



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 21, 2019 – 02:15 PM EST

PDB ID : 6O2P
EMDB ID: : EMD-0611
Title : Complex of ivacaftor with cystic fibrosis transmembrane conductance regulator (CFTR)
Authors : Liu, F.; Zhang, Z.; Chen, J.; Levit, A.; Shoichet, B.
Deposited on : 2019-02-24
Resolution : 3.30 Å (reported)
Based on PDB ID : 6MSM

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

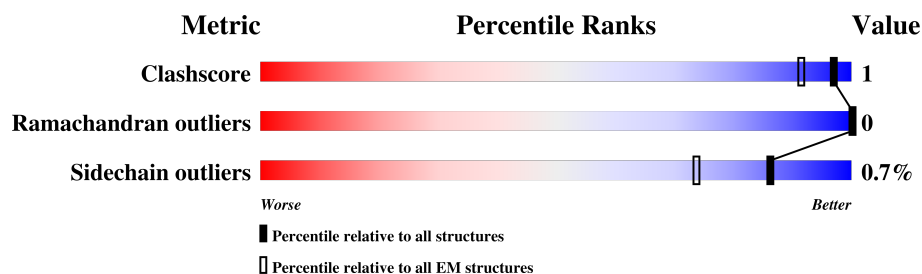
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1489	
2	B	17	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9767 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1179	Total	C	N	O	S	0	0
			9450	6173	1567	1663	47		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1371	GLN	GLU	engineered mutation	UNP P13569
A	1481	SER	-	expression tag	UNP P13569
A	1482	ASN	-	expression tag	UNP P13569
A	1483	SER	-	expression tag	UNP P13569
A	1484	LEU	-	expression tag	UNP P13569
A	1485	GLU	-	expression tag	UNP P13569
A	1486	VAL	-	expression tag	UNP P13569
A	1487	LEU	-	expression tag	UNP P13569
A	1488	PHE	-	expression tag	UNP P13569
A	1489	GLN	-	expression tag	UNP P13569

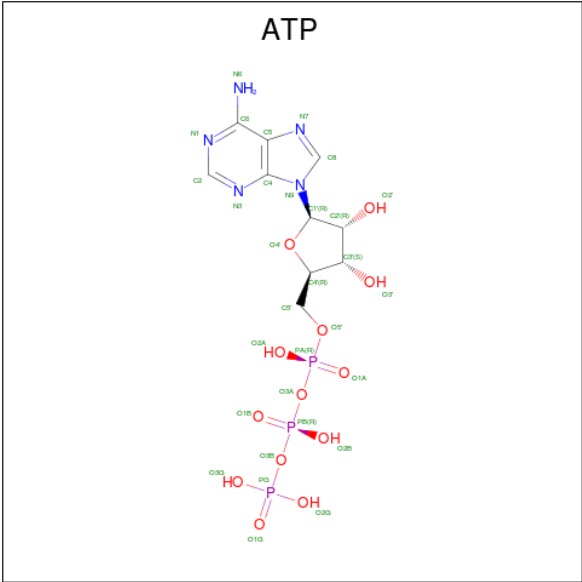
- Molecule 2 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

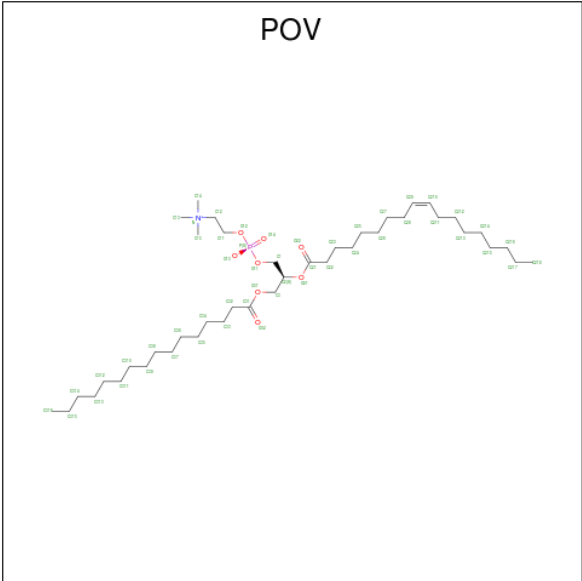
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Mg	0
			2	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



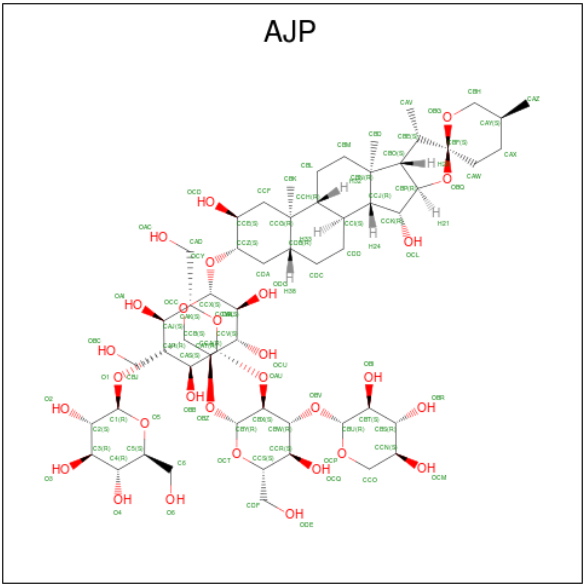
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			74	74	

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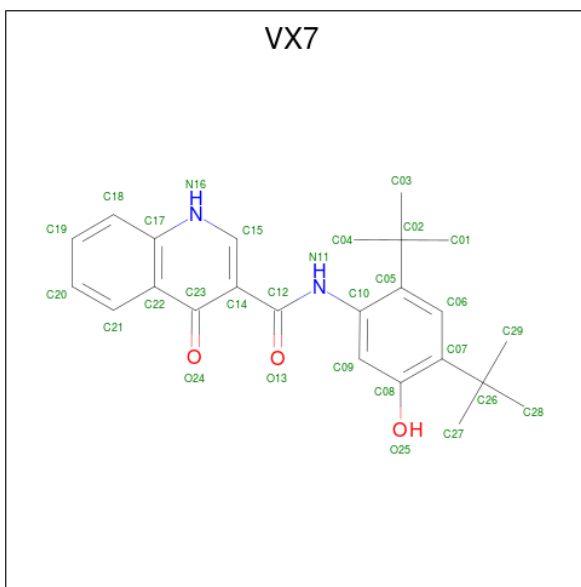
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			74	74	
5	A	1	Total	C	0
			74	74	
5	A	1	Total	C	0
			74	74	
5	A	1	Total	C	0
			74	74	
5	A	1	Total	C	0
			74	74	

- Molecule 6 is Digitonin (three-letter code: AJP) (formula: C₅₆H₉₂O₂₉).



Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C O	0
			65 45 20		

- Molecule 7 is N-(2,4-di-tert-butyl-5-hydroxyphenyl)-4-oxo-1,4-dihydroquinoline-3-carboxamide (three-letter code: VX7) (formula: C₂₄H₂₈N₂O₃).

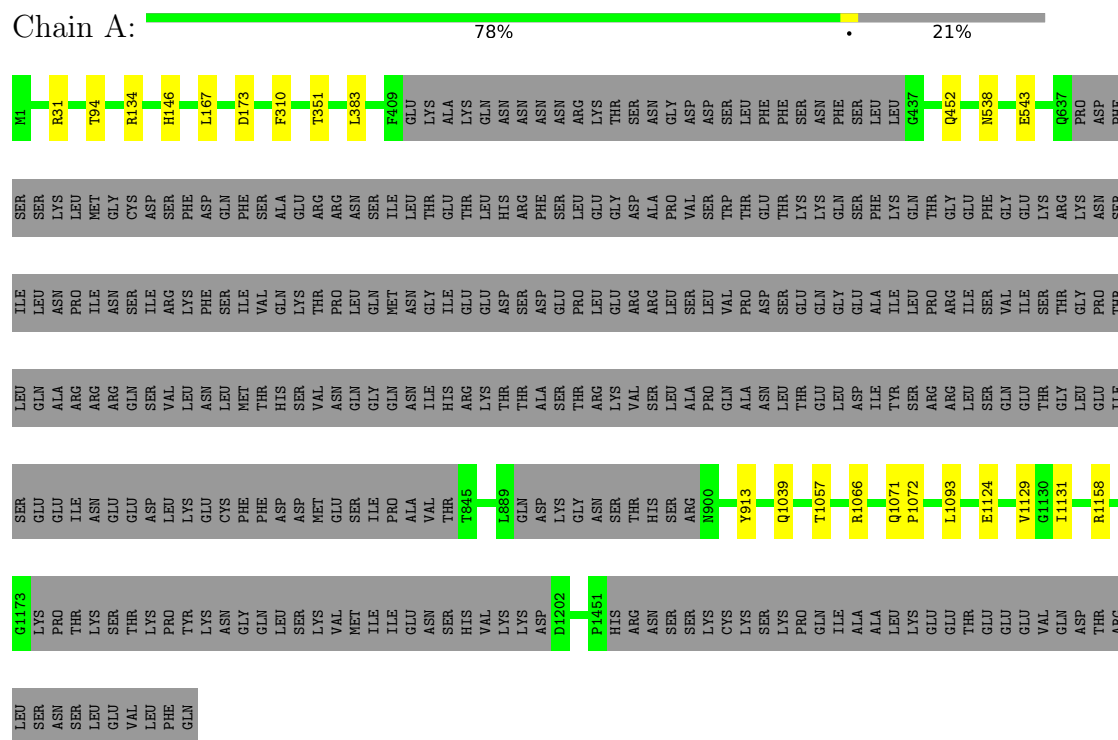


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	29	24	2	3	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: Cystic fibrosis transmembrane conductance regulator



- Molecule 2: Unknown Peptide



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	490750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.48	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: AJP, POV, MG, VX7, ATP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.70	0/9651	0.74	0/13050

There are no bond length outliers.

There are no bond angle outliers.

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	9450	0	9740	8	0
2	B	85	0	19	0	0
3	A	2	0	0	0	0
4	A	62	0	24	0	0
5	A	74	0	122	0	0
6	A	65	0	0	4	0
7	A	29	0	0	1	0
All	All	9767	0	9905	13	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.

All (13) 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)
6:A:1511:AJP:CCB	6:A:1511:AJP:CAD	2.85	0.54
1:A:913:TYR:HB2	1:A:1131:ILE:HG23	1.94	0.49
1:A:94:THR:HG23	1:A:134:ARG:HD3	1.94	0.48
6:A:1511:AJP:CBY	6:A:1511:AJP:CBJ	2.91	0.48
6:A:1511:AJP:CAV	6:A:1511:AJP:CBD	2.92	0.48
7:A:1512:VX7:O24	7:A:1512:VX7:N11	2.48	0.45
1:A:31:ARG:HA	1:A:1039:GLN:HE22	1.82	0.44
1:A:543:GLU:HG2	1:A:1057:THR:HG22	2.01	0.43
1:A:146:HIS:HB3	1:A:1093:LEU:HD21	2.01	0.42
1:A:310:PHE:HA	1:A:351:THR:HG21	2.02	0.41
1:A:1071:GLN:N	1:A:1072:PRO:CD	2.83	0.41
6:A:1511:AJP:OCC	6:A:1511:AJP:CAD	2.70	0.40
1:A:167:LEU:O	1:A:1066:ARG:NH1	2.51	0.40

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 PDB entries followed by that with respect to all EM entries.

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	A	1169/1489 (78%)	1116 (96%)	53 (4%)	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 PDB entries followed by that with respect to all EM entries.

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	1035/1322 (78%)	1028 (99%)	7 (1%)	85 91

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

Mol	Chain	Res	Type
1	A	173	ASP
1	A	383	LEU
1	A	452	GLN
1	A	538	ASN
1	A	1124	GLU
1	A	1129	VAL
1	A	1158	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	493	GLN
1	A	1039	GLN
1	A	1238	GLN
1	A	1268	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	ATP	A	1503	3	26,33,33	0.68	0	27,52,52	0.76	1 (3%)
4	ATP	A	1504	3	26,33,33	0.66	0	27,52,52	0.74	1 (3%)
5	POV	A	1505	-	9,9,51	0.08	0	8,8,59	0.07	0
5	POV	A	1506	-	13,13,51	0.08	0	12,12,59	0.07	0
5	POV	A	1507	-	10,10,51	0.08	0	9,9,59	0.07	0
5	POV	A	1508	-	14,14,51	0.95	1 (7%)	13,13,59	0.58	0
5	POV	A	1509	-	9,9,51	0.09	0	8,8,59	0.07	0
5	POV	A	1510	-	13,13,51	0.06	0	12,12,59	0.08	0
6	AJP	A	1511	-	73,73,95	0.39	0	107,116,149	0.88	5 (4%)
7	VX7	A	1512	-	29,31,31	2.22	6 (20%)	42,48,48	1.42	6 (14%)

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	ATP	A	1503	3	-	2/18/38/38	0/3/3/3
4	ATP	A	1504	3	-	2/18/38/38	0/3/3/3
5	POV	A	1505	-	-	0/7/7/55	-
5	POV	A	1506	-	-	2/11/11/55	-
5	POV	A	1507	-	-	0/8/8/55	-
5	POV	A	1508	-	-	1/12/12/55	-
5	POV	A	1509	-	-	0/7/7/55	-
5	POV	A	1510	-	-	1/11/11/55	-
6	AJP	A	1511	-	-	8/18/173/220	0/9/9/11
7	VX7	A	1512	-	-	0/20/20/20	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1512	VX7	C15-N16	5.74	1.41	1.31
7	A	1512	VX7	C26-C07	-5.15	1.45	1.54
7	A	1512	VX7	C02-C05	-5.11	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1512	VX7	C14-C12	-4.79	1.42	1.50
5	A	1508	POV	C29-C210	3.51	1.51	1.31
7	A	1512	VX7	C10-N11	-3.27	1.35	1.41
7	A	1512	VX7	C10-C05	2.53	1.43	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1512	VX7	C15-C14-C23	-5.49	117.21	119.97
6	A	1511	AJP	OBQ-CBP-CCK	4.75	120.09	110.23
7	A	1512	VX7	C15-N16-C17	3.27	120.92	116.92
6	A	1511	AJP	CBE-CBO-CBP	-2.46	99.71	104.35
6	A	1511	AJP	OBQ-CBP-CBO	-2.27	98.64	103.90
6	A	1511	AJP	CCJ-CBN-CBO	-2.26	96.27	100.22
7	A	1512	VX7	C10-N11-C12	-2.25	120.79	126.95
4	A	1503	ATP	C5-C6-N6	2.17	123.78	120.38
7	A	1512	VX7	C14-C15-N16	-2.12	120.97	124.34
4	A	1504	ATP	C5-C6-N6	2.11	123.70	120.38
6	A	1511	AJP	CBL-CBM-CBN	-2.07	109.22	112.80
7	A	1512	VX7	C29-C26-C07	2.05	114.79	110.87
7	A	1512	VX7	C03-C02-C05	2.04	114.77	110.87

There are no chirality outliers.

All (16) torsion outliers are listed below:

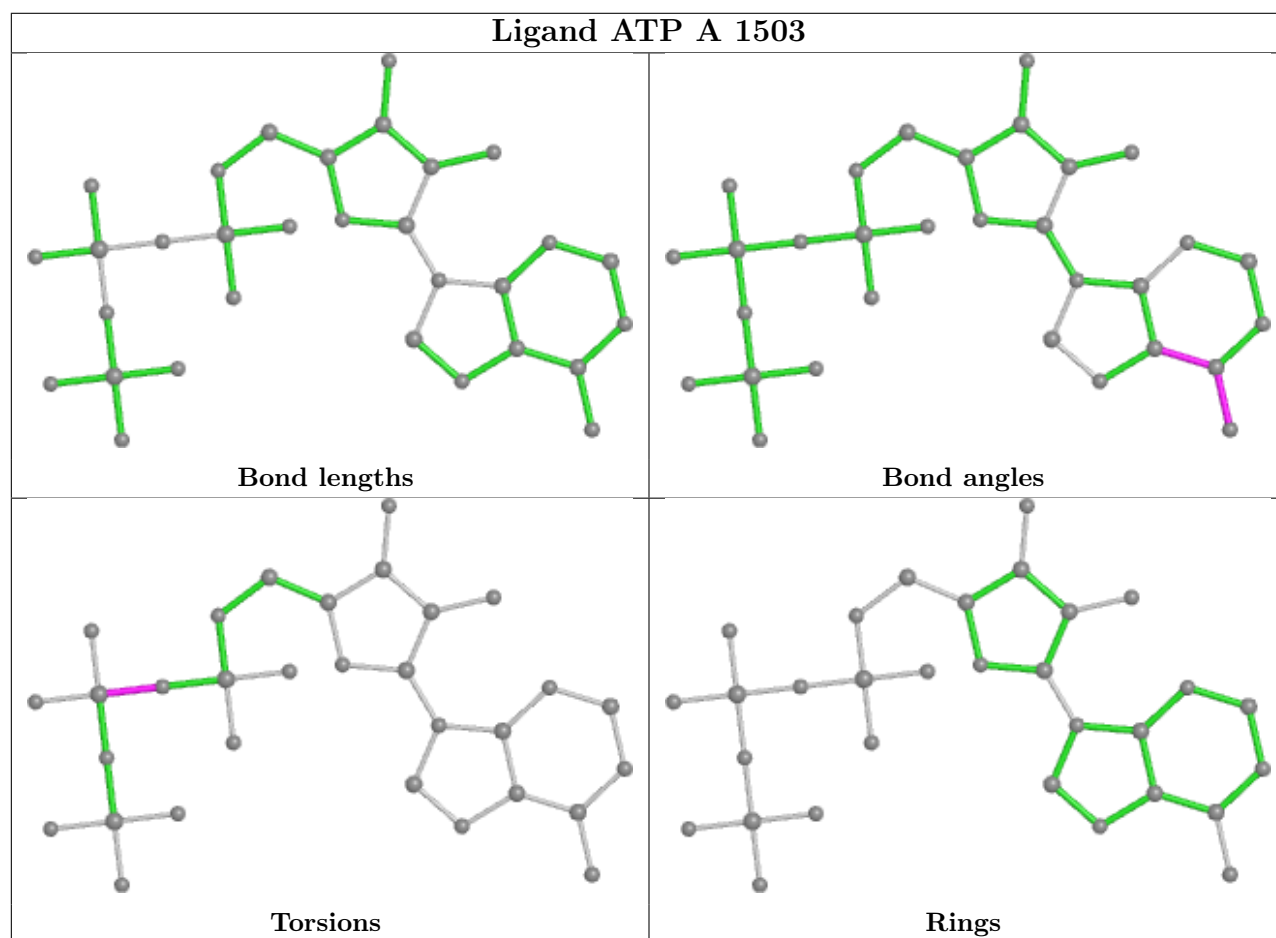
Mol	Chain	Res	Type	Atoms
6	A	1511	AJP	CDA-CCZ-OCY-CCX
6	A	1511	AJP	OAL-CAT-OAU-CBX
6	A	1511	AJP	CCB-CCA-OBZ-CBY
5	A	1506	POV	C33-C34-C35-C36
6	A	1511	AJP	OAC-CAD-CAK-OAL
6	A	1511	AJP	CBW-CBX-OAU-CAT
4	A	1504	ATP	PA-O3A-PB-O1B
6	A	1511	AJP	CCV-CCA-OBZ-CBY
6	A	1511	AJP	CCW-CCX-OCY-CCZ
4	A	1503	ATP	PA-O3A-PB-O2B
5	A	1508	POV	C29-C210-C211-C212
6	A	1511	AJP	OCC-CCX-OCY-CCZ
4	A	1504	ATP	PA-O3A-PB-O2B
5	A	1506	POV	C39-C310-C311-C312
5	A	1510	POV	C34-C35-C36-C37
4	A	1503	ATP	PA-O3A-PB-O1B

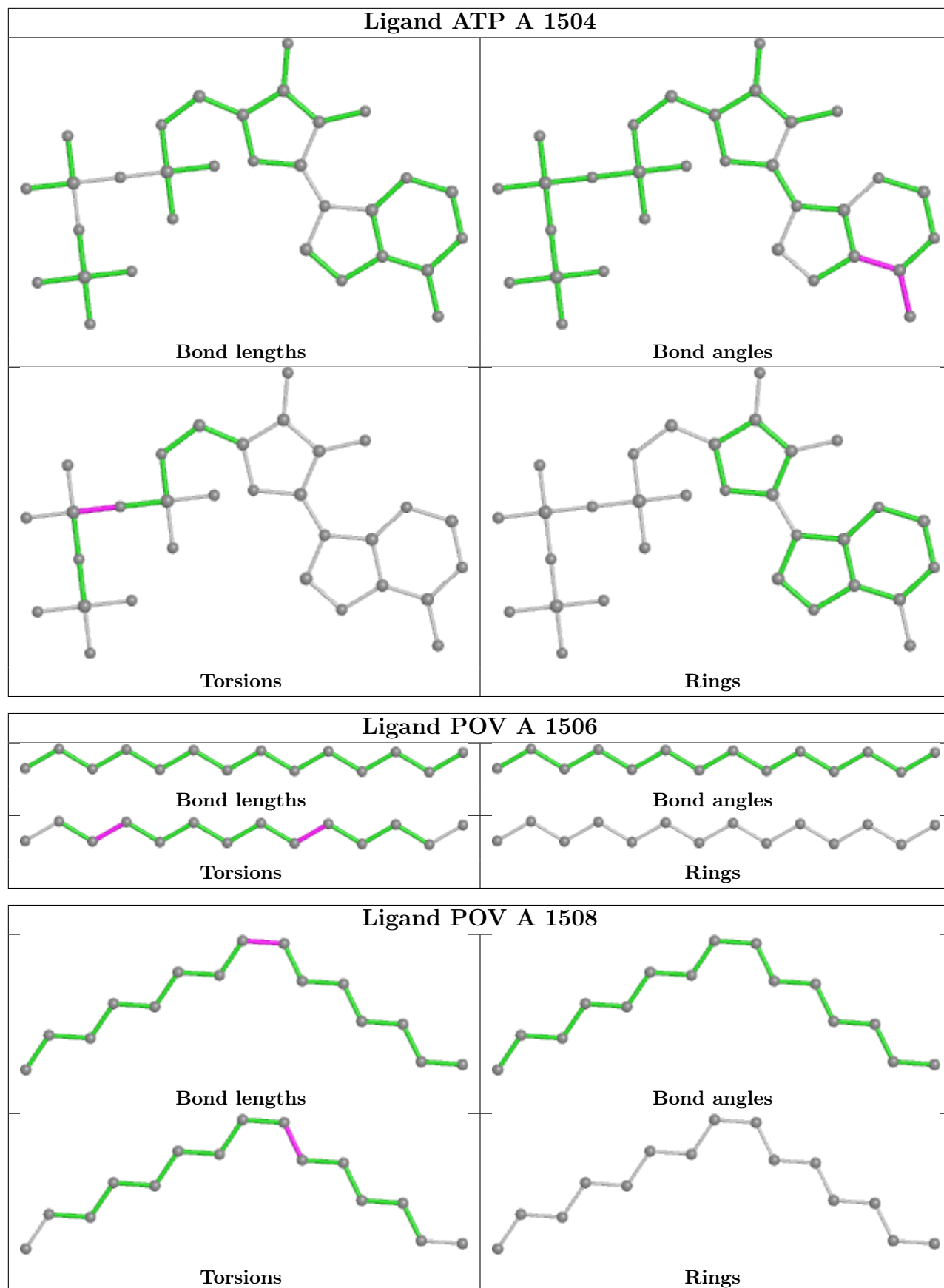
There are no ring outliers.

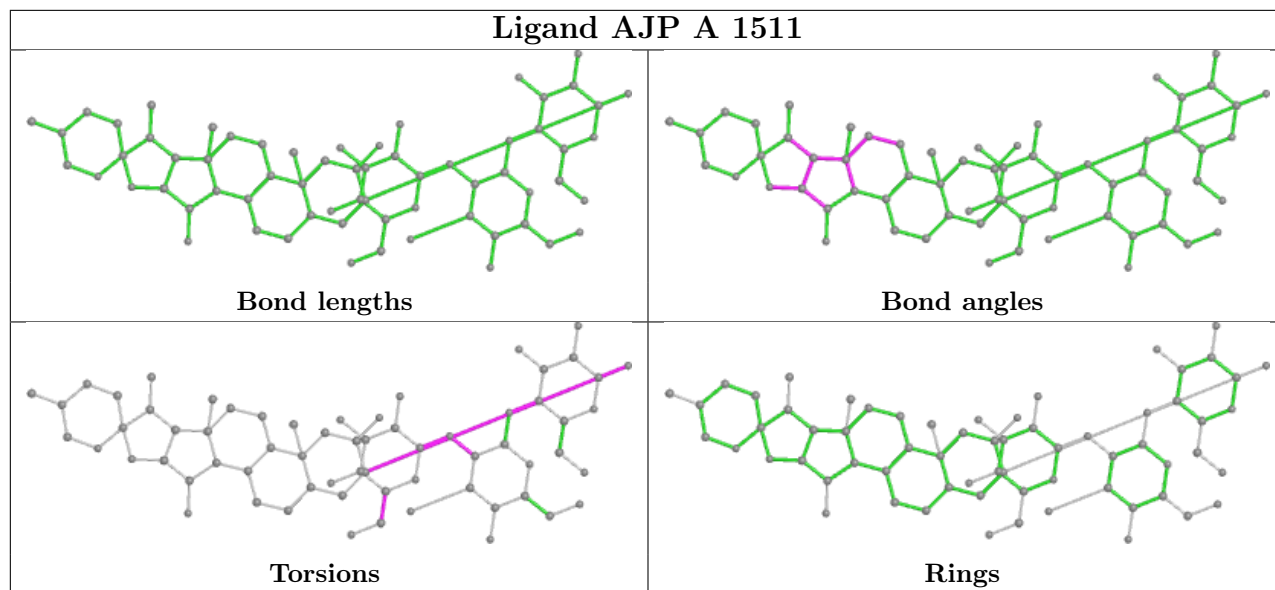
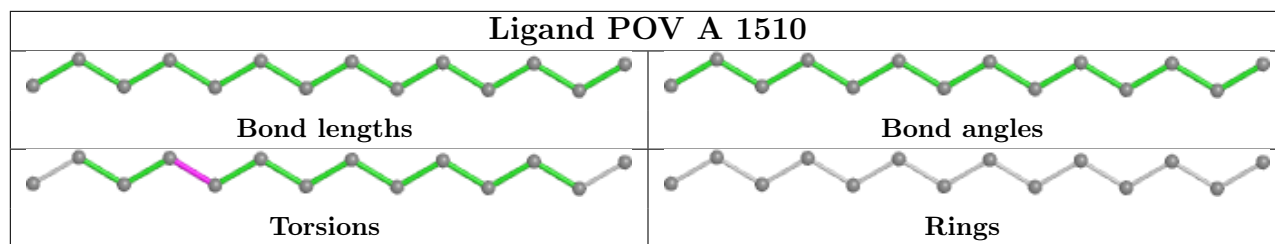
2 monomers are involved in 5 short contacts:

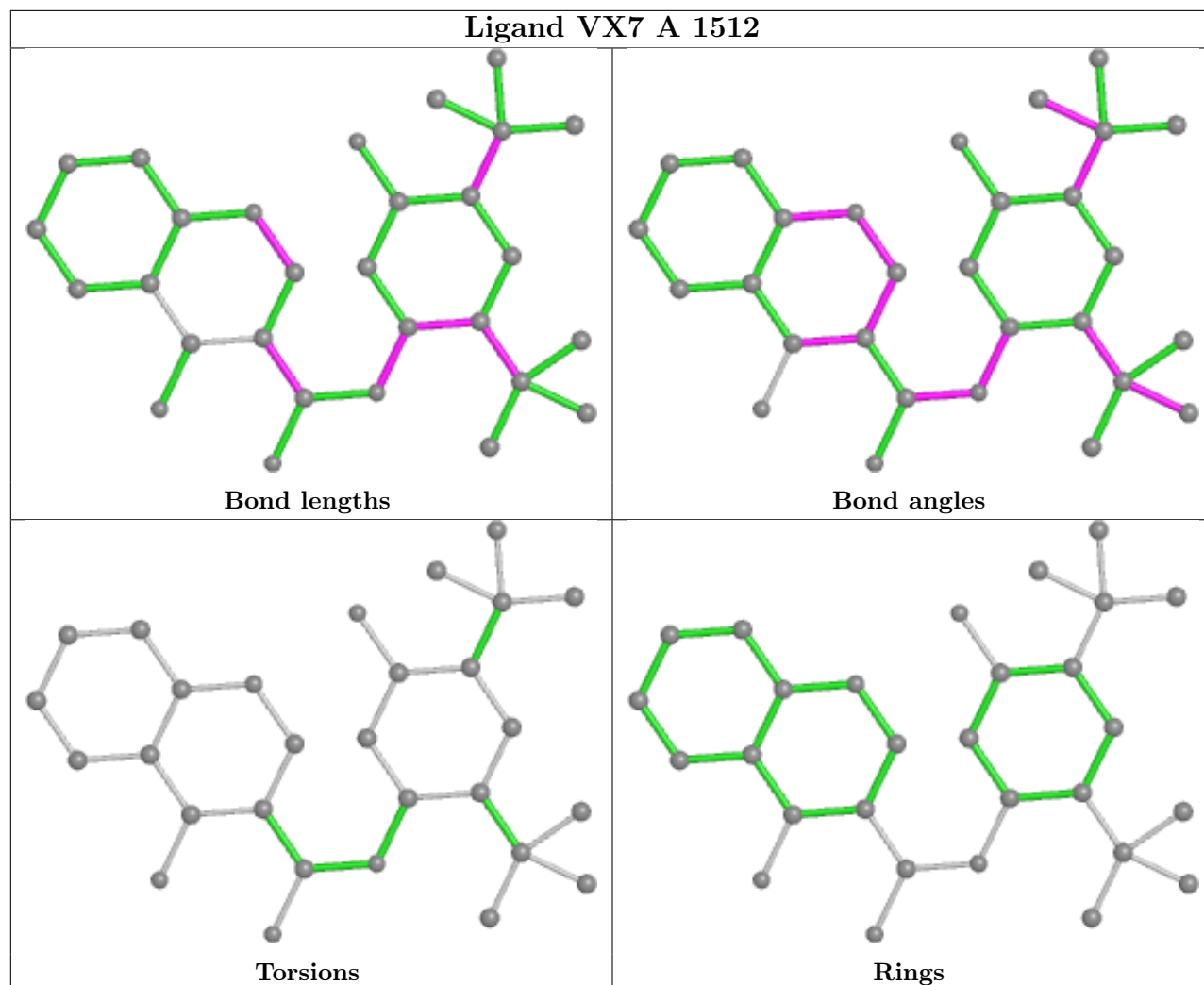
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1511	AJP	4	0
7	A	1512	VX7	1	0

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 than 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.