



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 02:07 PM JST

PDB ID : 8Z22
Title : Crystal structure of the liprin-alpha2/RIM1 complex
Authors : Jin, G.; Wei, Z.
Deposited on : 2024-04-12
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

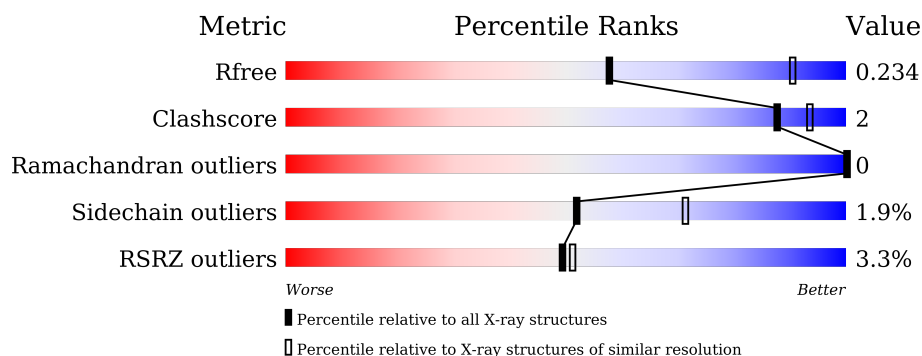
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
R_{free}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	175	<div> <div>2%</div> <div>82%</div> <div>15%</div> </div>
1	B	175	<div> <div>3%</div> <div>74%</div> <div>10%</div> <div>16%</div> </div>
2	C	111	<div> <div>3%</div> <div>79%</div> <div>5%</div> <div>16%</div> </div>
2	D	111	<div> <div>4%</div> <div>77%</div> <div>5%</div> <div>18%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3852 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 Regulating synaptic membrane exocytosis 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1150	738	193	212	7			
1	B	147	Total	C	N	O	S	0	0	0
			1138	732	189	210	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1160	HIS	-	expression tag	UNP A0A8I6GEN0
A	1161	MET	-	expression tag	UNP A0A8I6GEN0
A	1162	GLY	-	expression tag	UNP A0A8I6GEN0
A	1163	SER	-	expression tag	UNP A0A8I6GEN0
A	1164	GLU	-	expression tag	UNP A0A8I6GEN0
A	1165	PHE	-	expression tag	UNP A0A8I6GEN0
B	1160	HIS	-	expression tag	UNP A0A8I6GEN0
B	1161	MET	-	expression tag	UNP A0A8I6GEN0
B	1162	GLY	-	expression tag	UNP A0A8I6GEN0
B	1163	SER	-	expression tag	UNP A0A8I6GEN0
B	1164	GLU	-	expression tag	UNP A0A8I6GEN0
B	1165	PHE	-	expression tag	UNP A0A8I6GEN0

- Molecule 2 is a protein called Liprin-alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	93	Total	C	N	O	S	0	0	0
			782	471	145	160	6			
2	D	91	Total	C	N	O	S	0	0	0
			762	459	139	158	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	294	GLY	-	expression tag	UNP O75334
C	295	PRO	-	expression tag	UNP O75334
C	296	GLY	-	expression tag	UNP O75334
C	297	SER	-	expression tag	UNP O75334
C	298	GLU	-	expression tag	UNP O75334
C	299	PHE	-	expression tag	UNP O75334
D	294	GLY	-	expression tag	UNP O75334
D	295	PRO	-	expression tag	UNP O75334
D	296	GLY	-	expression tag	UNP O75334
D	297	SER	-	expression tag	UNP O75334
D	298	GLU	-	expression tag	UNP O75334
D	299	PHE	-	expression tag	UNP O75334

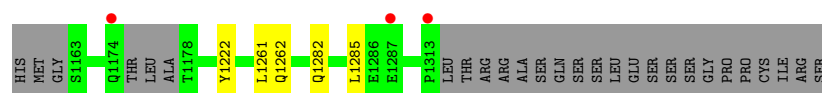
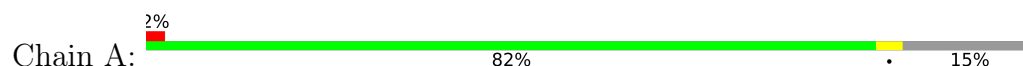
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	6	Total O 6 6	0	0
3	D	1	Total O 1 1	0	0

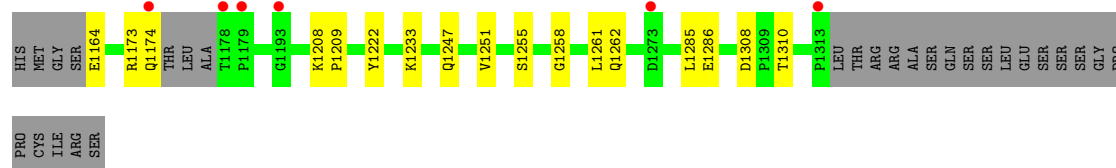
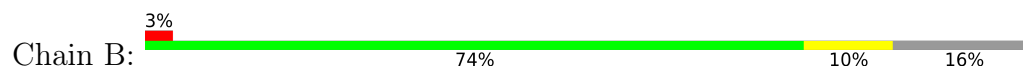
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

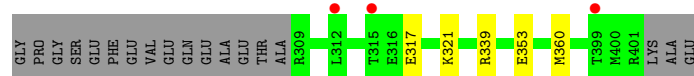
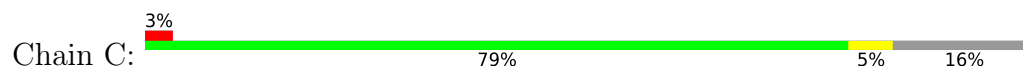
- Molecule 1: Regulating synaptic membrane exocytosis 1



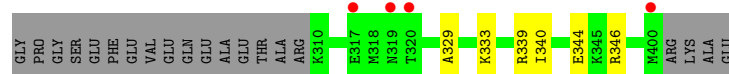
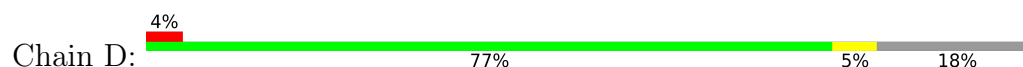
- Molecule 1: Regulating synaptic membrane exocytosis 1



- Molecule 2: Liprin-alpha-2



- Molecule 2: Liprin-alpha-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.66Å 92.70Å 66.58Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	38.80 – 2.75 38.80 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.80-2.75) 98.4 (38.80-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.205 , 0.234 0.208 , 0.234	Depositor DCC
R_{free} test set	17258 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3852	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/1173	0.45	0/1585
1	B	0.25	0/1161	0.45	0/1570
2	C	0.22	0/784	0.37	0/1041
2	D	0.22	0/764	0.34	0/1016
All	All	0.24	0/3882	0.42	0/5212

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	1150	0	1183	3	0
1	B	1138	0	1167	9	0
2	C	782	0	784	1	0
2	D	762	0	758	2	0
3	A	13	0	0	0	0
3	B	6	0	0	0	0
3	D	1	0	0	0	0
All	All	3852	0	3892	15	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 2.

All (15) 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:1261:LEU:HG	1:B:1285:LEU:HD11	1.76	0.68
1:B:1222:TYR:HB2	1:B:1262:GLN:HB2	1.79	0.65
2:C:317:GLU:HG3	2:C:321:LYS:HE3	1.84	0.59
1:B:1173:ARG:HH11	1:B:1310:THR:HB	1.71	0.55
1:A:1222:TYR:HB2	1:A:1262:GLN:HB2	1.89	0.55
1:A:1262:GLN:HG2	1:A:1282:GLN:HG2	1.88	0.55
1:B:1258:GLY:N	1:B:1286:GLU:OE1	2.38	0.55
1:A:1261:LEU:HG	1:A:1285:LEU:HD11	1.92	0.52
1:B:1233:LYS:HE3	1:B:1251:VAL:O	2.16	0.45
1:B:1174:GLN:OE1	1:B:1308:ASP:HB3	2.18	0.44
2:D:340:ILE:O	2:D:344:GLU:HG2	2.16	0.44
2:D:329:ALA:O	2:D:333:LYS:HG3	2.19	0.43
1:B:1261:LEU:HD23	1:B:1261:LEU:HA	1.85	0.42
1:B:1173:ARG:NH1	1:B:1310:THR:HB	2.33	0.42
1:B:1208:LYS:HA	1:B:1209:PRO:HD3	1.96	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	144/175 (82%)	141 (98%)	3 (2%)	0	100	100
1	B	143/175 (82%)	140 (98%)	3 (2%)	0	100	100
2	C	91/111 (82%)	91 (100%)	0	0	100	100
2	D	89/111 (80%)	89 (100%)	0	0	100	100
All	All	467/572 (82%)	461 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	127/150 (85%)	127 (100%)	0	100	100
1	B	125/150 (83%)	122 (98%)	3 (2%)	44	65
2	C	86/100 (86%)	83 (96%)	3 (4%)	31	52
2	D	84/100 (84%)	82 (98%)	2 (2%)	44	65
All	All	422/500 (84%)	414 (98%)	8 (2%)	52	71

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1164	GLU
1	B	1247	GLN
1	B	1255	SER
2	C	339	ARG
2	C	353	GLU
2	C	360	MET
2	D	339	ARG
2	D	346	ARG

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	148/175 (84%)	-0.09	3 (2%) 64 65	40, 57, 95, 119	0
1	B	147/175 (84%)	0.08	6 (4%) 42 44	39, 59, 108, 124	0
2	C	93/111 (83%)	0.38	3 (3%) 50 52	40, 70, 109, 143	0
2	D	91/111 (81%)	0.42	4 (4%) 39 41	48, 78, 117, 125	0
All	All	479/572 (83%)	0.15	16 (3%) 49 51	39, 63, 110, 143	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1193	GLY	3.3
1	B	1179	PRO	3.1
2	C	312	LEU	2.6
1	B	1178	THR	2.5
2	D	317	GLU	2.4
1	B	1174	GLN	2.4
1	B	1273	ASP	2.3
2	C	315	THR	2.3
2	D	319	ASN	2.3
1	A	1287	GLU	2.2
2	D	400	MET	2.2
1	B	1313	PRO	2.2
1	A	1313	PRO	2.1
2	D	320	THR	2.1
2	C	399	THR	2.0
1	A	1174	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.