



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:24 PM UTC

PDB ID : 1IJJ / pdb_00001ijj
Title : THE X-RAY CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN
RABBIT SKELETAL MUSCLE ACTIN AND LATRUNCULIN A AT 2.85
Å RESOLUTION
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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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

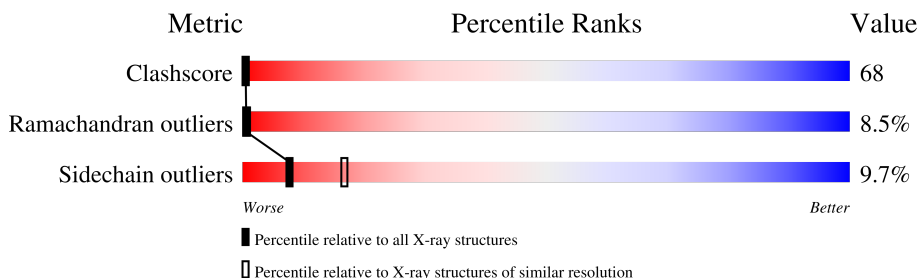
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

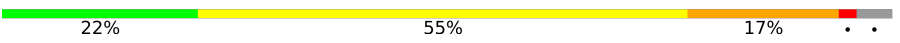
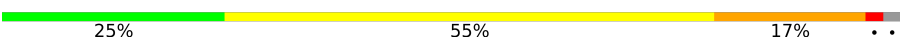
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)

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 $\leq 5\%$.

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 (CCD ID: MG) (formula: Mg).

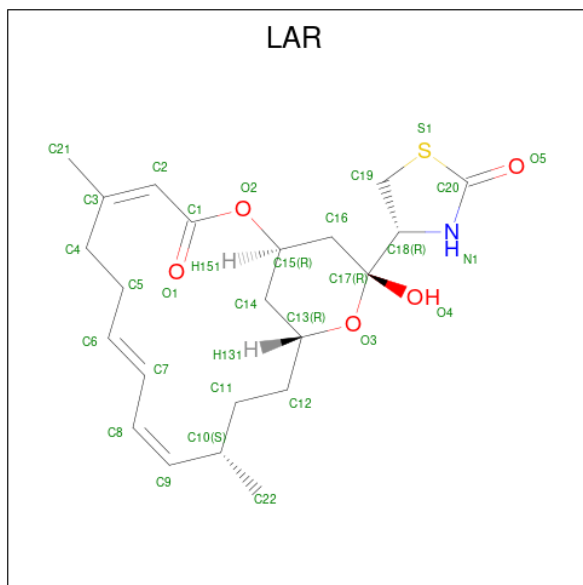
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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 (CCD ID: 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.

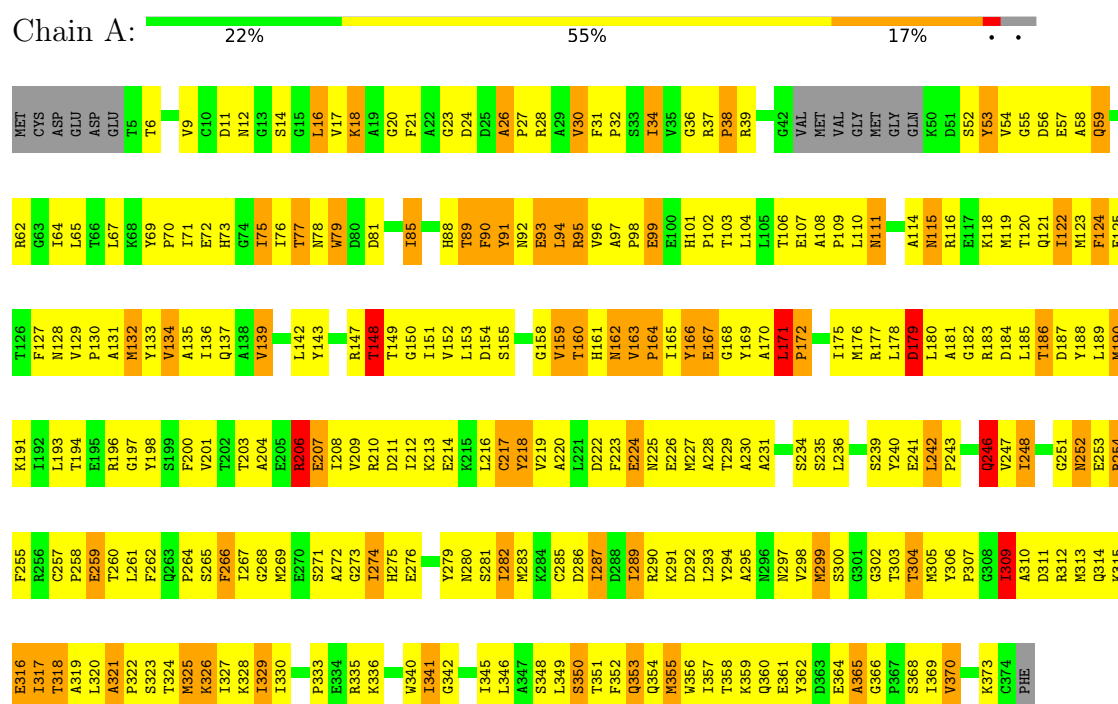
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	15	Total	O	0	0
			15	15		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



L594	T594	E595	R596	G597	Y598		T602	T603	A604	E605	R606	E607	I608	V609	R610	D611	I612	K613	E614	R615	L616	C617	Y618	V619	A620	L621	D622	F623	E624	N625	E626	M627	A628	T629	A630	A631	S632	S633	S634	S635	L636	E637	K638	S639	Y640	E641	L642	P643	D644	G645	Q646	V647	I648	T649	I650	G651	N652	E653	R654
F655	R656	C657	P658	E659	T660	L661	F662	Q663	P664	S665	F666	I667	G668	M669		G673	I674	H675	R676	T677	T678		S681	I682	M683	K684	C685	D686	I687	D688	I689	R690	K691	D692	L693	Y694	A695	R696	N697	V698	M699	S700	G701	G702	T703	T704	M705	Y706		I709	A710	D711	R712	M713	Q714	K715	E716	I717	T718
A719	L720	A721	P722	S723	T724	M725	K726	I727	K728	I729	I730	A731	F732	P733	E734	R735	K736		V739	W740	I741	G742	G743	S744	I745	L746	A747	S748	L749	S750	T751	F752	Q753	Q754	M755	W756	I757	T758	K759	Q760	E761	Y762		G766	P767	S768	I769	V770	H771	R772	K773	C774	PHE						

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LAR, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	3/2773 (0.1%)	1.44	45/3777 (1.2%)
1	B	1.00	5/2844 (0.2%)	1.45	49/3874 (1.3%)
All	All	1.00	8/5617 (0.1%)	1.44	94/7651 (1.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	774	CYS	C-O	-7.95	1.07	1.23
1	A	341	ILE	CA-CB	-7.49	1.46	1.54
1	A	325	MET	SD-CE	-7.04	1.61	1.79
1	B	741	ILE	CA-CB	-6.51	1.47	1.54
1	B	536	ILE	CA-CB	-6.22	1.46	1.54

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	704	THR	N-CA-C	-11.86	99.20	112.72
1	A	79	TRP	N-CA-C	10.62	122.44	111.07
1	B	774	CYS	CA-C-O	10.47	138.59	120.80
1	B	441	GLN	N-CA-C	-10.38	100.23	113.72
1	A	304	THR	N-CA-C	-9.91	101.83	112.93

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	2714	0	2584	367	0
1	B	2782	0	2652	377	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	742	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 68.

The worst 5 of 742 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%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	369/377 (98%)	270 (73%)	67 (18%)	32 (9%)	0	0
All	All	728/754 (97%)	519 (71%)	147 (20%)	62 (8%)	0	1

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%)	249 (90%)	27 (10%)	7	16
1	B	283/320 (88%)	256 (90%)	27 (10%)	8	17
All	All	559/640 (87%)	505 (90%)	54 (10%)	8	17

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	447	MET
1	B	548	THR
1	B	748	SER
1	B	464	ILE
1	B	509	PRO

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

Mol	Chain	Res	Type
1	B	487	HIS
1	B	528	ASN

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Mol	Chain	Res	Type
1	B	501	HIS
1	B	537	GLN
1	A	128	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	LAR	B	921	-	30,31,31	1.30	3 (10%)	32,43,43	1.34	4 (12%)
3	ATP	B	880	2	32,33,33	1.64	4 (12%)	48,52,52	0.93	3 (6%)
4	LAR	A	901	-	30,31,31	1.39	6 (20%)	32,43,43	1.62	6 (18%)
3	ATP	A	380	2	32,33,33	1.42	5 (15%)	48,52,52	1.06	4 (8%)

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	LAR	B	921	-	-	6/23/51/51	0/2/3/3
3	ATP	B	880	2	-	2/22/38/38	0/3/3/3
4	LAR	A	901	-	-	6/23/51/51	0/2/3/3
3	ATP	A	380	2	-	3/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	880	ATP	C5'-C4'	4.61	1.65	1.51
3	A	380	ATP	C5'-C4'	3.45	1.61	1.51
3	B	880	ATP	C2-N1	3.38	1.39	1.33
3	A	380	ATP	O2'-C2'	3.24	1.51	1.43
3	B	880	ATP	C2'-C3'	-3.04	1.45	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	LAR	C19-S1-C20	5.44	95.19	92.04
4	B	921	LAR	C19-S1-C20	4.99	94.93	92.04
4	B	921	LAR	C3-C2-C1	3.05	134.63	127.36
3	A	380	ATP	O3'-C3'-C4'	-2.91	102.73	111.08
4	A	901	LAR	C15-O2-C1	2.77	124.40	117.35

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

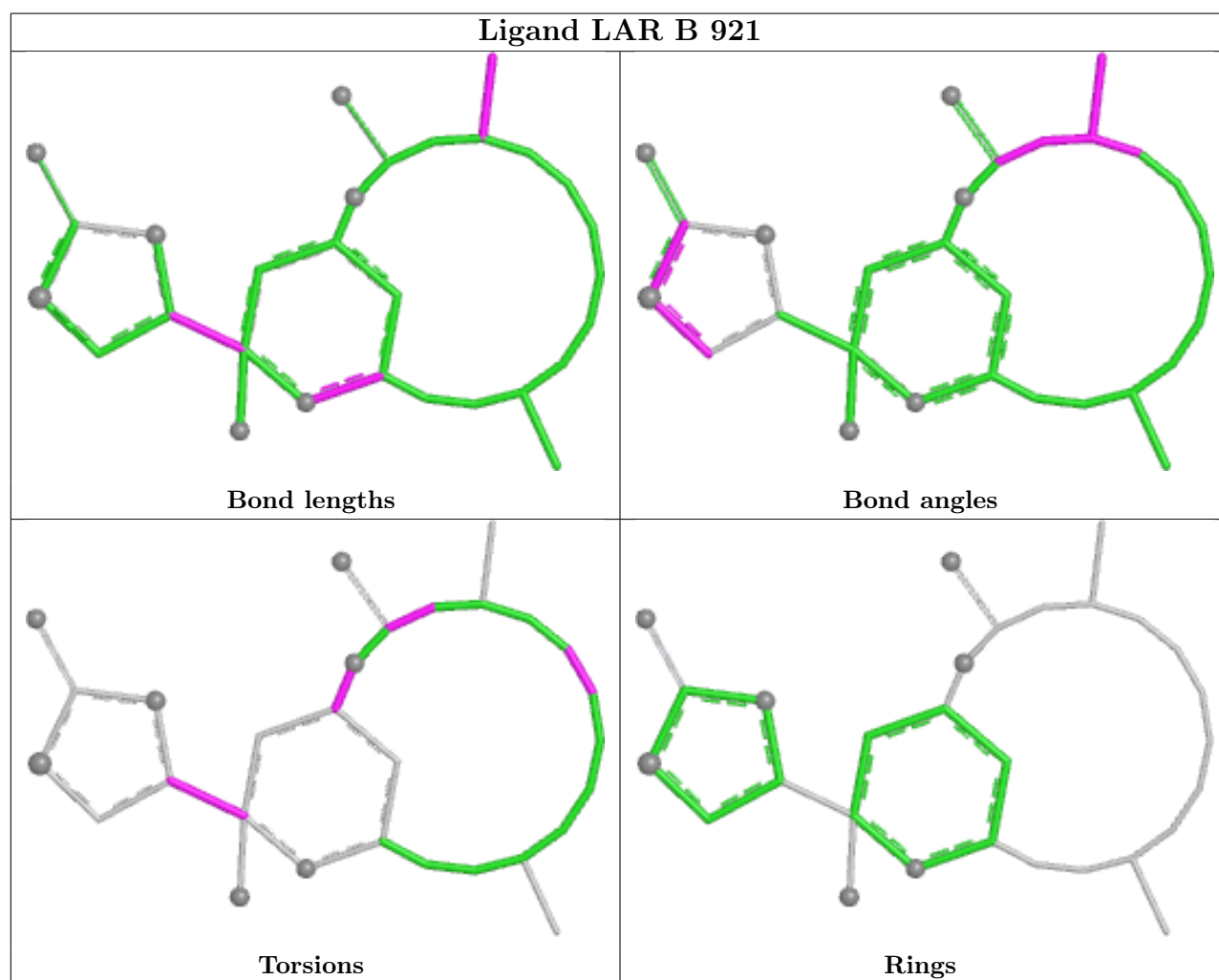
Mol	Chain	Res	Type	Atoms
3	A	380	ATP	PB-O3B-PG-O3G
4	A	901	LAR	O3-C17-C18-C19
4	B	921	LAR	O3-C17-C18-C19
3	B	880	ATP	PG-O3B-PB-O1B
4	B	921	LAR	C16-C15-O2-C1

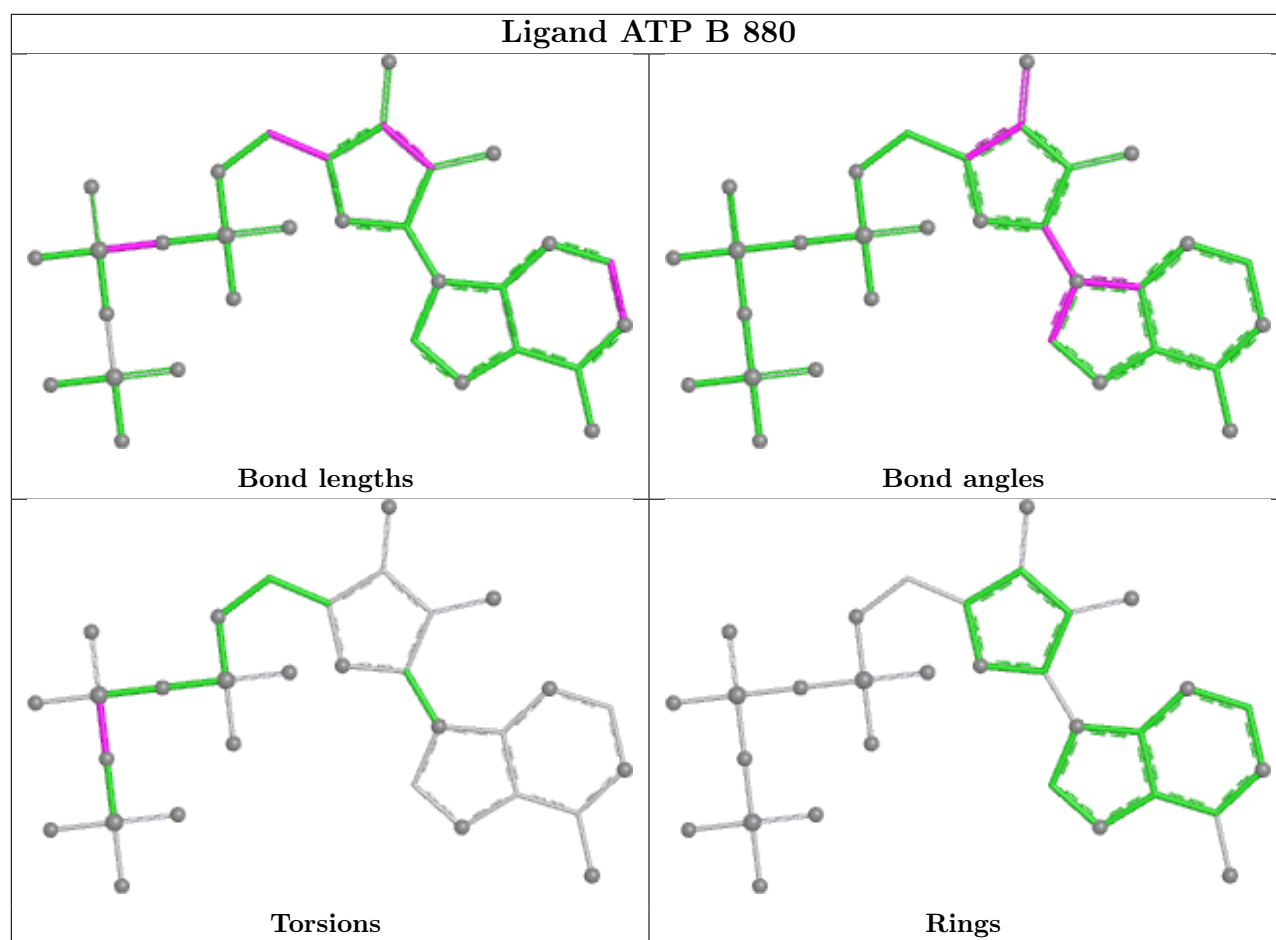
There are no ring outliers.

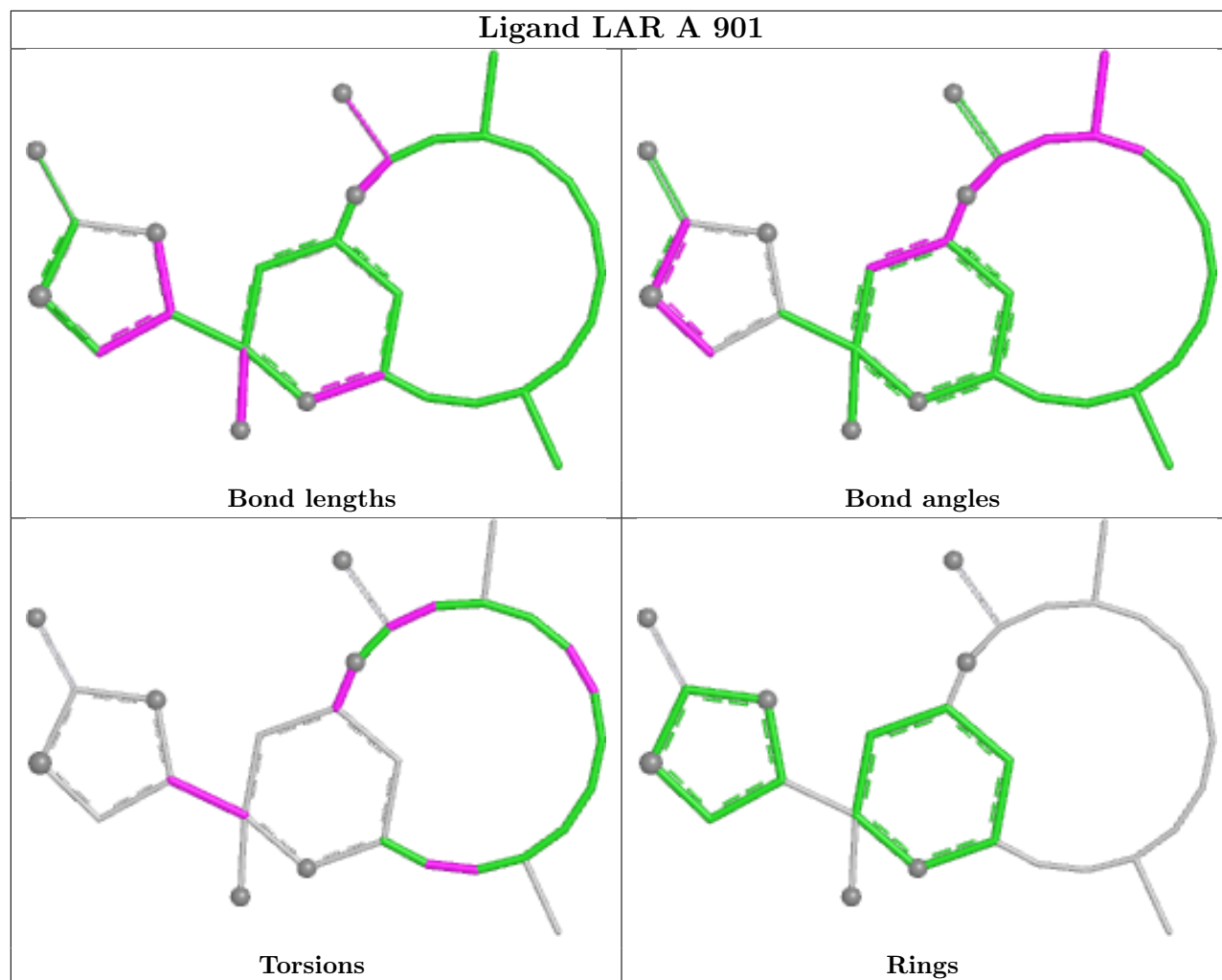
4 monomers are involved in 21 short contacts:

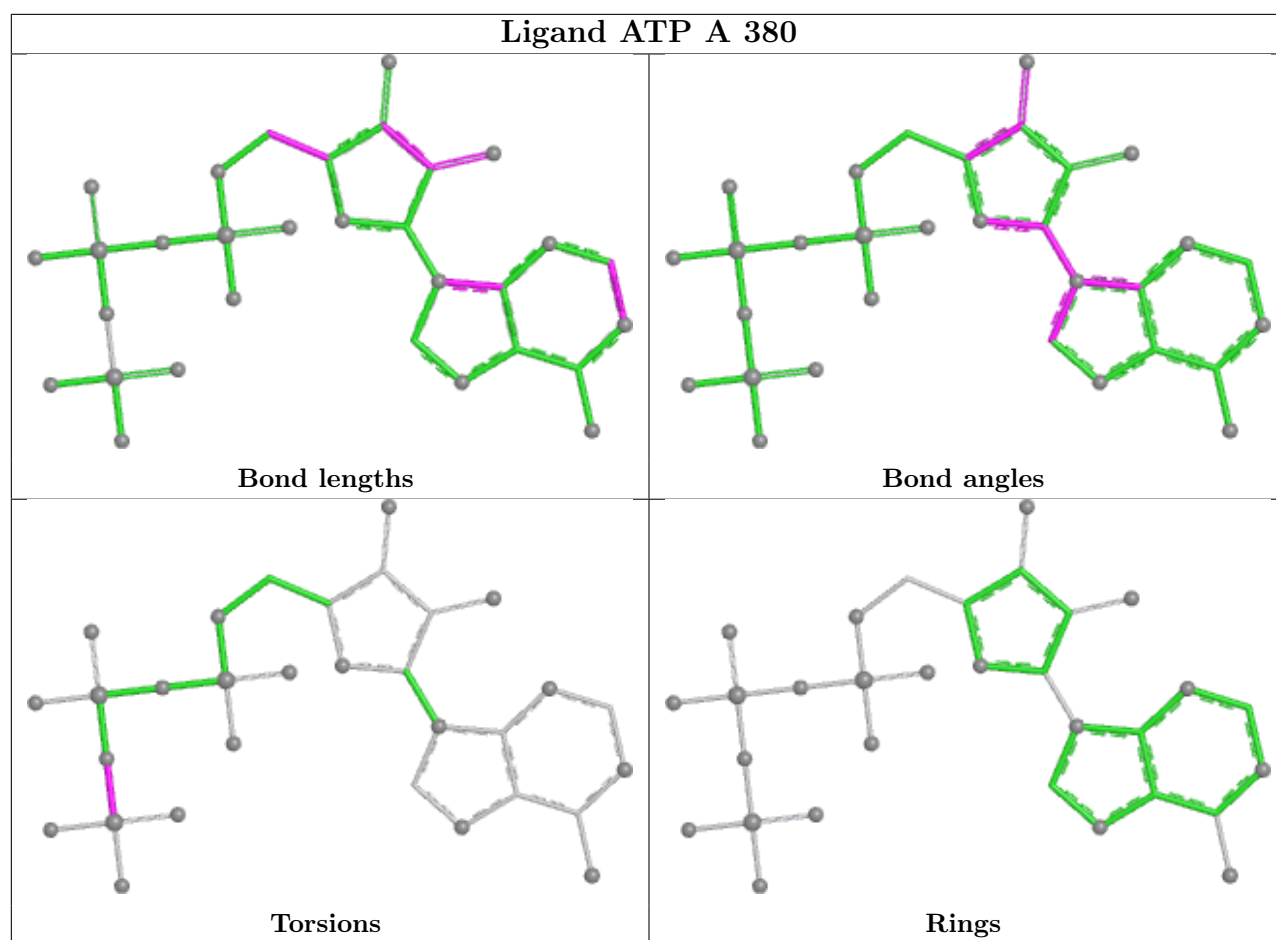
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	921	LAR	10	0
3	B	880	ATP	4	0
4	A	901	LAR	6	0
3	A	380	ATP	1	0

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.