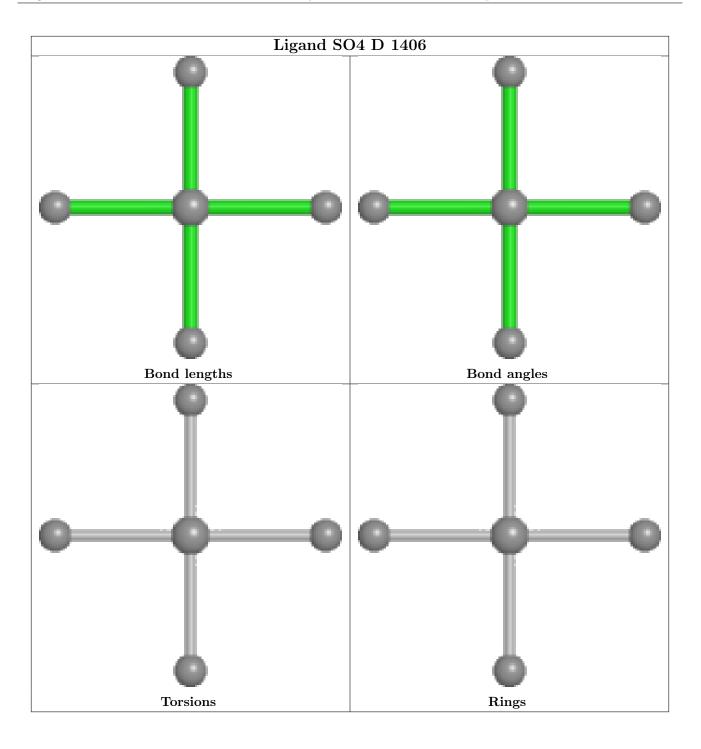




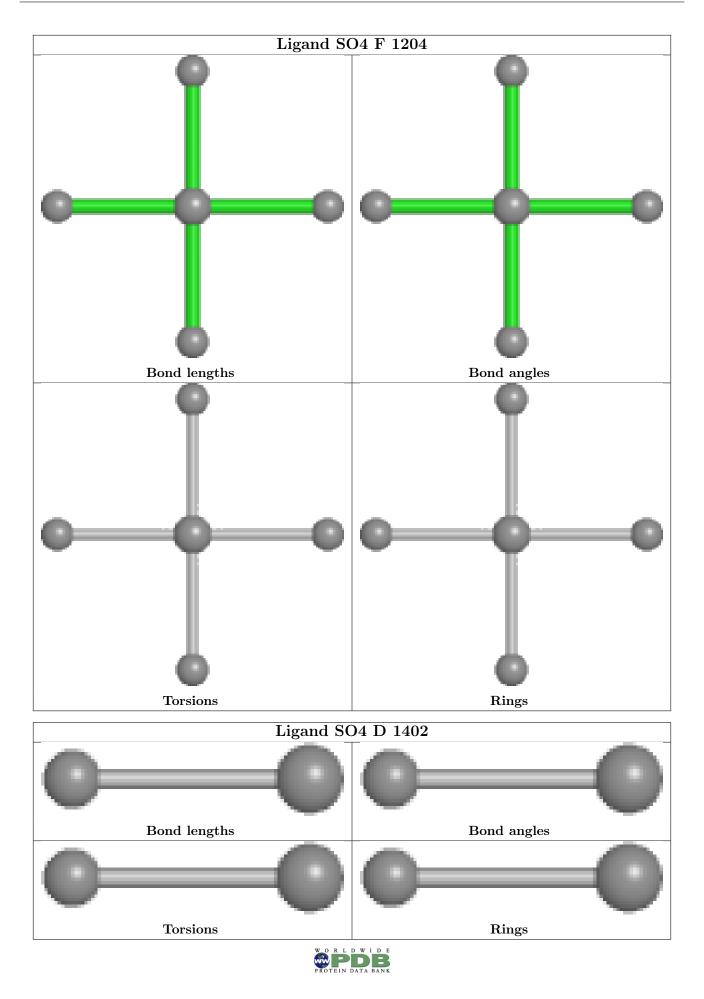


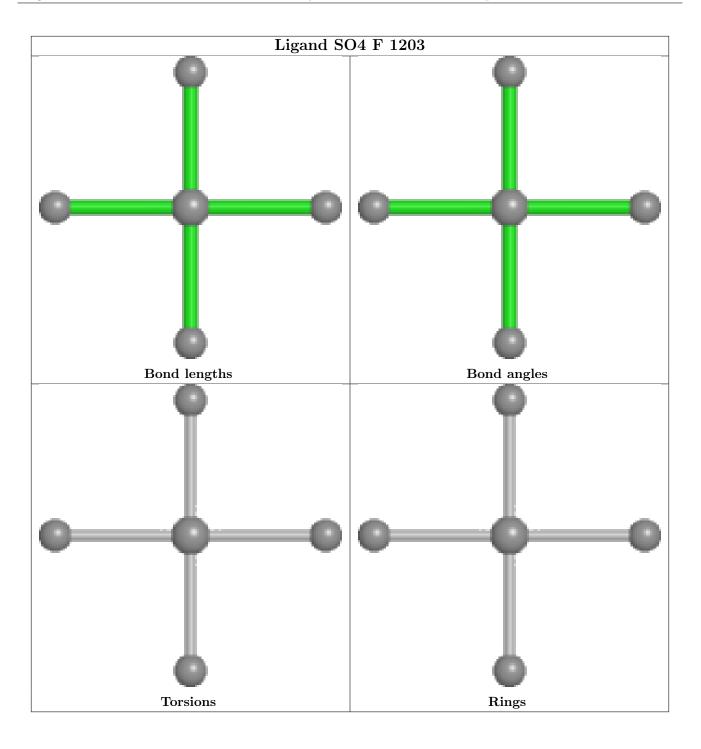




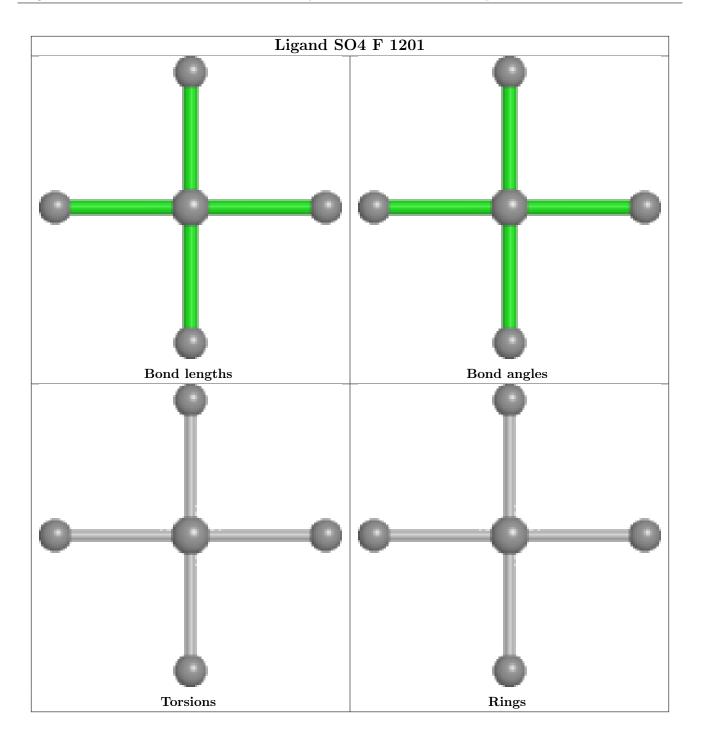




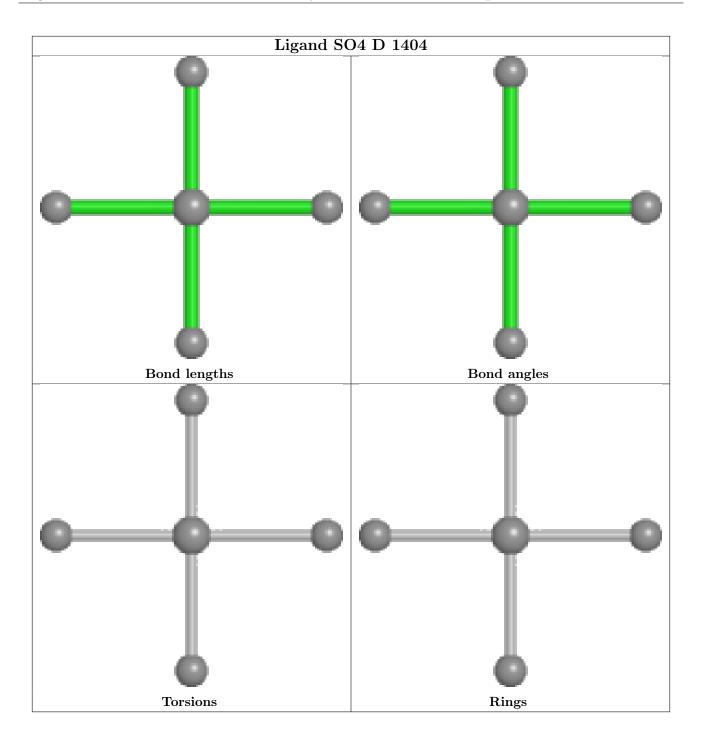




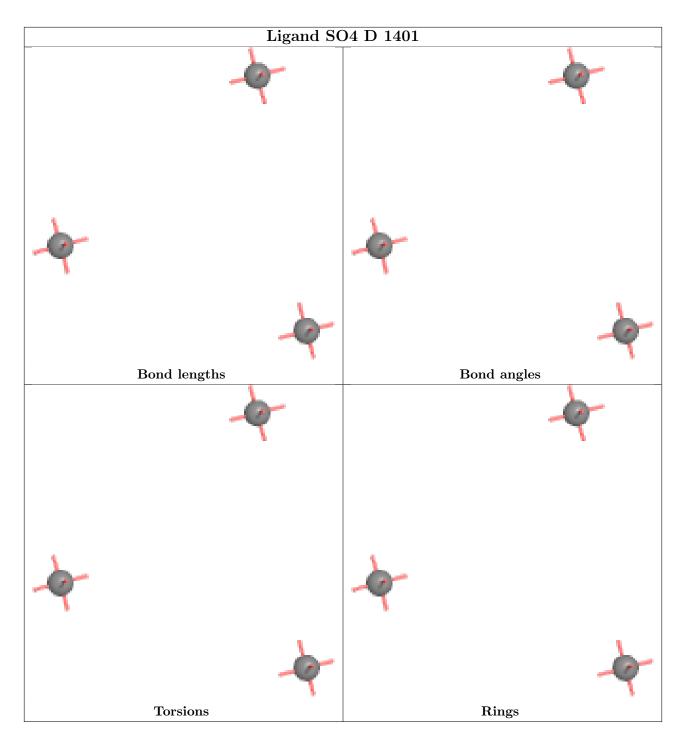












## 4.7 Other polymers (i)

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 (i)

## 5.1 Protein, DNA and RNA chains (i)

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

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

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

## 5.3 Carbohydrates (i)

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

## 5.4 Ligands (i)

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

### 5.5 Other polymers (i)

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

