



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:03 am BST

PDB ID : 1J36
Title : Crystal Structure of Drosophila AnCE
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Deposited on : 2003-01-20
Resolution : 2.40 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

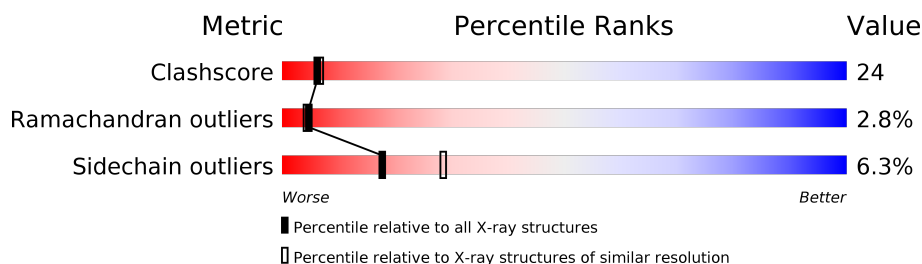
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	607	
1	B	607	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10263 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 angiotensin converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			
1	B	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			

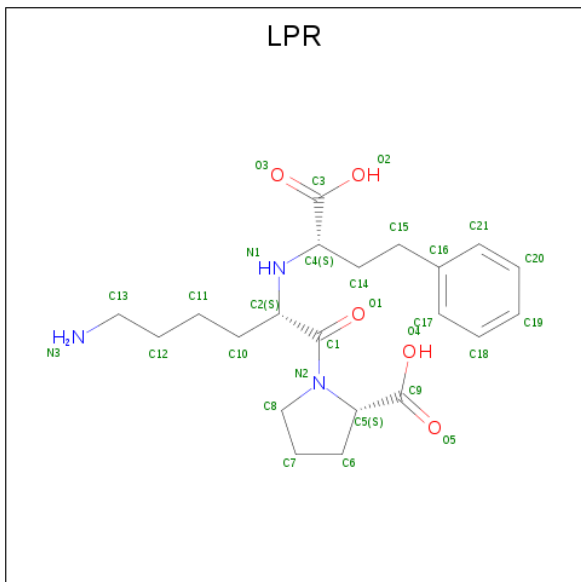
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ARG	GLY	CONFLICT	UNP Q10714
A	53	ALA	ASN	CONFLICT	UNP Q10714
A	607	ILE	THR	CONFLICT	UNP Q10714
A	616	HIS	-	EXPRESSION TAG	UNP Q10714
A	617	HIS	-	EXPRESSION TAG	UNP Q10714
A	618	HIS	-	EXPRESSION TAG	UNP Q10714
A	619	HIS	-	EXPRESSION TAG	UNP Q10714
A	620	HIS	-	EXPRESSION TAG	UNP Q10714
B	51	ARG	GLY	CONFLICT	UNP Q10714
B	53	ALA	ASN	CONFLICT	UNP Q10714
B	607	ILE	THR	CONFLICT	UNP Q10714
B	616	HIS	-	EXPRESSION TAG	UNP Q10714
B	617	HIS	-	EXPRESSION TAG	UNP Q10714
B	618	HIS	-	EXPRESSION TAG	UNP Q10714
B	619	HIS	-	EXPRESSION TAG	UNP Q10714
B	620	HIS	-	EXPRESSION TAG	UNP Q10714

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is [N2-[(S)-1-CARBOXY-3-PHENYLPROPYL]-L-LYSYL-L-PROLINE (three-letter code: LPR) (formula: C₂₁H₃₁N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	21	3	5		
3	B	1	Total	C	N	O	0	0
			29	21	3	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total	O	0	0
			196	196		
4	B	207	Total	O	0	0
			207	207		

M577	R485	A389	Q301	L194
S578	S486	M390	S309	M195
I582	E487	P391	M310	M196
A583	K488	G392	N311	F197
E584		V397		T198
Y585	D491		L315	E202
F586	S404			L317
E587	P493	T407	K322	E218
R590	A494		K327	
V591	K495	H410		R225
W592	Y496	L411	D330	P226
	I498		G331	L227
E596	E503	L416	R332	
M600	Y504	L417	D333	H232
M601	L505	K418	L334	R240
W602	R506	D419	V335	
H603	Y507		C336	
I604	L603	R422		V248
G605	V509	D423	W341	S249
W606		D424	D342	E250
I607	I513	E425	F343	T251
T608	Q514	A426	Y344	
	F515		L345	T254
V613	Q516	M429	I346	P255
S614		L433	D347	M256
S615	S620			H257
	I523	I439	R350	L258
H620	K524			L259
	A525	L442	Q353	M262
	G526	P443	T355	M263
	Q527		R356	A264
	Y528	F446	V357	
			T358	D272
		D449	Q359	I273
	M532	K450	D360	V274
	N531	Y451	Q361	S275
		R452	L362	P276
	L535	W453		F277
	P536	S454	V365	
	L537		H366	K280
	D538			P281
	M539	R457	L369	L282
	C540			V283
	D541	D461		D284
	I542	K462	Y374	V285
	Y543		L375	
	G544	W465	L376	
			Q377	M289
		L472	Y378	E290
	F552	R473	Q379	K291
	H553	D474	H380	Q292
		E475	Q381	A293
	L556	Y476	P382	T294
		S477	F383	T295
	G559	G478	V384	P296
		I479	Y385	L297
	F571		R386	
		P482		P290

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 121.22Å 94.74Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	92.2 (20.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10263	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: ZN, LPR

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	0.45	0/5031	0.67	3/6814 (0.0%)
1	B	0.46	0/5031	0.67	3/6814 (0.0%)
All	All	0.46	0/10062	0.67	6/13628 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	CYS	CA-CB-SG	-5.85	103.47	114.00
1	A	457	ARG	N-CA-C	-5.68	95.65	111.00
1	B	457	ARG	N-CA-C	-5.57	95.96	111.00
1	B	336	CYS	CA-CB-SG	-5.35	104.36	114.00
1	B	491	ASP	N-CA-C	5.17	124.97	111.00

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	4900	0	4696	217	0
1	B	4900	0	4696	240	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	29	0	29	1	0
3	B	29	0	29	1	0
4	A	196	0	0	10	0
4	B	207	0	0	31	0
All	All	10263	0	9450	458	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 24.

The worst 5 of 458 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:B:26:LYS:HE2	1:B:93:LEU:HD21	1.39	1.03
1:B:479:ILE:HA	4:B:947:HOH:O	1.57	1.01
1:A:26:LYS:HE2	1:A:93:LEU:HD21	1.40	0.98
1:B:347:ASP:H	1:B:379:GLN:NE2	1.68	0.92
1:A:347:ASP:H	1:A:379:GLN:NE2	1.67	0.91

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	596/607 (98%)	541 (91%)	39 (6%)	16 (3%)	5 5
1	B	596/607 (98%)	537 (90%)	42 (7%)	17 (3%)	4 4
All	All	1192/1214 (98%)	1078 (90%)	81 (7%)	33 (3%)	5 4

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	147	PRO
1	A	423	ASP
1	A	424	ASP
1	A	542	ILE

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	522/530 (98%)	490 (94%)	32 (6%)	18	30
1	B	522/530 (98%)	488 (94%)	34 (6%)	17	27
All	All	1044/1060 (98%)	978 (94%)	66 (6%)	18	28

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	601	ASN
1	B	119	THR
1	B	537	LEU
1	A	606	TRP
1	B	100	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	ASN
1	B	41	ASN
1	B	532	ASN
1	A	600	ASN
1	A	610	ASN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 2 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
3	LPR	A	801	2	24,30,30	1.96	7 (29%)	29,39,39	1.14	3 (10%)
3	LPR	B	802	2	24,30,30	1.99	11 (45%)	29,39,39	1.13	2 (6%)

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	LPR	A	801	2	-	4/22/40/40	0/2/2/2
3	LPR	B	802	2	-	4/22/40/40	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	LPR	C4-N1	4.24	1.53	1.47
3	A	801	LPR	C4-N1	4.24	1.53	1.47
3	B	802	LPR	C7-C6	-3.59	1.36	1.51
3	A	801	LPR	C7-C6	-3.56	1.37	1.51
3	A	801	LPR	O1-C1	2.95	1.27	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	LPR	C4-N1-C2	3.27	122.43	115.52
3	B	802	LPR	C4-N1-C2	3.22	122.35	115.52
3	B	802	LPR	C6-C7-C8	3.11	113.81	104.98
3	A	801	LPR	C6-C7-C8	2.99	113.46	104.98
3	A	801	LPR	C7-C6-C5	2.02	109.52	104.26

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	LPR	C2-C10-C11-C12
3	B	802	LPR	C2-C10-C11-C12
3	B	802	LPR	C10-C11-C12-C13
3	A	801	LPR	C10-C11-C12-C13
3	A	801	LPR	C14-C15-C16-C17

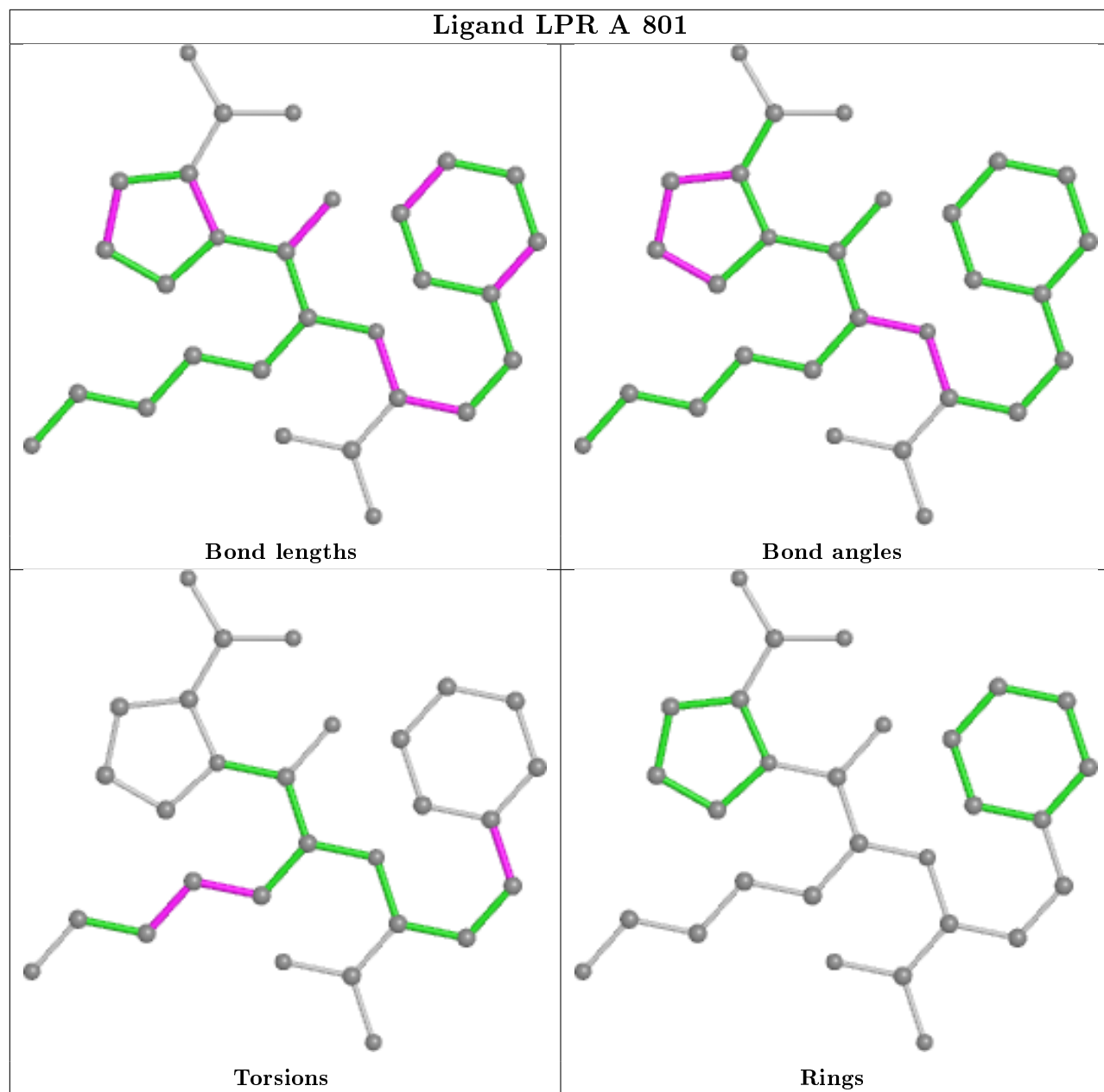
There are no ring outliers.

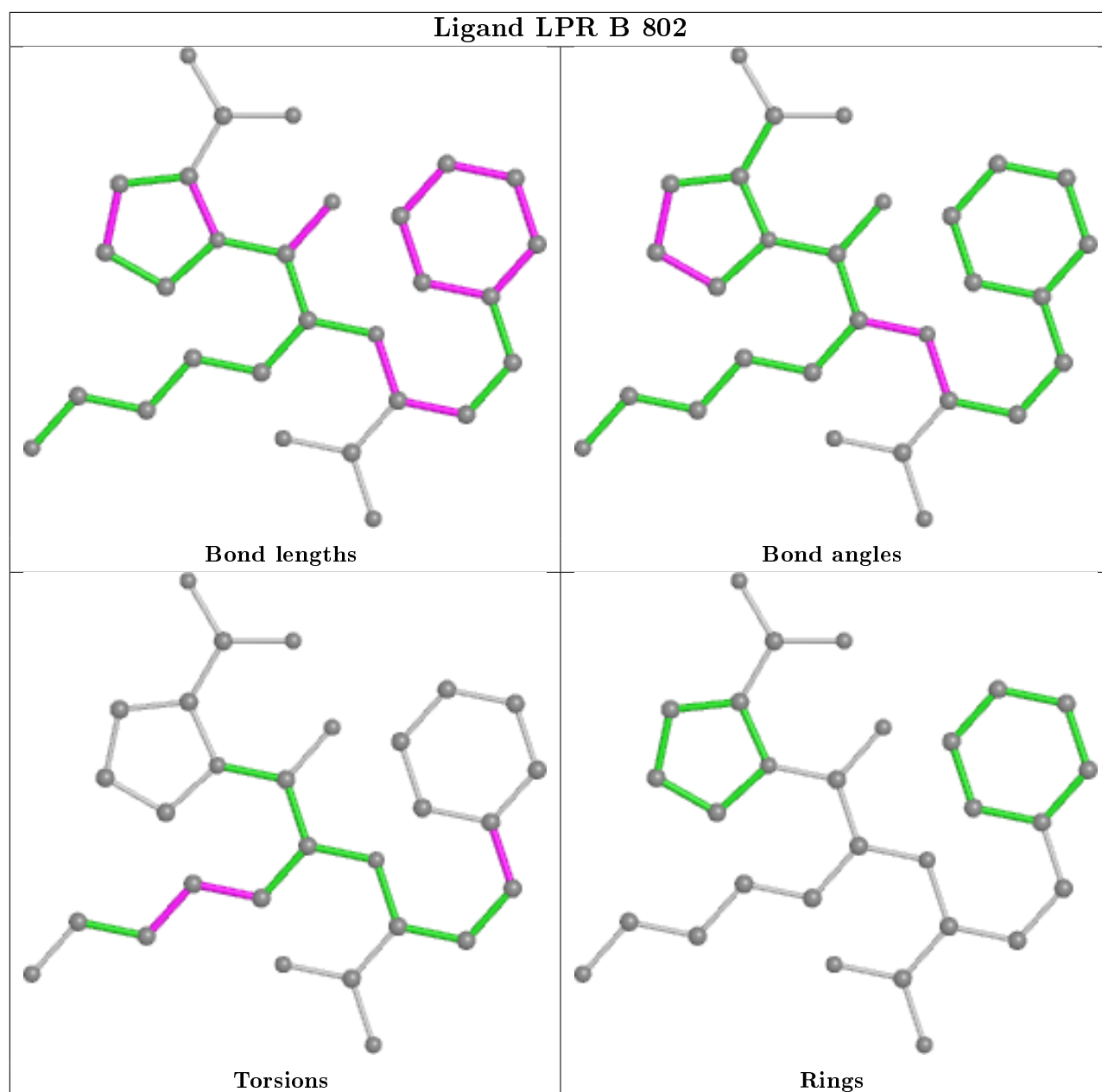
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	LPR	1	0
3	B	802	LPR	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.

Ligand LPR A 801





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.