



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:38 AM UTC

PDB ID : 5L5N / pdb_00005l5n
Title : Plexin A4 full extracellular region, domains 1 to 7 modeled, data to 8.5 angstrom, spacegroup P4(3)22
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Deposited on : 2016-05-28
Resolution : 8.50 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
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

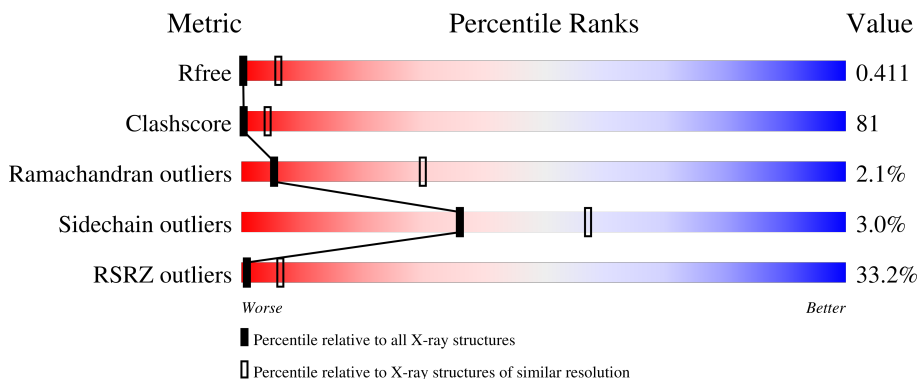
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.50 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	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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	1207	25% 22% 46% 7% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7189 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 Plexin-A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	915	Total	C	N	O	S	0	0	0
			7189	4533	1239	1357	60			

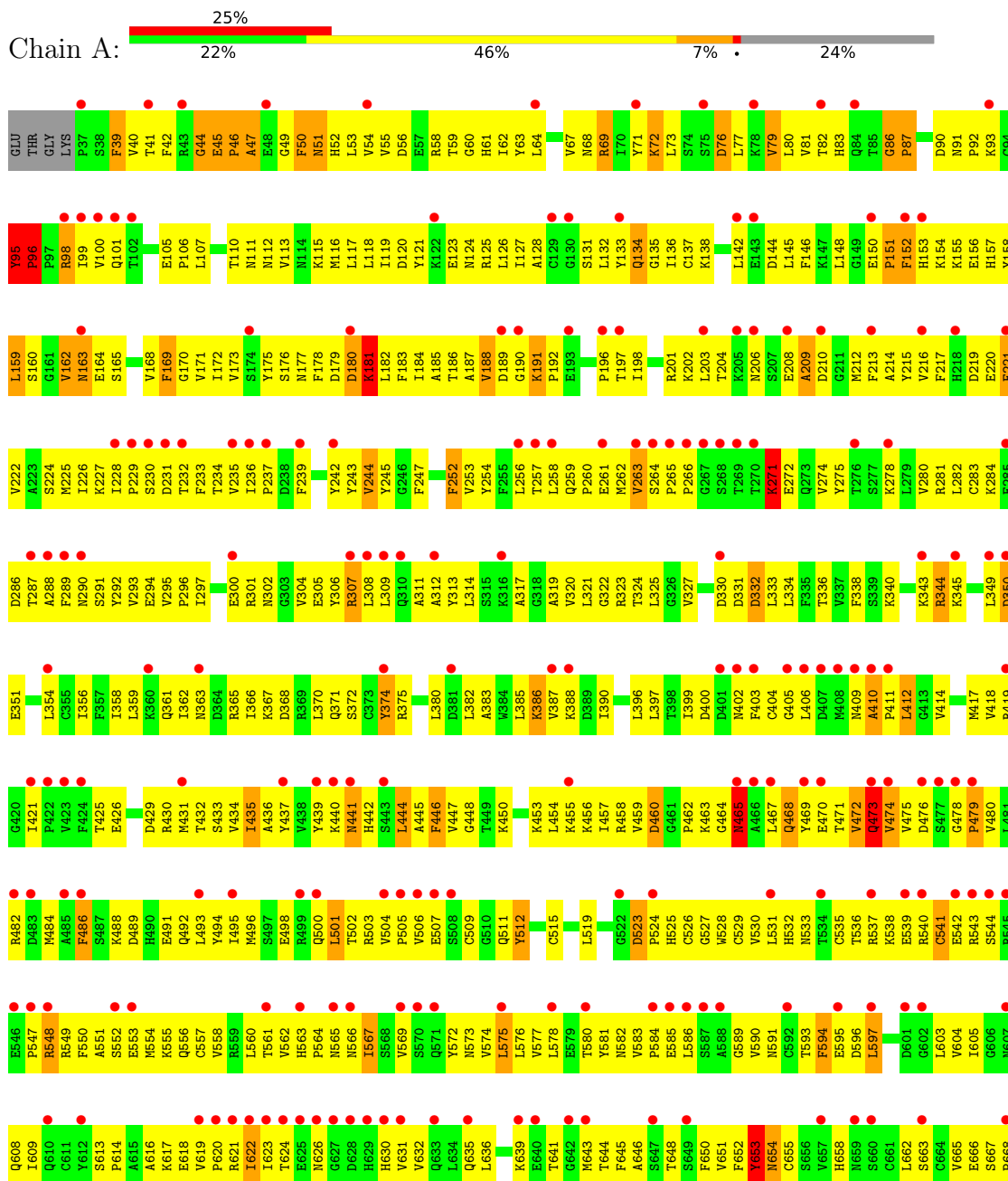
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	-	expression tag	UNP Q80UG2
A	34	THR	-	expression tag	UNP Q80UG2
A	35	GLY	-	expression tag	UNP Q80UG2
A	1230	GLY	-	expression tag	UNP Q80UG2
A	1231	ARG	-	expression tag	UNP Q80UG2
A	1232	THR	-	expression tag	UNP Q80UG2
A	1233	LYS	-	expression tag	UNP Q80UG2
A	1234	HIS	-	expression tag	UNP Q80UG2
A	1235	HIS	-	expression tag	UNP Q80UG2
A	1236	HIS	-	expression tag	UNP Q80UG2
A	1237	HIS	-	expression tag	UNP Q80UG2
A	1238	HIS	-	expression tag	UNP Q80UG2
A	1239	HIS	-	expression tag	UNP Q80UG2

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: Plexin-A4



GLY	ASN	ARG	GLY	K921	I859	Y799	G732	Y689
MET	VAL	ILE	PRO	P922	T860	L800	Q733	R670
VAL	VAL	GLU	ASP	S923	I861	Y801	R734	C671
TYR	VAL	PRO	ASN	Q924	I862	Y801	R734	H672
ILE	LEU	GLU	GLN	H925	I863	C803	G735	W673
ALA	TRP	TRP	PHE	A926	I864	G804	Y736	G674
PRO	SER	SER	GLY	G927	V865	A805		K675
PRO	ILE	ILE	SER	F928	V866	M806		Y676
ARG	VAL	VAL	GLN	V929	G867	R807		A677
VAL	SER	GLY	PRO	E930	G868	E808		H678
ALA	GLY	GLY	ASN	I931	R869	S809		V679
LYS	GLY	GLY	CYS	C932		C810		C680
ASN	ASN	THR	LEU	V933	T873	G811		T681
HIS	PHE	THR	PHE	A934	K874	L812		H682
HIS	HIS	PRO	HIS	V935	V875	C813		D683
HIS	LYS	ILE	ARG	C936	T876	Q747		T686
HIS	ASN	VAL	ALA	R937	I877	L814		F689
HIS	ASN	VAL	PHE	F939	R878	K815		E690
HIS	THR	GLY	SER	F940	G879	V750		E691
VAL	THR	THR	THR	M941	E880	D817		F694
LEU	TYR	THR	TYR	A942	N881	F813		K695
VAL	ILE	ASN	ILE	R943	L882	D819		L696
GLY	GLN	ASP	ILE		G883	F820		P697
GLU	GLY	LEU	CYS		L884	E821		E698
LEU	ASN	LEU	ASN		E885	C822		D699
LYS	THR	ILE	THR		F886	G823		C700
PRO	THR	GLN	THR		R887	W824		P701
CYS	ASN	ASN	THR		D888	C825		Q702
THR	THR	PRO	SER		F950	Q826		L703
VAL	VAL	GLU	GLU		I889	S827		L704
VAL	THR	ILE	GLU		M951	P828		V705
VAL	VAL	ARG	VAL		S891	G829		D707
SER	ASN	ALA	LEU		H882	Q830		K708
ASP	PHE	LYS	ASP		V893	C831		I709
VAL	THR	THR	THR		K894	T832		L710
GLN	THR	GLY	LYS		V895	L833		V711
LEU	LEU	GLY	GLY		A896	L833		P712
LEU	PRO	LYS	THR		G897	R834		V713
ASN	ASN	GLY	THR		V898	Q835		E714
GLU	VAL	ILE	VAL		E899	H836		V715
SER	VAL	ILE	GLN		C900	C837		I716
PRO	PHE	ASN	VAL		S901	P839		K717
ASN	GLY	ASN	ARG		P902	A839		P718
LEU	ALA	ALA	ARG		L903	H840		V719
ILE	PHE	CYS	ALA		V904	E841		T720
GLY	SER	VAL	ILE		D905	S842		L721
ARG	PRO	LEU	ARG		G906	W844		K722
LYS	SER	ALA	GLN		I908	E846		A723
VAL	ILE	THR	LEU		P909	L847		K724
MET	GLU	GLU	VAL		A910	S848		N725
ALA	GLU	MET	VAL		E911	G849		L726
ARG	THR	THR	PHE		Q912	A850		P727
VAL	LYS	CYS	GLN		I913	N851		Q728
PRO	GLY	PRO	TYR		V914	S852		P729
GLY	GLY	GLY	VAL		C915	D791		Q730
MET	ALA	THR	ALA		F916	K853		S731
GLU	PRO	PRO	ASP		M917	C854		
TYR	TYR	ILE	PRO		G918	T855		
SER	ILE	ALA	ALA		E919	N856		
PRO	LEU	LEU	LEU		A920	K857		
						R858		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	189.48Å 189.48Å 252.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.37 – 8.50 70.37 – 8.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (70.37-8.50) 99.3 (70.37-8.50)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 8.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.401 , 0.412 0.405 , 0.411	Depositor DCC
R_{free} test set	203 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	502.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 289.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% 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

5.1 Standard geometry

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	1.52	10/7343 (0.1%)	1.76	121/9940 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	653	TYR	C-N	-59.48	0.50	1.33
1	A	700	CYS	C-N	-27.17	0.70	1.33
1	A	49	GLY	C-N	9.92	1.45	1.33
1	A	180	ASP	C-N	7.50	1.44	1.33
1	A	49	GLY	CA-C	7.27	1.62	1.51

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	TYR	O-C-N	-38.56	89.64	121.65
1	A	747	GLN	CG-CD-OE1	-38.43	43.94	120.80
1	A	700	CYS	O-C-N	-17.09	101.67	121.32
1	A	747	GLN	CG-CD-NE2	-15.10	93.74	116.40
1	A	747	GLN	OE1-CD-NE2	15.09	137.69	122.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	653	TYR	Mainchain
1	A	700	CYS	Mainchain
1	A	863	ILE	Peptide
1	A	95	TYR	Peptide

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	7189	0	7049	1151	32
All	All	7189	0	7049	1151	32

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 81.

The worst 5 of 1151 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:468:GLN:HG3	1:A:524:PRO:CD	1.18	1.58
1:A:530:VAL:HG11	1:A:584:PRO:CD	1.11	1.56
1:A:439:TYR:CE2	1:A:538:LYS:NZ	1.78	1.51
1:A:468:GLN:CG	1:A:524:PRO:HD3	1.39	1.51
1:A:439:TYR:HE2	1:A:538:LYS:NZ	1.11	1.44

The worst 5 of 32 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:CA	1:A:234:THR:CA[5_455]	0.86	1.34
1:A:233:PHE:O	1:A:234:THR:OG1[5_455]	0.87	1.33
1:A:146:PHE:CE1	1:A:730:GLN:OE1[4_555]	1.03	1.17
1:A:146:PHE:CE1	1:A:730:GLN:CD[4_555]	1.26	0.94
1:A:146:PHE:CD1	1:A:730:GLN:OE1[4_555]	1.26	0.94

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	905/1207 (75%)	842 (93%)	44 (5%)	19 (2%)	5 30

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	181	LYS
1	A	191	LYS
1	A	410	ALA
1	A	465	ASN

5.3.2 Protein sidechains [i](#)

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	812/1067 (76%)	788 (97%)	24 (3%)	36 57

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	LEU
1	A	722	LYS
1	A	670	ARG
1	A	743	GLN
1	A	435	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	582	ASN
1	A	826	GLN
1	A	654	ASN
1	A	856	ASN
1	A	787	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	802:LYS	C	803:CYS	N	4.06

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	854:CYS	C	855:THR	N	3.30
1	A	557:CYS	C	558:VAL	N	2.81
1	A	506:VAL	C	507:GLU	N	2.58
1	A	700:CYS	C	701:PRO	N	0.70

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	915/1207 (75%)	1.74	304 (33%) 1 6	100, 150, 216, 216	0

The worst 5 of 304 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	815	LYS	11.7
1	A	633	GLN	11.2
1	A	649	SER	10.0
1	A	923	SER	9.9
1	A	621	ARG	9.6

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.