WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2023 – 07:43 PM EDT

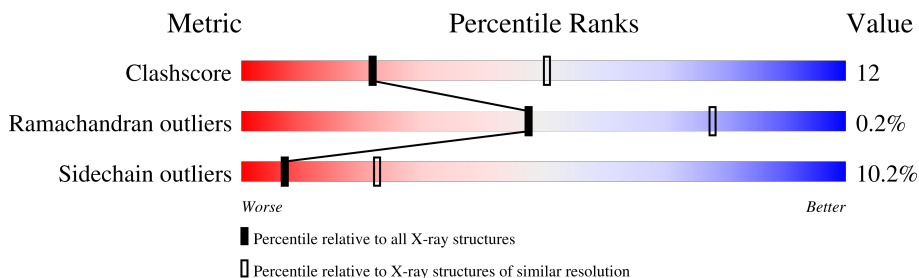|		
PDB ID	:	1D4M
Title	:	THE CRYSTAL STRUCTURE OF COXSACKIEVIRUS A9 TO 2.9 A RESOLUTION
Authors	:	Hendry, E.; Hatanaka, H.; Fry, E.; Smyth, M.; Tate, J.; Stanway, G.; Santti, J.; Maaronen, M.; Hyypia, T.; Stuart, D.
Deposited on	:	1999-10-04
Resolution	:	2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0.2%
Sidechain outliers		10.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	1	299	67% 22% 6% 5%
2	2	261	80% 13% • •
3	3	238	79% 16% 5%
4	4	68	74% 15% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	W71	1	501	-	-	X	-
5	W71	1	502	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 7051 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 PROTEIN (COXSACKIEVIRUS A9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	284	Total	C	N	O	S	0	0	0
			2261	1426	395	428	12			

- Molecule 2 is a protein called PROTEIN (COXSACKIEVIRUS A9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	252	Total	C	N	O	S	0	0	0
			1959	1239	332	372	16			

- Molecule 3 is a protein called PROTEIN (COXSACKIEVIRUS A9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1843	1173	302	350	18			

- Molecule 4 is a protein called PROTEIN (COXSACKIEVIRUS A9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	61	Total	C	N	O	S	0	0	0
			475	294	82	98	1			

- Molecule 5 is 5-(7-(4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (three-letter code: W71) (formula: $C_{20}H_{26}N_2O_3$).

W71
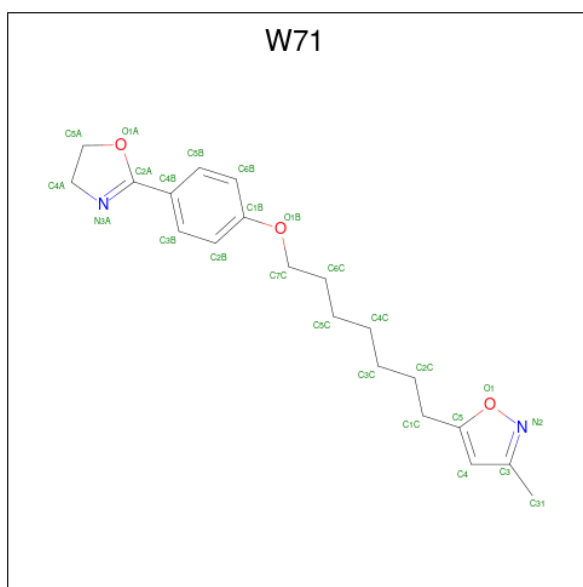
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total	C	N	O	0	0
			25	20	2	3		
5	1	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).

MYR
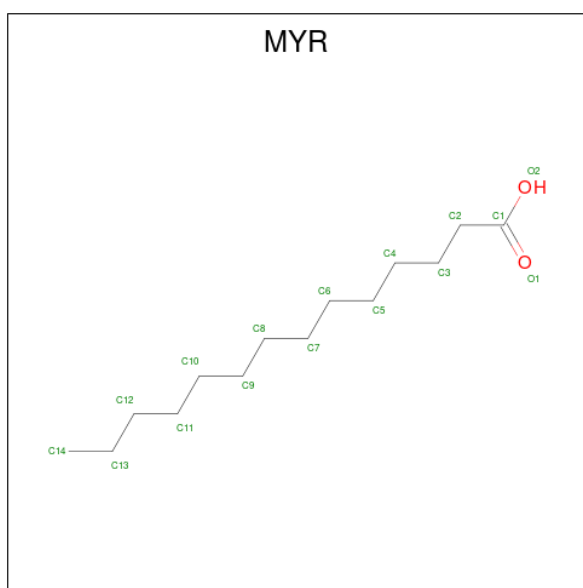
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	162	Total 162	O 162	0	0
7	2	146	Total 146	O 146	0	0
7	3	112	Total 112	O 112	0	0
7	4	28	Total 28	O 28	0	0

3 Residue-property plots ⓘ

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.
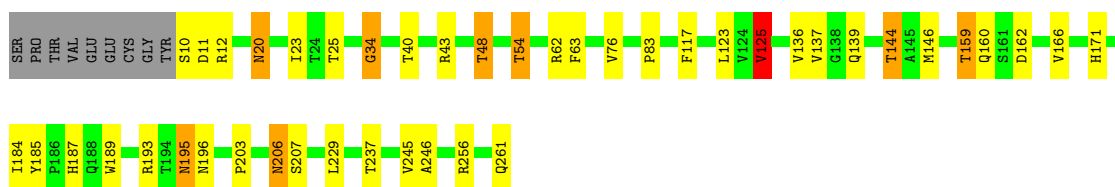
Note EDS was not executed.

• Molecule 1: PROTEIN (COXSACKIEVIRUS A9)

Chain 1:
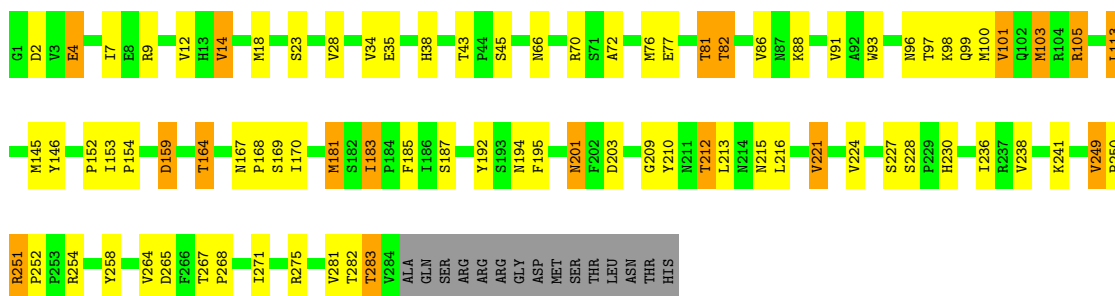
• Molecule 2: PROTEIN (COXSACKIEVIRUS A9)

Chain 2:

• Molecule 3: PROTEIN (COXSACKIEVIRUS A9)

Chain 3:

• Molecule 4: PROTEIN (COXSACKIEVIRUS A9)

Chain 4:
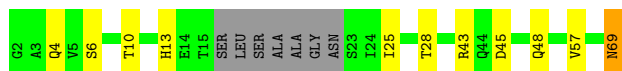
4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	487.30Å 358.10Å 305.70Å 90.00° 128.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	41.0 (20.00-2.90)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7051	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, W71

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	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	1	0.58	0/2325	0.81	0/3172
2	2	0.55	0/2009	0.81	2/2740 (0.1%)
3	3	0.55	0/1892	0.80	0/2581
4	4	0.60	0/483	0.88	0/652
All	All	0.56	0/6709	0.81	2/9145 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	125	VAL	CB-CA-C	-5.86	100.27	111.40
2	2	195	ASN	CB-CA-C	-5.75	98.91	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	195	ASN	Mainchain

5.2 Too-close contacts ⓘ

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	1	2261	0	2192	75	0
2	2	1959	0	1878	39	0
3	3	1843	0	1802	46	0
4	4	475	0	456	8	0
5	1	50	0	52	22	0
6	4	15	0	27	1	0
7	1	162	0	0	18	0
7	2	146	0	0	7	0
7	3	112	0	0	4	0
7	4	28	0	0	3	0
All	All	7051	0	6407	155	0

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 12.

The worst 5 of 155 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:97:THR:H	5:1:502:W71:H313	1.16	1.04
5:1:501:W71:H312	5:1:502:W71:H2C2	1.43	1.00
1:1:82:THR:HB	7:1:617:HOH:O	1.60	0.99
1:1:4:GLU:HG2	4:4:4:GLN:HG2	1.50	0.92
1:1:97:THR:N	5:1:502:W71:H313	1.92	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	Percentiles	
1	1	282/299 (94%)	264 (94%)	17 (6%)	1 (0%)	34	66
2	2	250/261 (96%)	227 (91%)	22 (9%)	1 (0%)	34	66
3	3	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
4	4	57/68 (84%)	55 (96%)	2 (4%)	0	100	100
All	All	825/866 (95%)	774 (94%)	49 (6%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	224	VAL
2	2	34	GLY

5.3.2 Protein sidechains ⓘ

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	1	254/267 (95%)	222 (87%)	32 (13%)	4	13
2	2	209/217 (96%)	190 (91%)	19 (9%)	9	28
3	3	211/211 (100%)	194 (92%)	17 (8%)	11	33
4	4	53/57 (93%)	47 (89%)	6 (11%)	6	18
All	All	727/752 (97%)	653 (90%)	74 (10%)	7	22

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	96	LYS
4	4	28	THR
3	3	119	VAL
3	3	225	LEU
1	1	238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20

such sidechains are listed below:

Mol	Chain	Res	Type
3	3	56	ASN
3	3	206	ASN
4	4	44	GLN
4	4	4	GLN
2	2	97	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	W71	1	501	-	24,27,27	2.09	5 (20%)	29,34,34	3.05	6 (20%)
6	MYR	4	1	4	14,14,15	0.46	0	13,13,15	0.66	0
5	W71	1	502	-	24,27,27	1.92	6 (25%)	29,34,34	3.20	4 (13%)

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
5	W71	1	501	-	-	6/14/22/22	0/3/3/3
6	MYR	4	1	4	-	7/11/12/13	-
5	W71	1	502	-	-	6/14/22/22	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	501	W71	C4-C5	-6.06	1.31	1.39
5	1	502	W71	C2A-N3A	5.58	1.34	1.27
5	1	501	W71	C2A-N3A	4.58	1.33	1.27
5	1	502	W71	O1A-C2A	3.98	1.42	1.36
5	1	501	W71	O1A-C2A	3.51	1.41	1.36

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	502	W71	O1A-C2A-N3A	-11.64	108.23	118.23
5	1	501	W71	O1A-C2A-N3A	-10.68	109.05	118.23
5	1	502	W71	O1A-C2A-C4B	9.85	128.90	115.85
5	1	501	W71	O1A-C2A-C4B	9.03	127.81	115.85
5	1	502	W71	C4A-N3A-C2A	6.06	112.18	106.77

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	502	W71	C5-C1C-C2C-C3C
5	1	501	W71	C6B-C1B-O1B-C7C
5	1	501	W71	C5-C1C-C2C-C3C
5	1	501	W71	C2B-C1B-O1B-C7C
5	1	502	W71	C6B-C1B-O1B-C7C

There are no ring outliers.

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	501	W71	9	0
6	4	1	MYR	1	0
5	1	502	W71	22	0

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 W71 1 501

Bond lengths   Bond angles   Torsions   Rings

Ligand W71 1 502

Bond lengths   Bond angles   Torsions   Rings
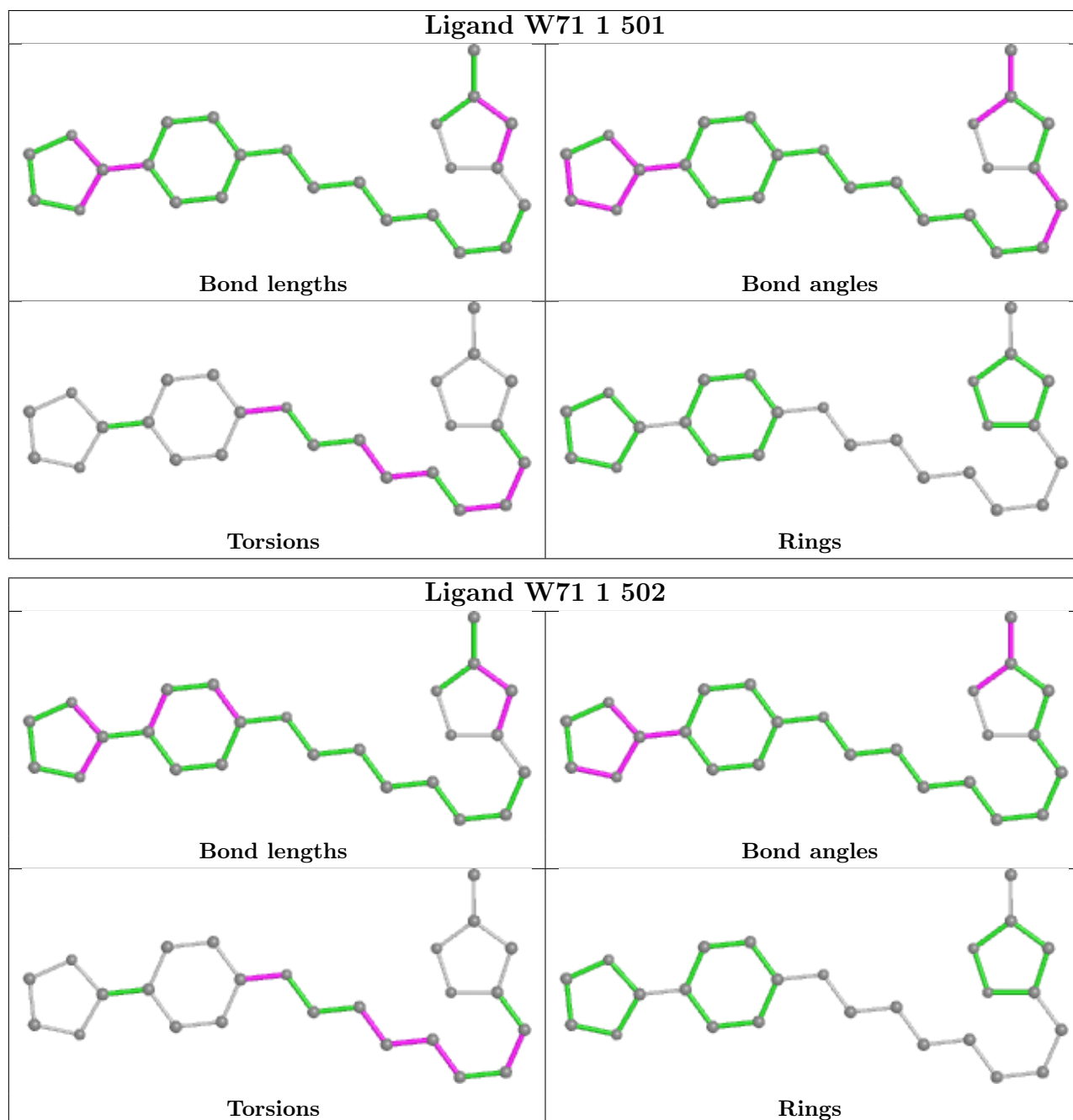
5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.