



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2020 – 04:57 pm BST

PDB ID : 1IJJ
Title : THE X-RAY CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN
RABBIT SKELETAL MUSCLE ACTIN AND LATRUNCULIN A AT 2.85
Å RESOLUTION
Authors : Vorobiev, S.M.; Bubb, M.R.; Almo, S.C.
Deposited on : 2001-04-26
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.11

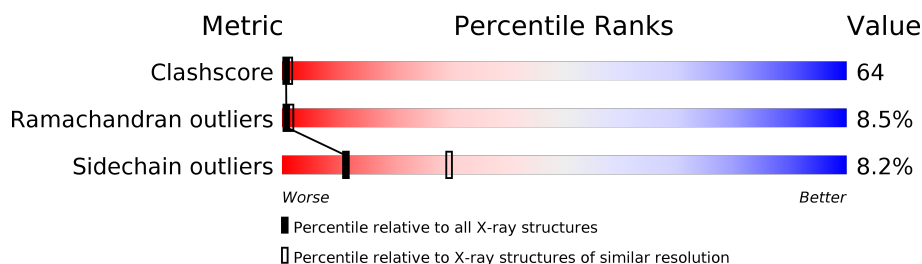
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5674 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.

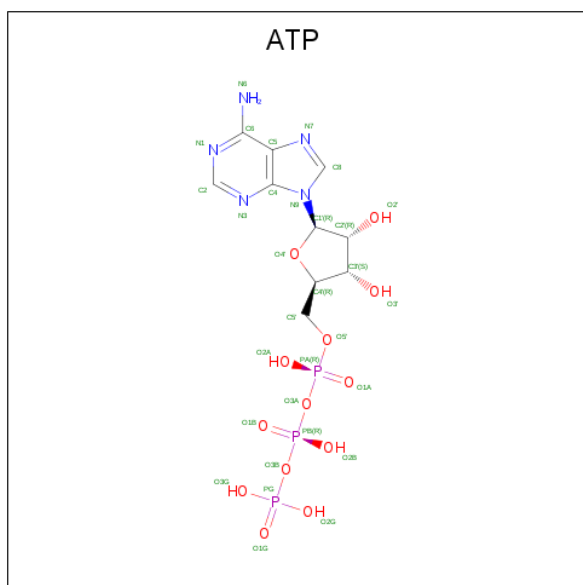
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2714	1722	457	516	19			
1	B	371	Total	C	N	O	S	0	0	0
			2782	1766	468	528	20			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

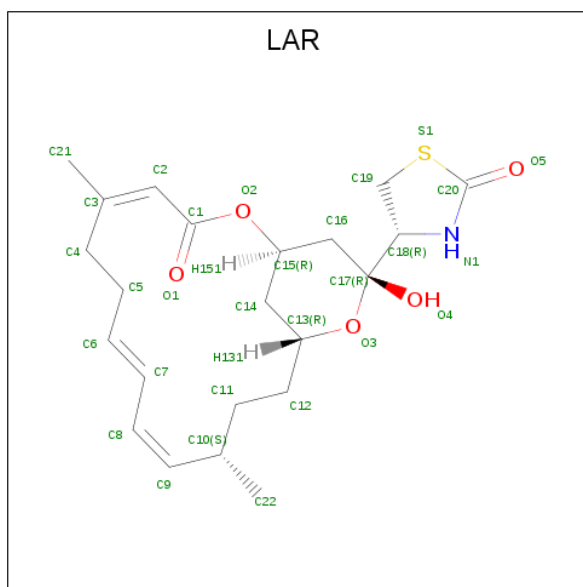
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
4	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 5 is water.

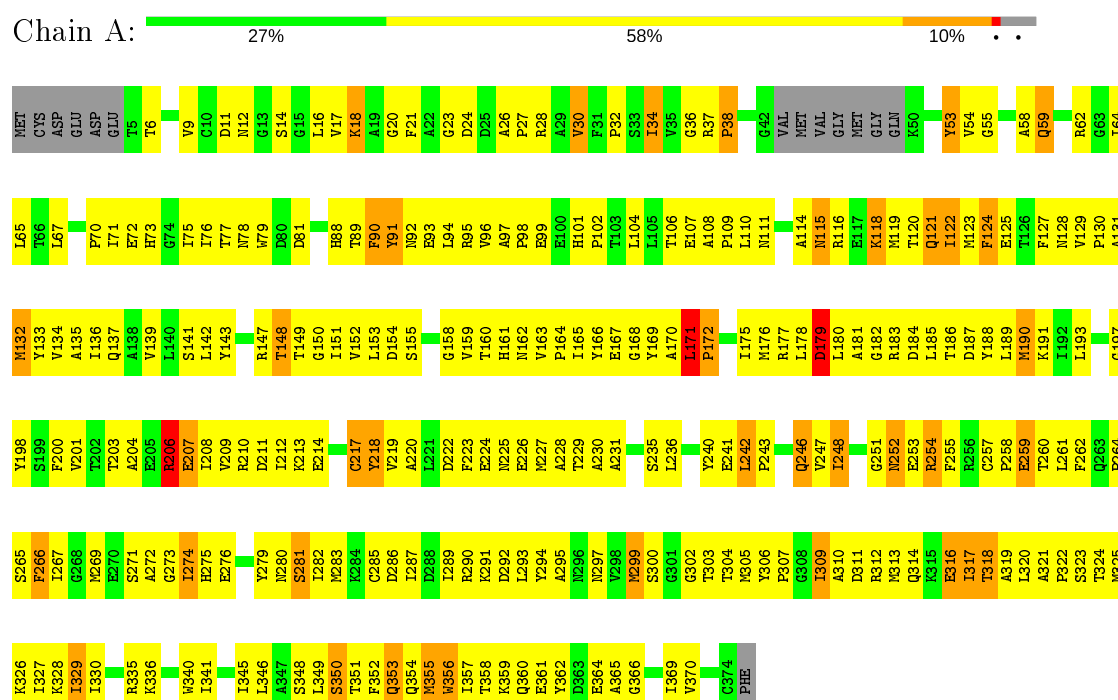
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	15	Total	O	0	0
			15	15		

3 Residue-property plots

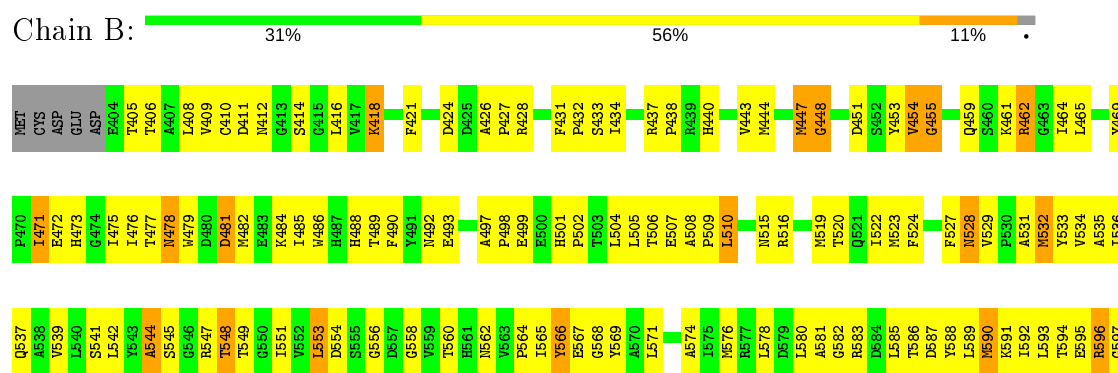
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



I727	F662	T602	T598
K728	Q663	T602	
A731	P664	T602	
F732	S665	T603	
F733	F666	A604	
E734	I667	E605	
R735	G668	R606	
K736	M669	E607	
		V608	
V739	G673	V609	
F740	I674	R610	
I741	H675	D611	
G742	E676	I612	
G743	I677	K613	
S744	T678	L616	
L745	S681	G617	
L746	I682	X618	
	M683	V619	
L749	K684	A620	
S750	C685	L621	
T751	D686	D622	
F752	I687	F623	
Q753	D688	E624	
Q754	I689	M625	
M755	R690	E626	
F756	K691	M627	
I757	D692	A628	
T758	L693	T629	
K759	E694	A630	
Q760	A695		
E761	N696	S633	
Y762	N697	S634	
	V698	S635	
G766	M699	L636	
F767	S700	E637	
S768	G701	K638	
I769	G702	S639	
V770	T703	Y640	
H771	T704	E641	
R772	M705	L642	
K773	Y706	P643	
G774		D644	
PHE	I709	G645	
	A710	Q646	
	D711	V647	
		I648	
	Q714	T649	
	K715	I650	
	E716	G651	
	I717	N652	
	T718	E653	
	A719	R654	
	L720	F655	
	A721	R656	
	F722	C657	
	S723	P658	
	T724	E659	
	M725	T660	
	K726	L661	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.30Å 102.18Å 124.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.85	Depositor
% Data completeness (in resolution range)	96.9 (15.00-2.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5674	wwPDB-VP
Average B, all atoms (Å ²)	76.0	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: MG, ATP, LAR

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	A	0.80	1/2773 (0.0%)	0.98	2/3777 (0.1%)
1	B	0.79	1/2844 (0.0%)	0.97	5/3874 (0.1%)
All	All	0.80	2/5617 (0.0%)	0.97	7/7651 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	774	CYS	C-O	-8.26	1.07	1.23
1	A	356	TRP	CB-CG	-5.04	1.41	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	LEU	CA-CB-CG	-9.46	93.55	115.30
1	B	774	CYS	CA-C-O	8.81	138.59	120.10
1	B	571	LEU	CA-CB-CG	-7.82	97.32	115.30
1	A	200	PHE	N-CA-C	-5.63	95.80	111.00
1	B	510	LEU	CA-CB-CG	-5.32	103.08	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2714	0	2584	344	0
1	B	2782	0	2652	353	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	4	0
4	A	29	0	31	6	0
4	B	29	0	31	10	0
5	A	41	0	0	1	0
5	B	15	0	0	0	0
All	All	5674	0	5322	695	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 64.

The worst 5 of 695 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:A:190:MET:HB3	1:A:209:VAL:HG11	1.26	1.16
1:B:590:MET:CG	1:B:609:VAL:HG11	1.79	1.13
1:B:588:TYR:HE2	1:B:657:CYS:HA	1.03	1.09
1:B:588:TYR:CE2	1:B:657:CYS:HA	1.88	1.08
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.30	1.07

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	A	359/377 (95%)	249 (69%)	80 (22%)	30 (8%)	<div>11</div>
1	B	369/377 (98%)	270 (73%)	67 (18%)	32 (9%)	<div>11</div>
All	All	728/754 (97%)	519 (71%)	147 (20%)	62 (8%)	<div>11</div>

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	PRO
1	A	90	PHE
1	A	207	GLU
1	A	274	ILE
1	A	318	THR

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	A	276 / 320 (86%)	254 (92%)	22 (8%)	12	31
1	B	283 / 320 (88%)	259 (92%)	24 (8%)	10	28
All	All	559 / 640 (87%)	513 (92%)	46 (8%)	11	29

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ILE
1	B	478	ASN
1	B	697	ASN
1	A	355	MET
1	B	447	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	B	473	HIS
1	B	697	ASN
1	B	412	ASN
1	B	478	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
3	ATP	A	380	2	26,33,33	1.51	6 (23%)	31,52,52	1.26	3 (9%)
3	ATP	B	880	2	26,33,33	1.65	5 (19%)	31,52,52	1.14	3 (9%)
4	LAR	B	921	-	30,31,31	1.60	4 (13%)	32,43,43	1.44	5 (15%)
4	LAR	A	901	-	30,31,31	1.55	7 (23%)	32,43,43	1.79	7 (21%)

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
3	ATP	A	380	2	-	3/18/38/38	0/3/3/3
3	ATP	B	880	2	-	2/18/38/38	0/3/3/3
4	LAR	B	921	-	-	6/23/51/51	0/2/3/3
4	LAR	A	901	-	-	6/23/51/51	0/2/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	921	LAR	C20-N1	-5.60	1.26	1.34
3	B	880	ATP	C5'-C4'	4.43	1.65	1.51
4	A	901	LAR	C20-N1	-3.63	1.29	1.34
3	A	380	ATP	O2'-C2'	3.40	1.51	1.43
3	A	380	ATP	C5'-C4'	3.32	1.61	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	LAR	C19-S1-C20	5.95	95.19	92.00
4	B	921	LAR	C19-S1-C20	5.46	94.93	92.00
4	A	901	LAR	O5-C20-N1	3.89	131.05	126.81
3	A	380	ATP	C5-C6-N6	3.45	125.60	120.35
3	B	880	ATP	C1'-N9-C4	-3.25	120.93	126.64

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	LAR	O3-C17-C18-C19
3	A	380	ATP	PB-O3B-PG-O3G
4	B	921	LAR	O3-C17-C18-C19
3	B	880	ATP	PG-O3B-PB-O1B
4	B	921	LAR	C16-C15-O2-C1

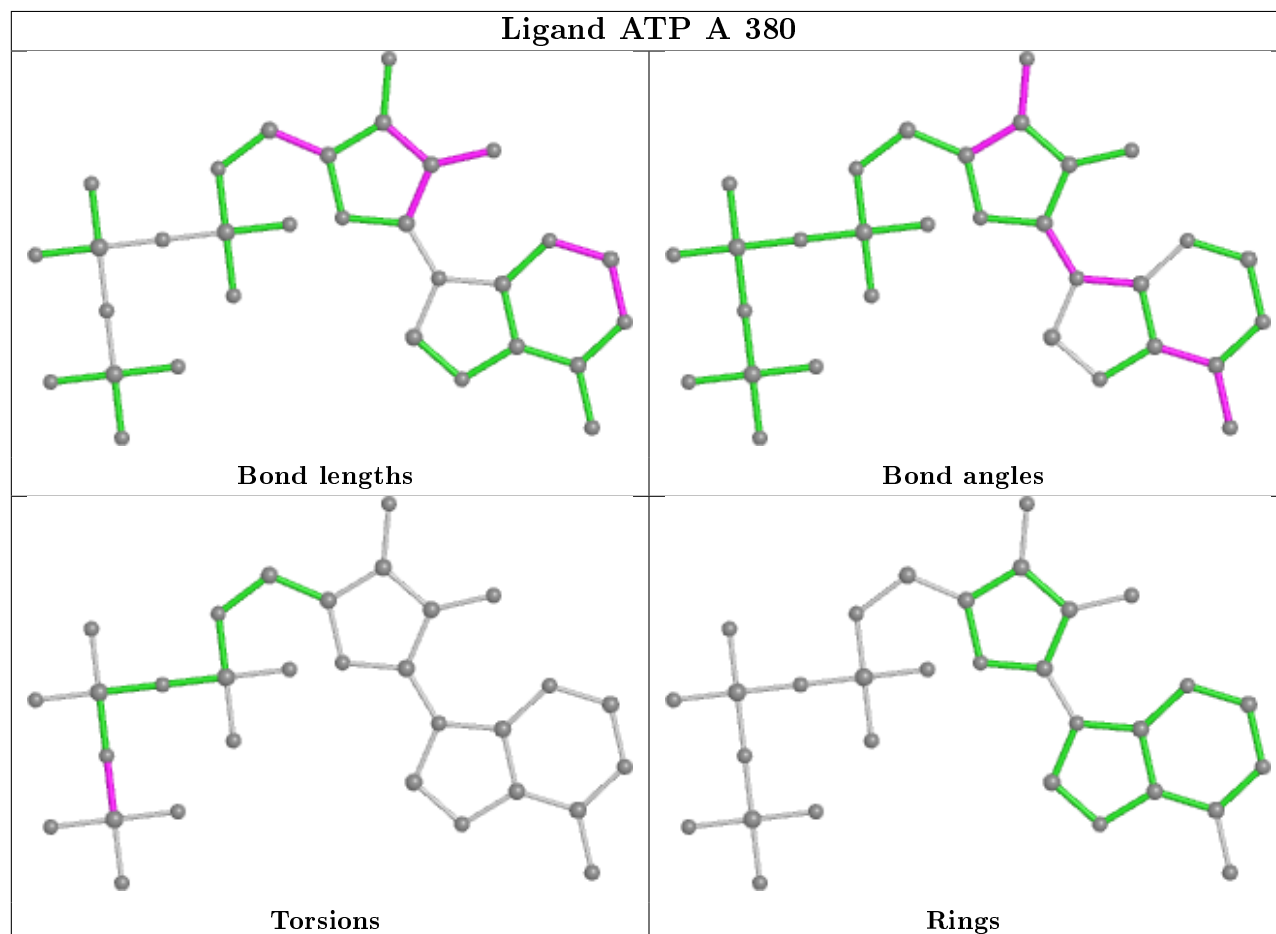
There are no ring outliers.

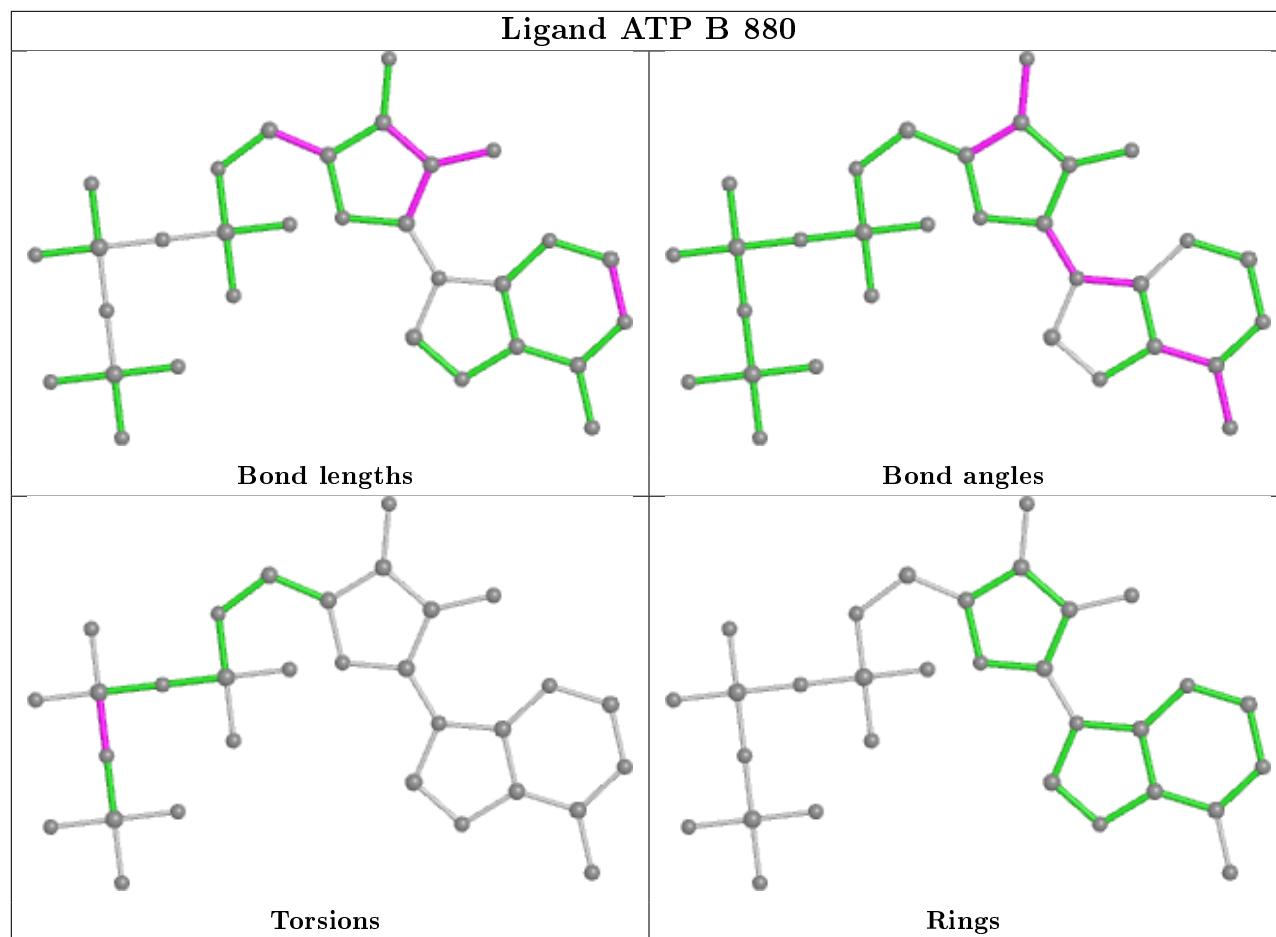
4 monomers are involved in 21 short contacts:

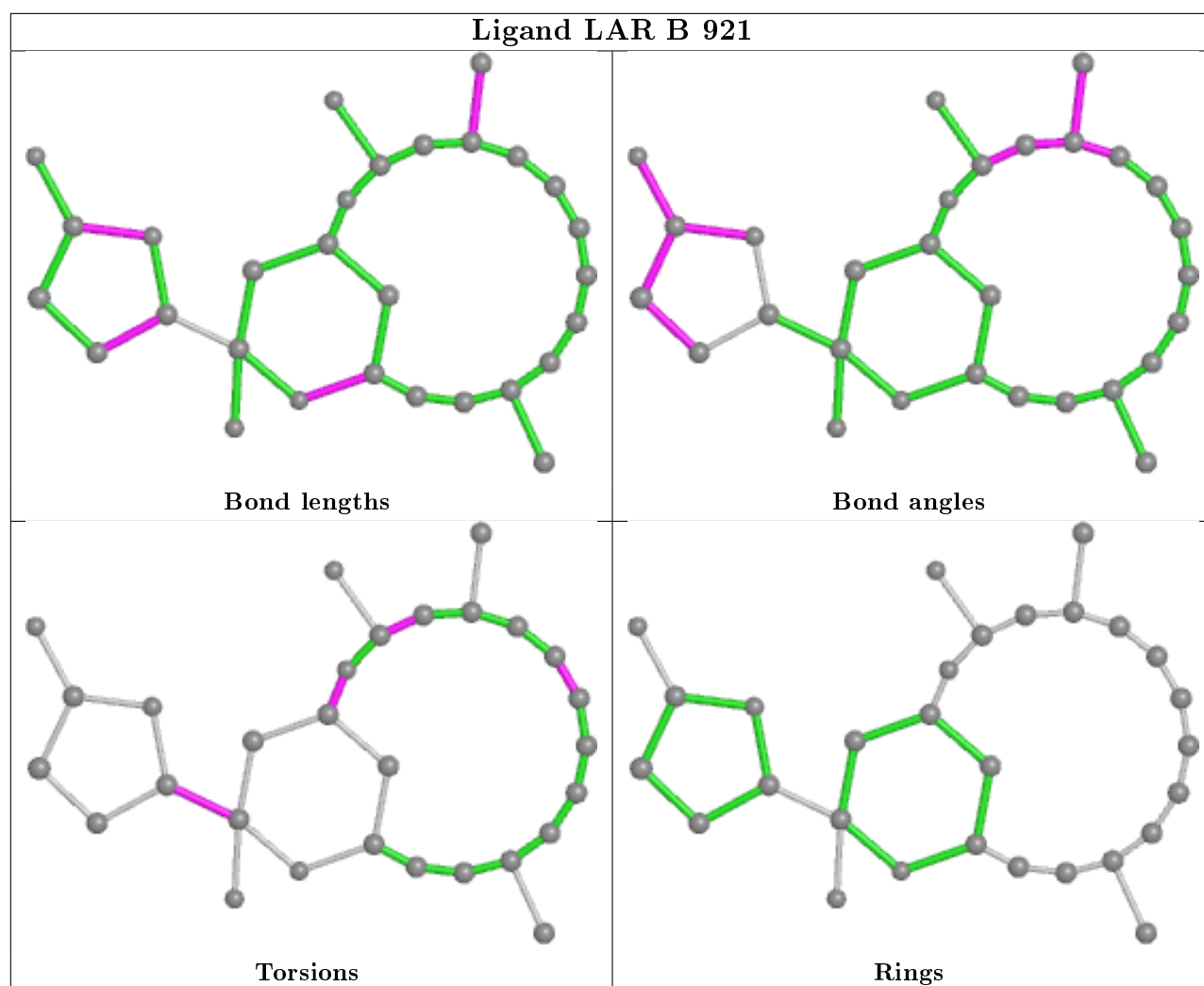
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	380	ATP	1	0
3	B	880	ATP	4	0
4	B	921	LAR	10	0
4	A	901	LAR	6	0

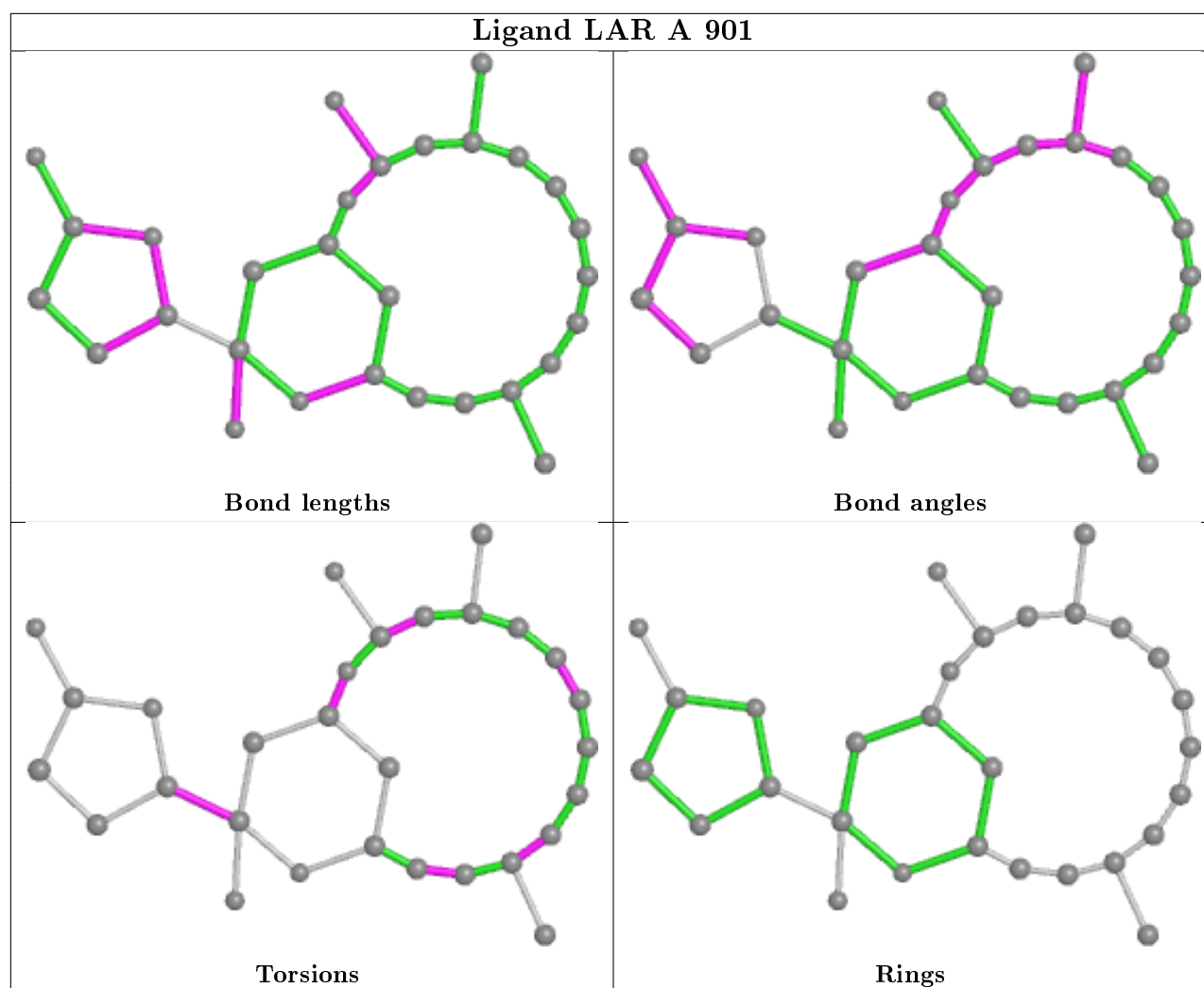
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

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.