

Full wwPDB X-ray Structure Validation Report (i)

Jan 22, 2023 - 12:19 am GMT

PDB ID : 8ABT

Title : Crystal structure of NaLdpA in complex with the product analog Resveratrol

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Deposited on : 2022-07-04

Resolution : 1.39 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: 4.02b-467

Mogul : 1.8.4, 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)

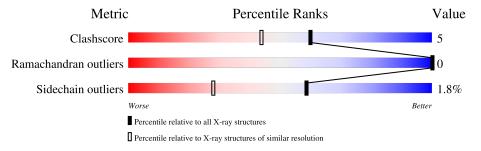
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.39 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	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	A	251	86%	7%	6%
1	В	251	82%	12%	• 6%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8033 atoms, of which 3722 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 SnoaL-like domain-containing protein.

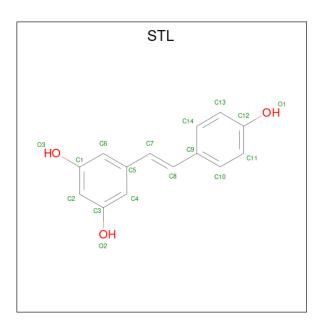
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	235	Total 3737	C 1223	H 1837	N 325	O 346	S 6	41	1	0
1	В	236	Total 3775	C 1232		N 330	O 346	S 6	42	2	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	LEU	-	expression tag	UNP Q2G4I2
A	245	GLU	-	expression tag	UNP Q2G4I2
A	246	HIS	-	expression tag	UNP Q2G4I2
A	247	HIS	-	expression tag	UNP Q2G4I2
A	248	HIS	-	expression tag	UNP Q2G4I2
A	249	HIS	-	expression tag	UNP Q2G4I2
A	250	HIS	-	expression tag	UNP Q2G4I2
A	251	HIS	-	expression tag	UNP Q2G4I2
В	244	LEU	-	expression tag	UNP Q2G4I2
В	245	GLU	-	expression tag	UNP Q2G4I2
В	246	HIS	-	expression tag	UNP Q2G4I2
В	247	HIS	-	expression tag	UNP Q2G4I2
В	248	HIS	-	expression tag	UNP Q2G4I2
В	249	HIS	-	expression tag	UNP Q2G4I2
В	250	HIS	-	expression tag	UNP Q2G4I2
В	251	HIS	-	expression tag	UNP Q2G4I2

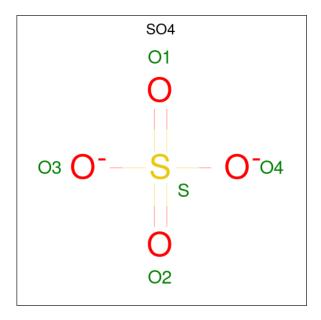
• Molecule 2 is RESVERATROL (three-letter code: STL) (formula: $C_{14}H_{12}O_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Λ	1	Total	С	Н	О	9	0	
	A	1	29	14	12	3	2		
2	D	1	Total	С	Н	О	2	0	
	2 B	1	29	14	12	3	2	U	

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S	0	0
		_	5 4 1 Total O S		
3	A	1	5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
			5 4 1 Total O S		
3	A	1	5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
			Total O S	_	_
3	A	1	5 4 1	0	0
3	В	1	Total O S	0	0
			5 4 1 Total O S		
3	В	1	5 4 1	0	0
3	В	1	Total O S	0	0
			5 4 1	_	_

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	207	Total O 207 207	0	0
4	В	206	Total O 206 206	0	0

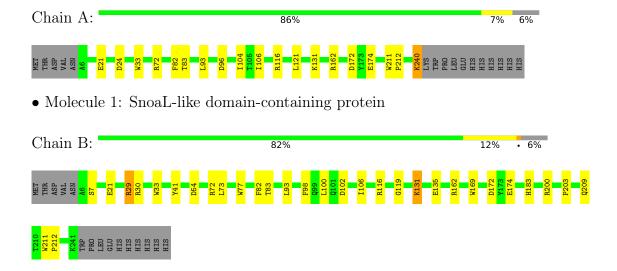


3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: SnoaL-like domain-containing protein





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 63	Depositor	
Cell constants	78.05Å 78.05Å 159.54Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	51.57 - 1.39	Depositor	
% Data completeness	100.0 (51.57-1.39)	Depositor	
(in resolution range)	,	-	
R_{merge}	0.14	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	0.35 (at 1.39Å)	Xtriage	
Refinement program	REFMAC 5.8.0267	Depositor	
R, R_{free}	0.237 , 0.259	Depositor	
Wilson B-factor (A^2)	14.4	Xtriage	
Anisotropy	0.393	Xtriage	
L-test for twinning ²	$< L > = 0.45, < L^2> = 0.28$	Xtriage	
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage	
Total number of atoms	8033	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	20.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, STL

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	Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.87	1/1959 (0.1%)	0.99	5/2660~(0.2%)	
1	В	0.90	$2/1976 \ (0.1\%)$	1.07	10/2681 (0.4%)	
All	All	0.88	3/3935 (0.1%)	1.03	$15/5341 \ (0.3\%)$	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
1	В	174	GLU	CD-OE2	9.87	1.36	1.25
1	A	174	GLU	CD-OE2	8.67	1.35	1.25
1	В	174	GLU	CD-OE1	5.36	1.31	1.25

All (15) bond angle outliers are listed below:

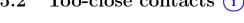
Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	В	29	ARG	NE-CZ-NH2	12.91	126.75	120.30
1	В	162	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	В	29	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	В	30	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	116	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	116	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	В	116	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	В	72	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	162	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	В	162	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	В	41	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	A	162	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	72	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	В	41	TYR	CB-CG-CD1	5.17	124.10	121.00
1	В	116	ARG	NE-CZ-NH1	5.16	122.88	120.30



There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)



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	1900	1837	1831	11	1
1	В	1914	1861	1856	20	0
2	A	17	12	11	2	0
2	В	17	12	11	2	0
3	A	35	0	0	2	1
3	В	15	0	0	1	0
4	A	207	0	0	3	0
4	В	206	0	0	4	0
All	All	4311	3722	3709	35	1

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 (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)	
1:B:172:ASP:OD1	2:B:301:STL:O1	1.62	1.17	
1:A:82:PHE:O	1:A:93:LEU:HD21	1.86	0.76	
1:A:82:PHE:O	1:A:93:LEU:CD2	2.34	0.76	
1:B:83:THR:HG22	1:B:93:LEU:HD23	1.69	0.75	
1:A:83:THR:HG22	1:A:93:LEU:HD23	1.73	0.68	
1:B:82:PHE:O	1:B:93:LEU:CD2	2.42	0.68	
3:B:303:SO4:O3	4:B:401:HOH:O	2.11	0.67	
3:A:306:SO4:O3	4:A:401:HOH:O	2.10	0.66	
1:B:82:PHE:O	1:B:93:LEU:HD21	1.99	0.63	
1:B:209:GLN:NE2	4:B:403:HOH:O	2.33	0.61	
4:A:491:HOH:O	1:B:135:GLU:HG2	2.02	0.60	
1:B:29:ARG:HD3	1:B:102:ASP:CG	2.24	0.58	
1:B:82:PHE:O	1:B:93:LEU:HD22	2.05	0.57	
1:A:82:PHE:O	1:A:93:LEU:HD22	2.05	0.56	
1:B:172:ASP:OD1	2:B:301:STL:C12	2.52	0.56	

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Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)	
1:B:29:ARG:HD3	1:B:102:ASP:OD2	2.05	0.56	
1:B:200[A]:ARG:HH22	1:B:203:PRO:HD3	1.73	0.52	
1:A:21:GLU:HG3	1:A:106:ILE:HD12	1.91	0.52	
3:A:303:SO4:O2	4:A:402:HOH:O	2.20	0.50	
1:B:83:THR:HG22	1:B:93:LEU:CD2	2.39	0.50	
1:B:131:LYS:HZ2	1:B:131:LYS:H	1.58	0.50	
1:A:172:ASP:OD1	2:A:301:STL:O1	2.33	0.47	
1:B:21:GLU:HG3	1:B:106:ILE:HD12	2.00	0.43	
1:B:169:TRP:HA	1:B:211:TRP:HB2	2.01	0.43	
1:B:211:TRP:CD2	1:B:212:PRO:HA	2.53	0.43	
1:A:240:LYS:N	1:A:240:LYS:HD3	2.34	0.42	
1:A:211:TRP:CD2	1:A:212:PRO:HA	2.55	0.42	
1:A:82:PHE:C	1:A:93:LEU:HD21	2.40	0.42	
1:B:54:ASP:HB2	4:B:564:HOH:O	2.20	0.41	
1:B:98:PHE:O	1:B:119:GLY:HA2	2.21	0.41	
1:A:24:ASP:HB2	1:A:106:ILE:HD13	2.03	0.41	
1:A:96:ASP:O	1:A:121:LEU:HA	2.21	0.40	
2:A:301:STL:H10	2:A:301:STL:H7	1.74	0.40	
1:B:7:SER:HB2	4:B:490:HOH:O	2.21	0.40	
1:B:73:LEU:O	1:B:77:TRP:HB3	2.21	0.40	

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:H	3:A:308:SO4:O2[2_655]	1.57	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	Percentile	es
1	A	234/251 (93%)	228 (97%)	6 (3%)	0	100 100	

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Mol	Chain	Analysed	ysed Favoured		Outliers	Perce	ntiles
1	В	236/251 (94%)	230 (98%)	6 (2%)	0	100	100
All	All	470/502 (94%)	458 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	193/208 (93%)	190 (98%)	3 (2%)	62 33		
1	В	195/208 (94%)	191 (98%)	4 (2%)	53 21		
All	All	388/416 (93%)	381 (98%)	7 (2%)	59 28		

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TRP
1	A	131	LYS
1	A	240	LYS
1	В	33	TRP
1	В	100	LEU
1	В	131	LYS
1	В	183	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	80	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands 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).

Mal	Trino	Chain	Dag	Link	Во	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	В	304	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	306	-	4,4,4	0.31	0	6,6,6	0.16	0
3	SO4	В	302	-	4,4,4	0.33	0	6,6,6	0.66	0
3	SO4	В	303	-	4,4,4	0.26	0	6,6,6	0.30	0
3	SO4	A	304	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SO4	A	302	-	4,4,4	0.53	0	6,6,6	0.59	0
3	SO4	A	305	-	4,4,4	0.50	0	6,6,6	0.38	0
2	STL	A	301	-	18,18,18	0.43	0	24,24,24	1.10	1 (4%)
2	STL	В	301	-	18,18,18	0.34	0	24,24,24	0.46	0
3	SO4	A	303	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	A	307	-	4,4,4	0.28	0	6,6,6	0.06	0
3	SO4	A	308	-	4,4,4	0.44	0	6,6,6	0.09	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
2	STL	A	301	-	-	0/5/5/5	0/2/2/2
2	STL	В	301	-	-	0/5/5/5	0/2/2/2



There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	A	301	STL	C4-C5-C7	-2.34	113.62	120.60

There are no chirality outliers.

There are no torsion outliers.

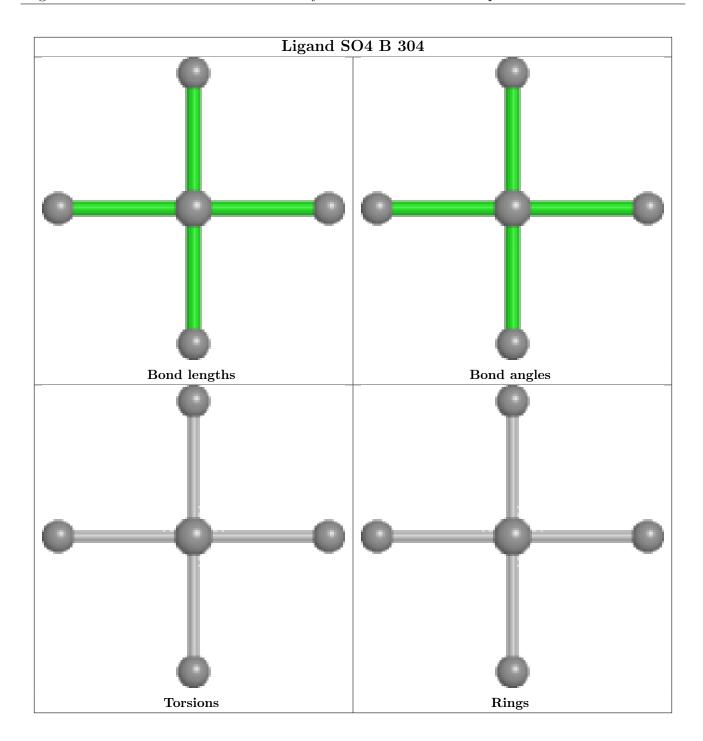
There are no ring outliers.

6 monomers are involved in 8 short contacts:

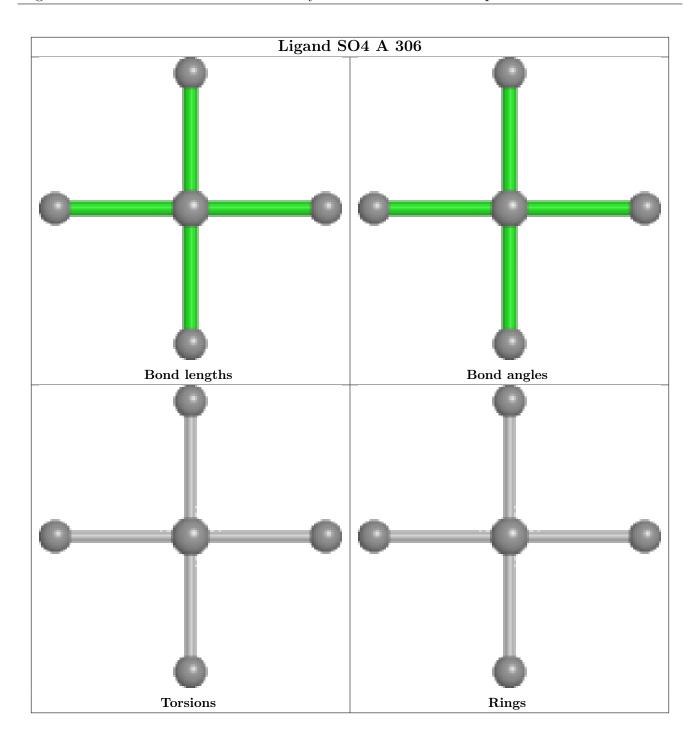
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	306	SO4	1	0
3	В	303	SO4	1	0
2	A	301	STL	2	0
2	В	301	STL	2	0
3	A	303	SO4	1	0
3	A	308	SO4	0	1

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 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.

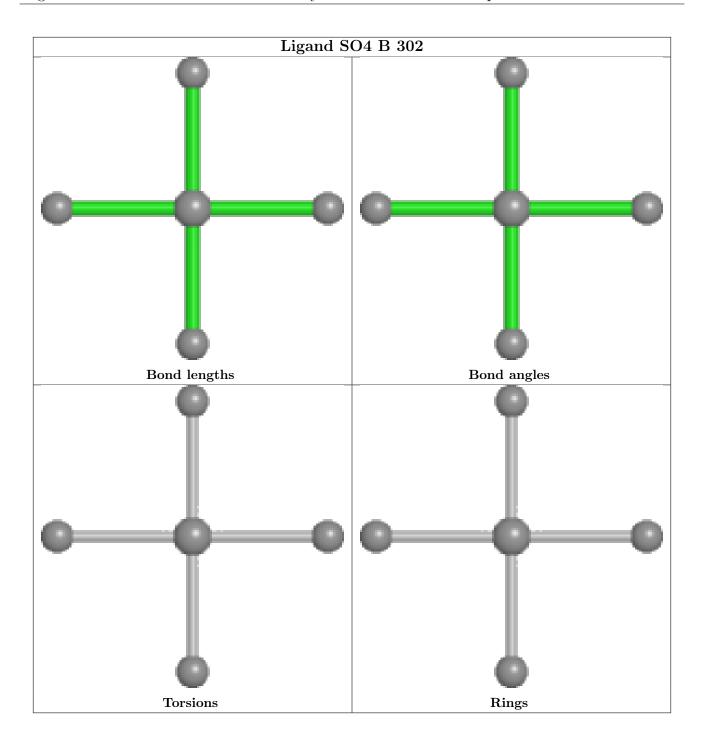




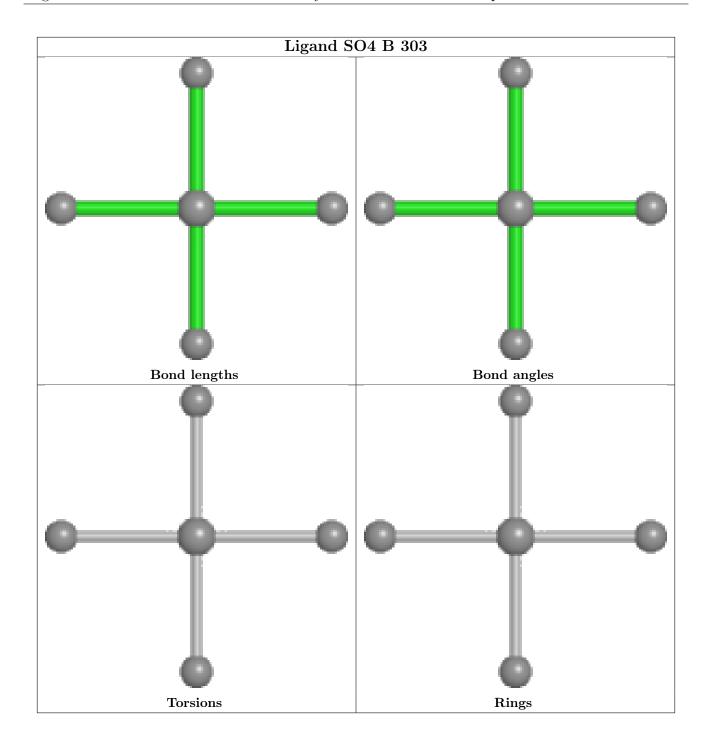




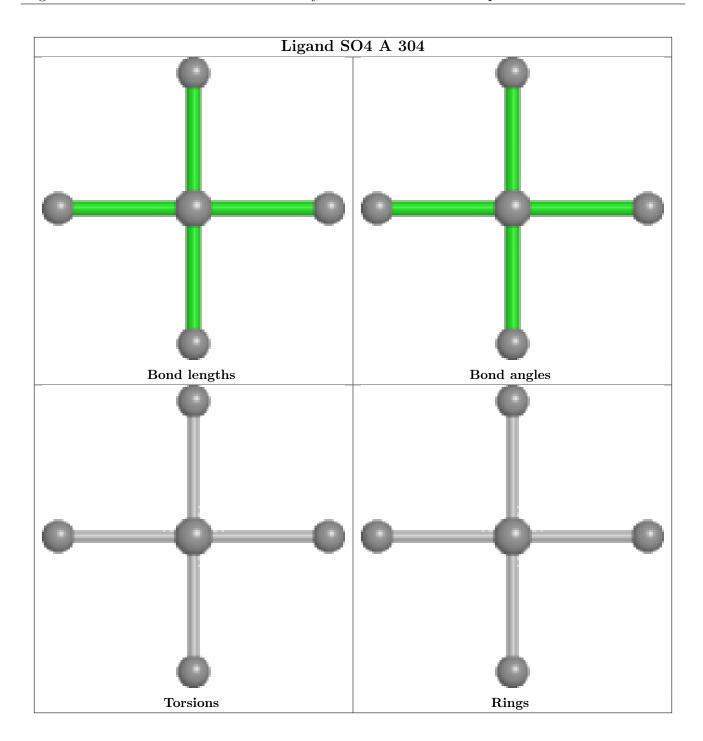




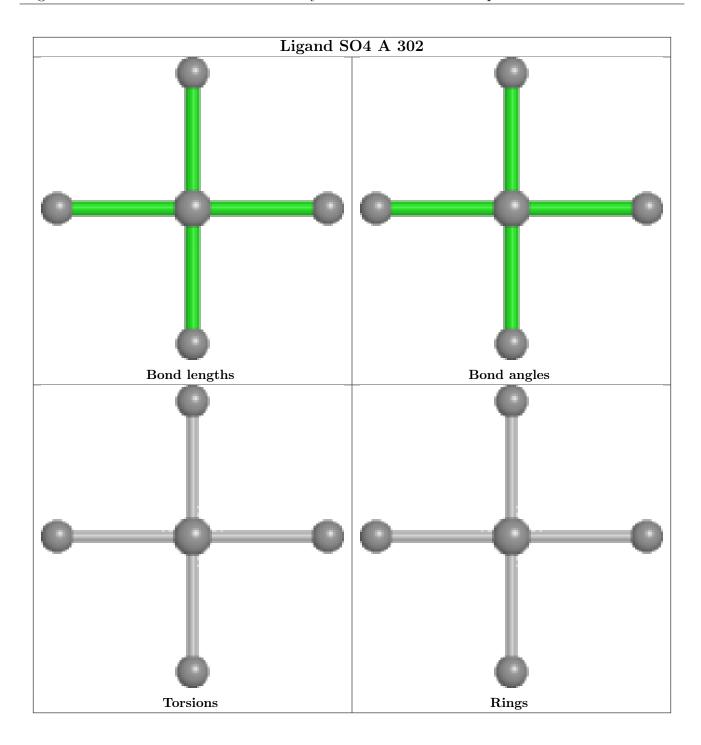




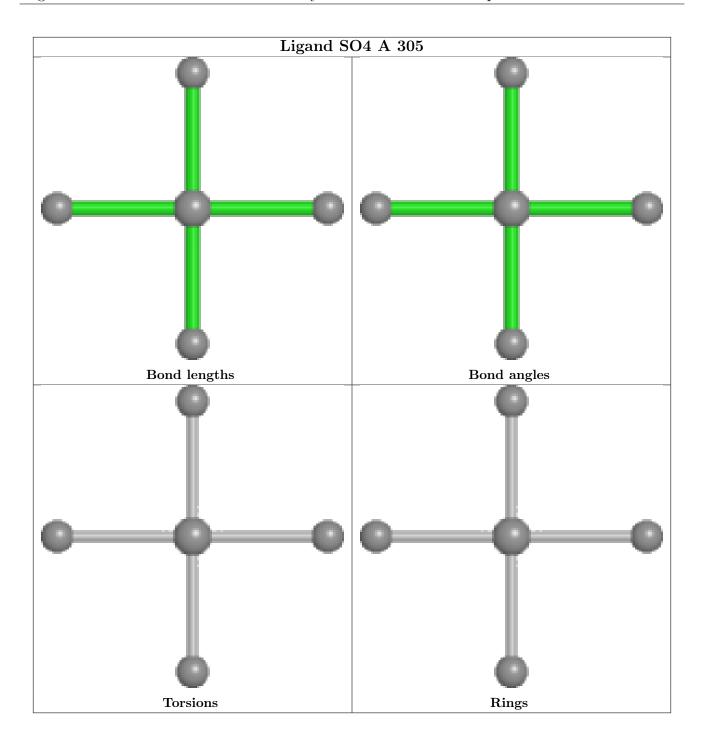




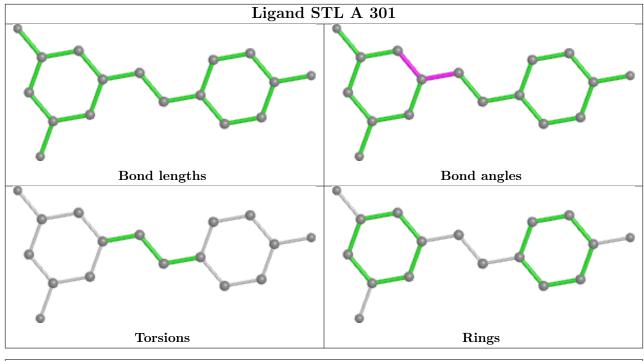


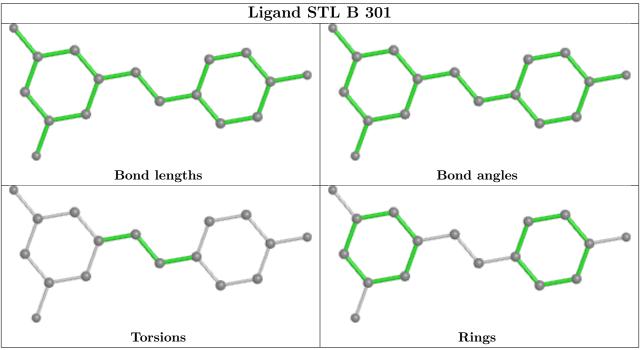




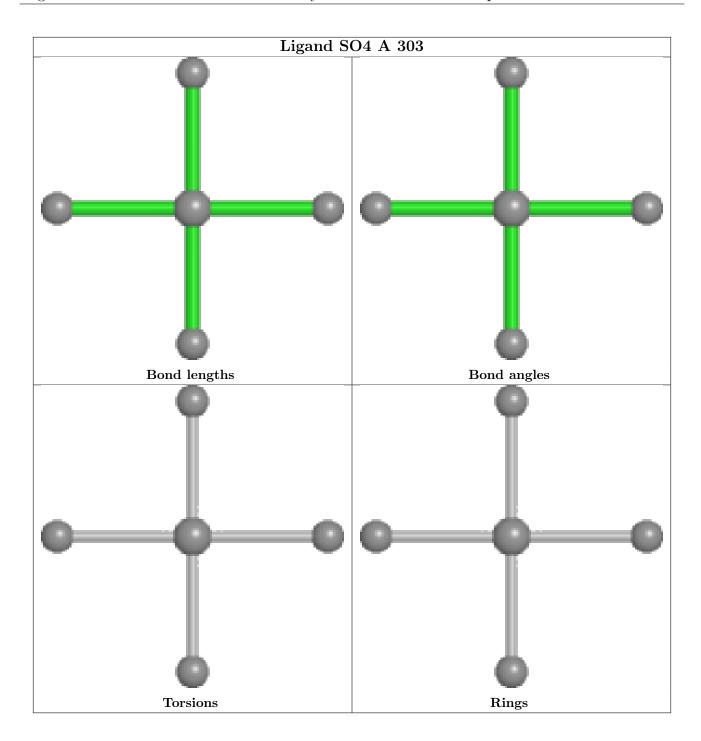




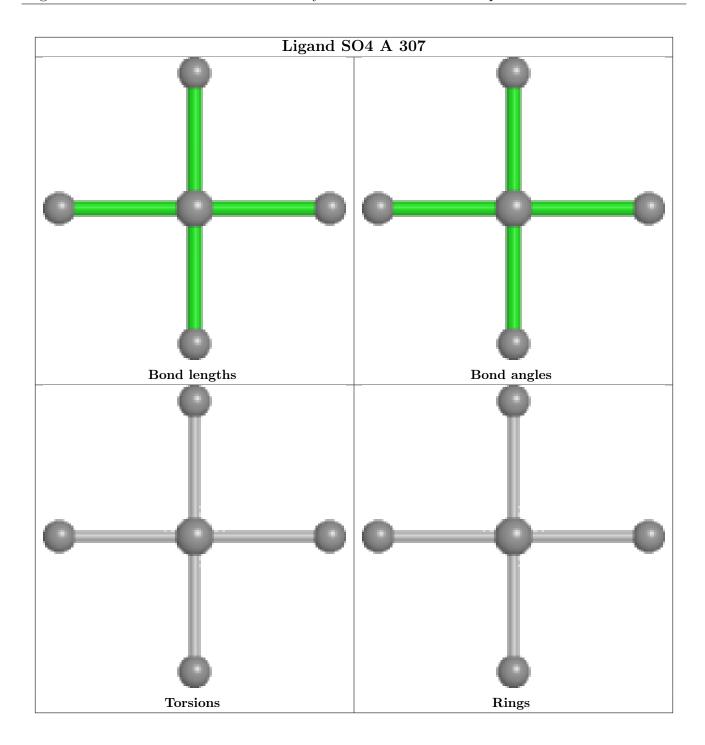




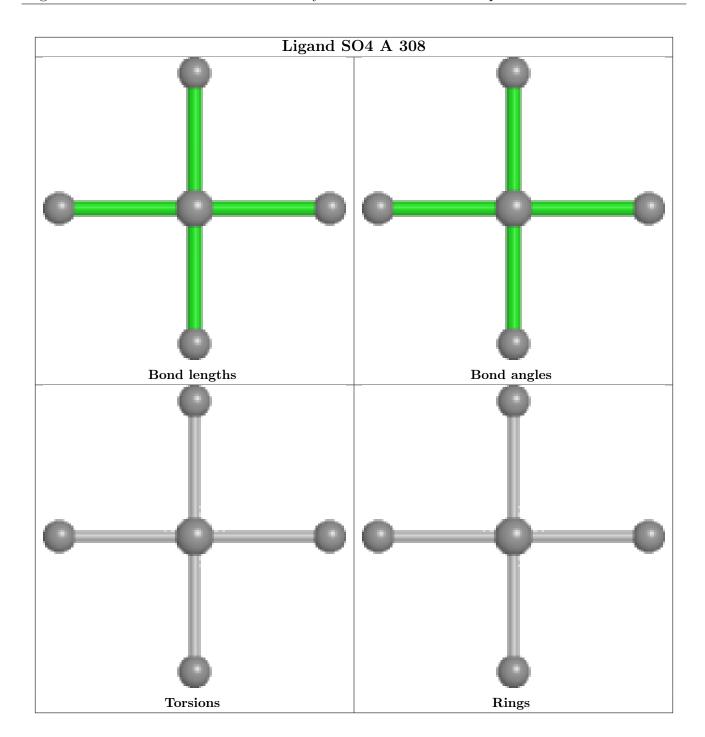












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

