W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2022 – 01:07 am GMT

PDB ID	:	7QB5
Title	:	Coxsackievirus A24v (CVA24v) in complex with a dimeric C2-C9-linked sialic acid inhibitor
Authors	:	Zocher, G.; Stehle, T.
Deposited on	:	2021-11-18
Resolution	:	1.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

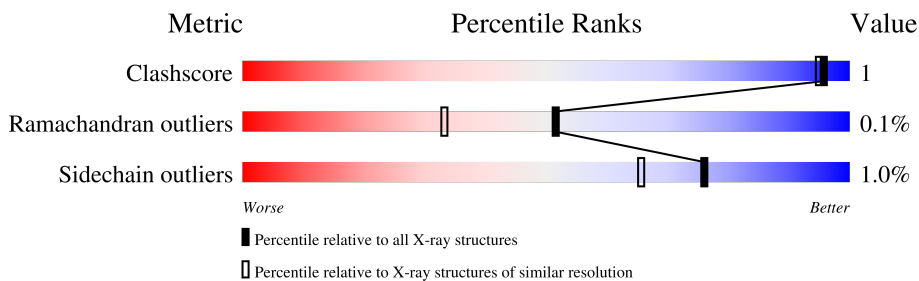|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.73 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		1
Ramachandran outliers		0.1%
Sidechain outliers		1.0%

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	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)

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	111	305	89% · · 8%
2	222	271	94% · ·
3	333	240	94% · ·
4	444	69	78% · 17%

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2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 7489 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	111	281	Total 2291	C 1462	N 382	O 439	S 8	0	10	0

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	222	264	Total 2072	C 1323	N 342	O 393	S 14	0	5	0

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	333	234	Total 1846	C 1188	N 289	O 347	S 22	0	11	0

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	444	57	Total 432	C 271	N 70	O 90	S 1	0	2	0

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).

SIA
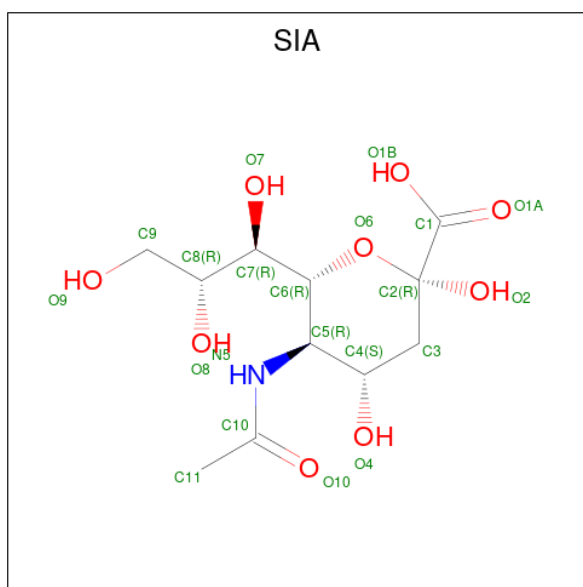
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	111	1	21	11	1	9	0	0

- Molecule 6 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).

HEZ
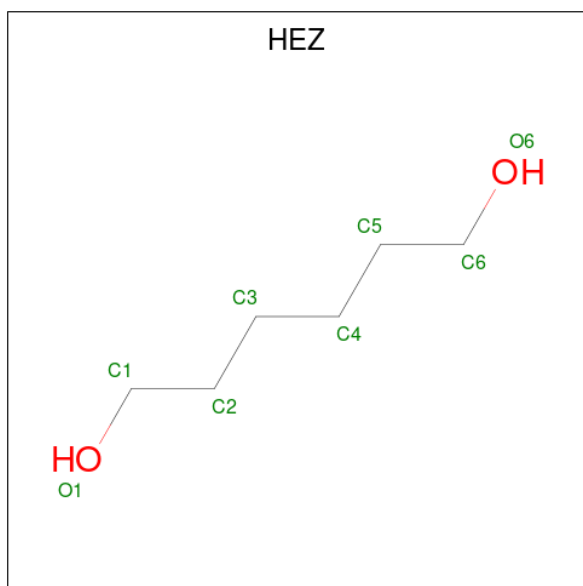
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	111	1	8	6	2	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	111	3	Total 3	Ca 3	0	0
7	222	1	Total 1	Ca 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	111	3	Total 3	Cl 3	0	0
8	222	1	Total 1	Cl 1	0	0

- Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	111	289	Total 289	O 289	0	0
9	222	238	Total 238	O 238	0	0
9	333	220	Total 220	O 220	0	0
9	444	64	Total 64	O 64	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 failed to run properly.

• Molecule 1: Capsid protein VP1

Chain 111:
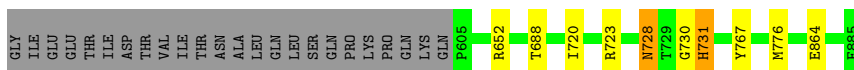
• Molecule 2: Capsid protein VP2

Chain 222:

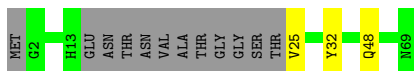• Molecule 3: Capsid protein VP3

Chain 333:

• Molecule 4: Capsid protein VP4

Chain 444:

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	305.76Å 365.71Å 366.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 1.73	Depositor
% Data completeness (in resolution range)	90.9 (49.92-1.73)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.206	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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.

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5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, HEZ, CA, SIA

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	111	0.60	0/2385	0.76	0/3258
2	222	0.61	0/2143	0.77	0/2927
3	333	0.61	0/1926	0.75	0/2624
4	444	0.65	0/445	0.72	0/601
All	All	0.61	0/6899	0.76	0/9410

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	222	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	222	151	LEU	Peptide

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	111	2291	0	2231	6	0
2	222	2072	0	2000	3	0
3	333	1846	0	1845	5	0
4	444	432	0	415	3	0
5	111	21	0	18	0	0
6	111	8	0	14	0	0
7	111	3	0	0	0	0
7	222	1	0	0	0	0
8	111	3	0	0	0	0
8	222	1	0	0	1	0
9	111	289	0	0	0	0
9	222	238	0	0	0	0
9	333	220	0	0	0	0
9	444	64	0	0	0	0
All	All	7489	0	6523	14	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 1.

The worst 5 of 14 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)
3:333:360:GLN:HE22	4:444:32:TYR:H	1.32	0.78
1:111:652:ARG:HH11	4:444:48:GLN:HE22	1.43	0.66
4:444:25:VAL:O	4:444:25:VAL:HG12	2.01	0.59
3:333:472[A]:SER:OG	3:333:530[A]:THR:OG1	2.26	0.53
1:111:728:ASN:HD22	1:111:728:ASN:H	1.58	0.52

There are no symmetry-related clashes.

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	Percentiles	
1	111	289/305 (95%)	278 (96%)	11 (4%)	0	100	100
2	222	267/271 (98%)	253 (95%)	13 (5%)	1 (0%)	34	18
3	333	242/240 (101%)	230 (95%)	12 (5%)	0	100	100
4	444	55/69 (80%)	53 (96%)	2 (4%)	0	100	100
All	All	853/885 (96%)	814 (95%)	38 (4%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	222	117	ASN

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	111	256/268 (96%)	250 (98%)	6 (2%)	50	31
2	222	223/225 (99%)	222 (100%)	1 (0%)	91	86
3	333	216/212 (102%)	215 (100%)	1 (0%)	88	83
4	444	47/57 (82%)	47 (100%)	0	100	100
All	All	742/762 (97%)	734 (99%)	8 (1%)	76	62

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	333	488	MET
2	222	332	ARG
1	111	731	HIS
1	111	728	ASN
1	111	864	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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
5	SIA	111	901	-	21,21,21	1.04	2 (9%)	25,31,31	1.07	2 (8%)
6	HEZ	111	902	-	7,7,7	0.63	0	6,6,6	0.37	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
5	SIA	111	901	-	-	9/20/38/38	0/1/1/1
6	HEZ	111	902	-	-	5/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	111	901	SIA	O2-C2	3.32	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	111	901	SIA	C3-C2	2.01	1.54	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	111	901	SIA	O1A-C1-C2	-3.54	118.23	123.59
5	111	901	SIA	O2-C2-C1	-2.17	106.36	110.76

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	111	901	SIA	O1A-C1-C2-O2
5	111	901	SIA	O1A-C1-C2-O6
5	111	901	SIA	O1B-C1-C2-O2
5	111	901	SIA	O1B-C1-C2-O6
6	111	902	HEZ	O1-C1-C2-C3

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 SIA 111 901

Bond lengths

Bond angles

Torsions

Rings
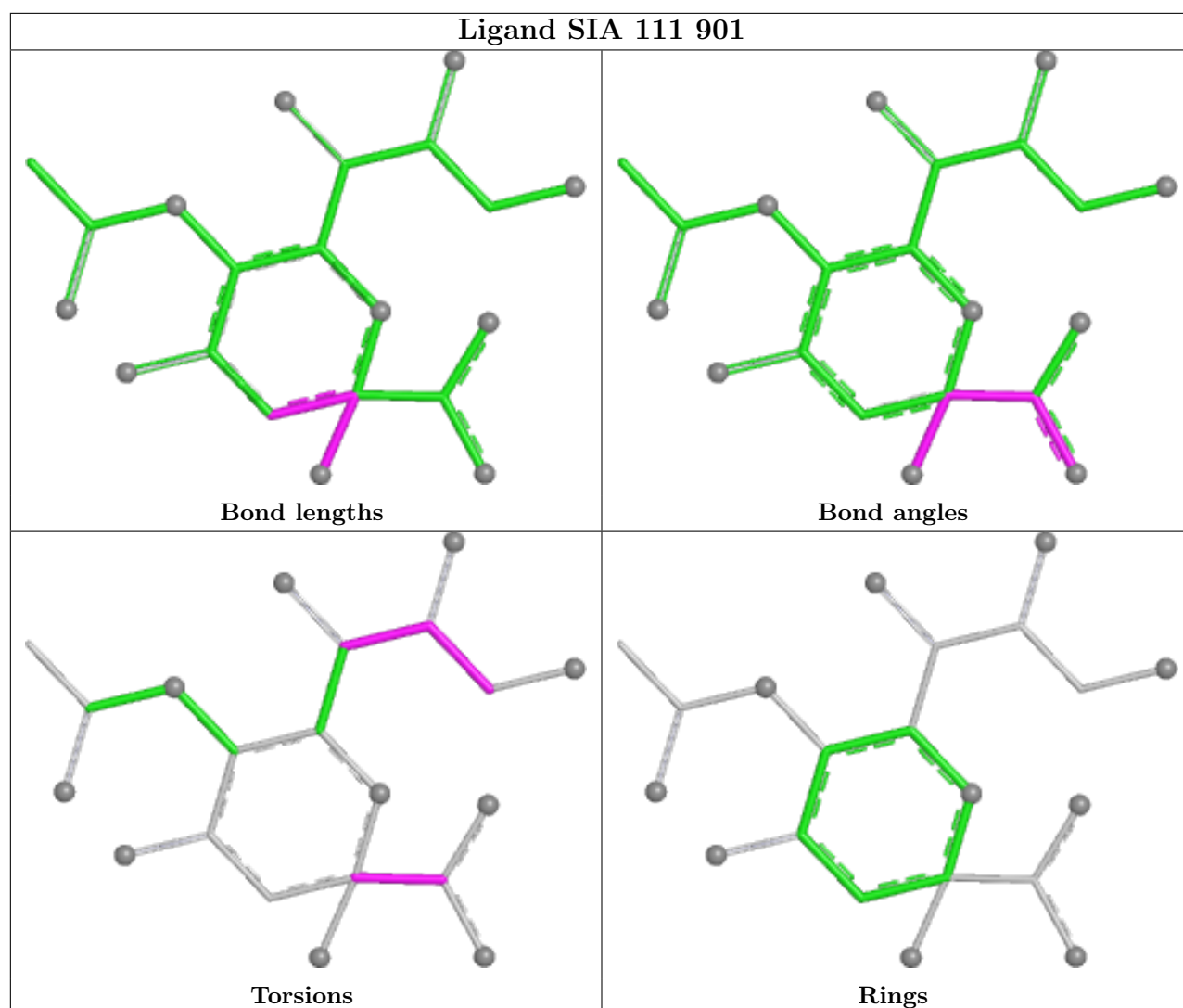
5.7 Other polymers ⓘ

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 failed to run properly - this section is therefore empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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