



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:33 PM UTC

PDB ID : 5J1I / pdb_00005j1i
Title : Structure of the spectrin repeats 7, 8, and 9 of the plakin domain of plectin
Authors : Ortega, E.; DE PEREDA, J.M.
Deposited on : 2016-03-29
Resolution : 2.80 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

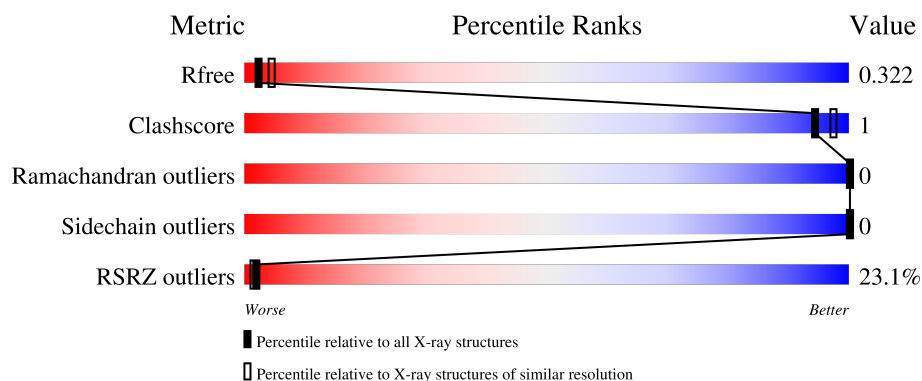
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	373	24% 89% 7%
1	B	373	19% 89% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5179 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 Plectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	1
			2550	1581	473	491	5			
1	B	345	Total	C	N	O	S	0	0	0
			2629	1626	486	511	6			

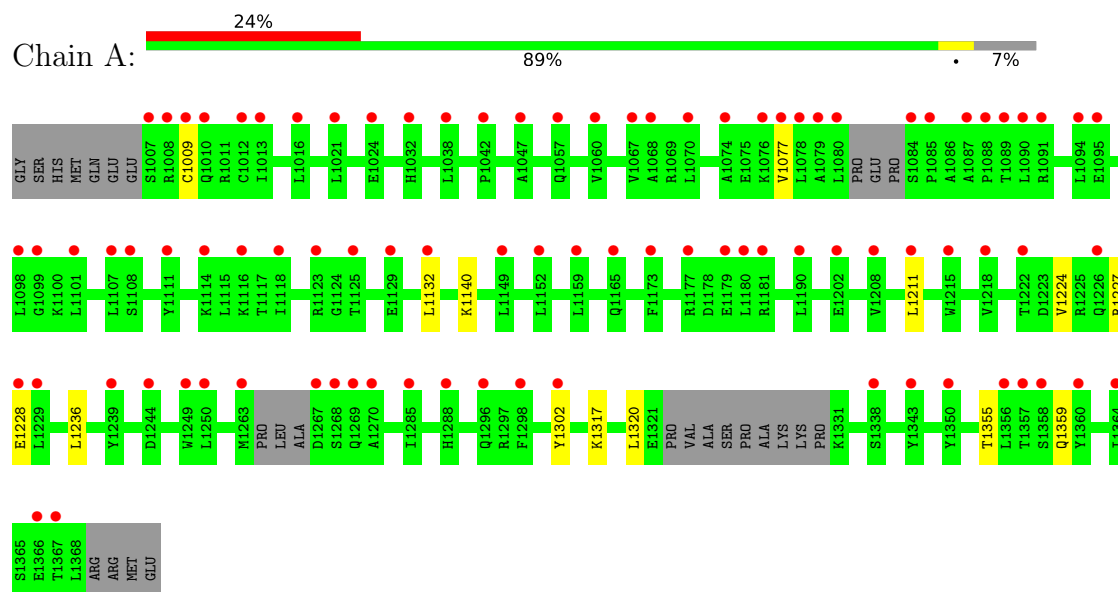
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1000	GLY	-	expression tag	UNP Q15149
A	1001	SER	-	expression tag	UNP Q15149
A	1002	HIS	-	expression tag	UNP Q15149
A	1003	MET	-	expression tag	UNP Q15149
B	1000	GLY	-	expression tag	UNP Q15149
B	1001	SER	-	expression tag	UNP Q15149
B	1002	HIS	-	expression tag	UNP Q15149
B	1003	MET	-	expression tag	UNP Q15149

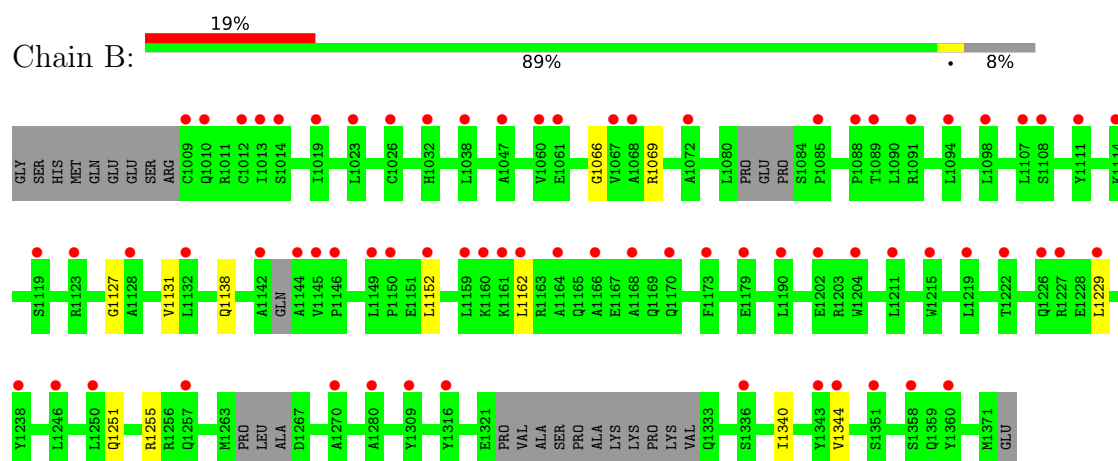
3 Residue-property plots

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 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: Plectin



• Molecule 1: Plectin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	75.24Å 90.70Å 154.54Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	48.88 – 2.80 48.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	55.6 (48.88-2.80) 55.7 (48.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.81Å)	Xtriage
Refinement program	PHENIX dev_2299	Depositor
R, R_{free}	0.296 , 0.322 0.294 , 0.322	Depositor DCC
R_{free} test set	695 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5179	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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	0.24	0/2574	0.51	1/3488 (0.0%)
1	B	0.23	0/2654	0.46	0/3587
All	All	0.23	0/5228	0.49	1/7075 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1227	ARG	CA-CB-CG	-5.43	103.24	114.10

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	2550	0	2392	7	0
1	B	2629	0	2513	6	0
All	All	5179	0	4905	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)
1:B:1138:GLN:OE1	1:B:1162:LEU:HD13	1.99	0.62
1:A:1355:THR:O	1:A:1359:GLN:HG2	2.09	0.52
1:A:1236:LEU:HD13	1:A:1302:TYR:CZ	2.45	0.51
1:B:1152:LEU:HD11	1:B:1229:LEU:HB3	1.93	0.50
1:A:1132:LEU:HD12	1:A:1211:LEU:HD22	1.94	0.49
1:A:1224:VAL:O	1:A:1228:GLU:HG2	2.12	0.49
1:A:1140:LYS:HG2	1:A:1317:LYS:HG3	1.97	0.47
1:B:1066:GLY:HA2	1:B:1069:ARG:NH1	2.31	0.45
1:B:1127:GLY:O	1:B:1131:VAL:HG23	2.18	0.44
1:A:1009:CYS:HB2	1:A:1077:VAL:HG11	2.00	0.42
1:B:1251:GLN:O	1:B:1255:ARG:HG3	2.20	0.41
1:A:1140:LYS:HE3	1:A:1320:LEU:HB2	2.03	0.40
1:B:1340:ILE:O	1:B:1344:VAL:HG23	2.21	0.40

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	339/373 (91%)	338 (100%)	1 (0%)	0	100	100
1	B	335/373 (90%)	334 (100%)	1 (0%)	0	100	100
All	All	674/746 (90%)	672 (100%)	2 (0%)	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	230/319 (72%)	230 (100%)	0	100	100
1	B	250/319 (78%)	250 (100%)	0	100	100
All	All	480/638 (75%)	480 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1135	HIS
1	A	1194	HIS
1	A	1210	GLN
1	A	1288	HIS
1	A	1301	GLN
1	B	1226	GLN
1	B	1257	GLN
1	B	1288	HIS
1	B	1301	GLN
1	B	1319	GLN

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

6.1 Protein, DNA and RNA chains

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	347/373 (93%)	1.45	89 (25%)  	46, 71, 126, 146	0
1	B	345/373 (92%)	1.34	71 (20%)  	58, 81, 108, 130	0
All	All	692/746 (92%)	1.40	160 (23%)  	46, 78, 117, 146	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1094	LEU	6.5
1	B	1226	GLN	5.5
1	A	1078	LEU	5.3
1	B	1150	PRO	4.8
1	B	1222	THR	4.7
1	B	1215	TRP	4.6
1	A	1080	LEU	4.3
1	A	1074	ALA	4.2
1	A	1090	LEU	4.2
1	A	1098	LEU	4.1
1	B	1023	LEU	4.1
1	A	1089	THR	4.1
1	B	1132	LEU	4.1
1	B	1013	ILE	3.9
1	A	1208	VAL	3.8
1	A	1085	PRO	3.8
1	A	1215	TRP	3.8
1	A	1021	LEU	3.8
1	A	1007	SER	3.7
1	B	1091	ARG	3.7
1	B	1047	ALA	3.7
1	B	1257	GLN	3.7
1	B	1098	LEU	3.7
1	B	1012	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	1358	SER	3.6
1	A	1070	LEU	3.6
1	A	1091	ARG	3.5
1	A	1067	VAL	3.5
1	B	1250	LEU	3.5
1	A	1267	ASP	3.5
1	A	1270	ALA	3.4
1	B	1094	LEU	3.4
1	B	1343	TYR	3.4
1	A	1087	ALA	3.3
1	B	1162	LEU	3.3
1	A	1107	LEU	3.3
1	A	1077	VAL	3.3
1	A	1226	GLN	3.2
1	B	1010	GLN	3.2
1	B	1360	TYR	3.2
1	A	1060	VAL	3.2
1	B	1026	CYS	3.2
1	A	1152	LEU	3.2
1	A	1357	THR	3.1
1	A	1076	LYS	3.1
1	A	1288	HIS	3.1
1	A	1108	SER	3.1
1	A	1268	SER	3.1
1	A	1024	GLU	3.1
1	A	1111	TYR	3.0
1	B	1111	TYR	3.0
1	A	1132	LEU	3.0
1	B	1089	THR	3.0
1	A	1350	TYR	2.9
1	A	1180	LEU	2.9
1	B	1085	PRO	2.9
1	A	1298	PHE	2.9
1	B	1019	ILE	2.9
1	B	1152	LEU	2.9
1	B	1219	LEU	2.9
1	A	1211	LEU	2.9
1	A	1038	LEU	2.8
1	A	1367	THR	2.8
1	B	1179	GLU	2.8
1	A	1079	ALA	2.8
1	A	1149	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1227	ARG	2.8
1	A	1190	LEU	2.8
1	B	1309	TYR	2.8
1	A	1013	ILE	2.8
1	A	1084	SER	2.8
1	B	1344	VAL	2.7
1	A	1239	TYR	2.7
1	B	1211	LEU	2.7
1	B	1123	ARG	2.7
1	B	1246	LEU	2.7
1	B	1088	PRO	2.7
1	A	1356	LEU	2.7
1	B	1107	LEU	2.7
1	A	1118	ILE	2.7
1	B	1166	ALA	2.7
1	A	1012	CYS	2.7
1	A	1016	LEU	2.7
1	B	1159	LEU	2.7
1	A	1366	GLU	2.6
1	B	1072	ALA	2.6
1	A	1179	GLU	2.6
1	B	1144	ALA	2.6
1	B	1108	SER	2.6
1	A	1032	HIS	2.6
1	A	1088	PRO	2.6
1	A	1285	ILE	2.6
1	A	1057	GLN	2.6
1	A	1302	TYR	2.5
1	B	1145	VAL	2.5
1	A	1009	CYS	2.5
1	A	1218	VAL	2.5
1	A	1068	ALA	2.5
1	B	1280	ALA	2.5
1	B	1316	TYR	2.5
1	B	1190	LEU	2.4
1	B	1336	SER	2.4
1	A	1202	GLU	2.4
1	B	1009	CYS	2.4
1	B	1060	VAL	2.4
1	A	1095	GLU	2.4
1	A	1222	THR	2.4
1	B	1142	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1360	TYR	2.4
1	A	1114	LYS	2.3
1	B	1067	VAL	2.3
1	B	1032	HIS	2.3
1	A	1116	LYS	2.3
1	B	1146	PRO	2.3
1	A	1173	PHE	2.3
1	B	1149	LEU	2.3
1	B	1119	SER	2.3
1	B	1061	GLU	2.3
1	B	1160	LYS	2.3
1	B	1161	LYS	2.3
1	A	1181	ARG	2.3
1	B	1014	SER	2.3
1	A	1269	GLN	2.2
1	A	1008	ARG	2.2
1	A	1249	TRP	2.2
1	B	1068	ALA	2.2
1	A	1099	GLY	2.2
1	B	1114	LYS	2.2
1	A	1250	LEU	2.2
1	B	1038	LEU	2.2
1	A	1129	GLU	2.2
1	B	1168	ALA	2.2
1	A	1125	THR	2.2
1	A	1229	LEU	2.2
1	B	1128	ALA	2.2
1	B	1164	ALA	2.2
1	A	1177	ARG	2.1
1	A	1364	ILE	2.1
1	A	1159	LEU	2.1
1	B	1173	PHE	2.1
1	A	1123	ARG	2.1
1	A	1228	GLU	2.1
1	B	1202	GLU	2.1
1	A	1101	LEU	2.1
1	B	1351	SER	2.1
1	B	1170	GLN	2.1
1	A	1244	ASP	2.1
1	A	1343	TYR	2.1
1	A	1296	GLN	2.1
1	A	1042	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1010	GLN	2.0
1	A	1165	GLN	2.0
1	B	1229	LEU	2.0
1	A	1263	MET	2.0
1	A	1338	SER	2.0
1	A	1358	SER	2.0
1	A	1047	ALA	2.0
1	B	1270	ALA	2.0
1	B	1204	TRP	2.0
1	B	1238	TYR	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 oligosaccharides 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.