



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 05:36 PM EDT

PDB ID : 4GZA / pdb_00004gza
Title : Complex of mouse Plexin A2 - Semaphorin 3A - Neuropilin-1
Authors : Janssen, B.J.C.; Malinauskas, T.; Siebold, C.; Jones, E.Y.
Deposited on : 2012-09-06
Resolution : 7.00 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

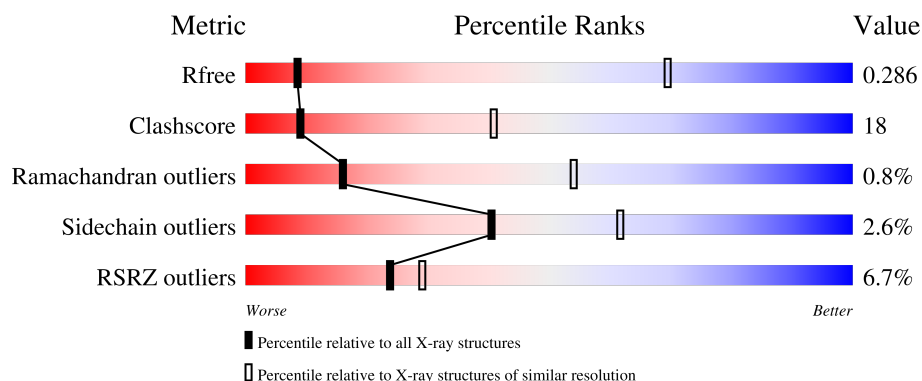
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1167 (10.00-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	681	7% 70% 25% • •
1	B	681	6% 72% 22% • •
1	C	681	7% 72% 23% • •
1	D	681	4% 72% 22% • •
1	E	681	7% 73% 22% • •

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Mol	Chain	Length	Quality of chain
1	F	681	8% 72% 23% 1%
2	G	538	5% 42% 41% 10%
3	H	577	1% 17% 80% 2%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35655 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-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	B	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	C	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	D	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	E	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	F	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP P70207
A	704	GLY	-	expression tag	UNP P70207
A	705	THR	-	expression tag	UNP P70207
A	706	LYS	-	expression tag	UNP P70207
A	707	HIS	-	expression tag	UNP P70207
A	708	HIS	-	expression tag	UNP P70207
A	709	HIS	-	expression tag	UNP P70207
A	710	HIS	-	expression tag	UNP P70207
A	711	HIS	-	expression tag	UNP P70207
A	712	HIS	-	expression tag	UNP P70207
B	32	GLU	-	expression tag	UNP P70207
B	704	GLY	-	expression tag	UNP P70207
B	705	THR	-	expression tag	UNP P70207
B	706	LYS	-	expression tag	UNP P70207
B	707	HIS	-	expression tag	UNP P70207
B	708	HIS	-	expression tag	UNP P70207
B	709	HIS	-	expression tag	UNP P70207

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Chain	Residue	Modelled	Actual	Comment	Reference
B	710	HIS	-	expression tag	UNP P70207
B	711	HIS	-	expression tag	UNP P70207
B	712	HIS	-	expression tag	UNP P70207
C	32	GLU	-	expression tag	UNP P70207
C	704	GLY	-	expression tag	UNP P70207
C	705	THR	-	expression tag	UNP P70207
C	706	LYS	-	expression tag	UNP P70207
C	707	HIS	-	expression tag	UNP P70207
C	708	HIS	-	expression tag	UNP P70207
C	709	HIS	-	expression tag	UNP P70207
C	710	HIS	-	expression tag	UNP P70207
C	711	HIS	-	expression tag	UNP P70207
C	712	HIS	-	expression tag	UNP P70207
D	32	GLU	-	expression tag	UNP P70207
D	704	GLY	-	expression tag	UNP P70207
D	705	THR	-	expression tag	UNP P70207
D	706	LYS	-	expression tag	UNP P70207
D	707	HIS	-	expression tag	UNP P70207
D	708	HIS	-	expression tag	UNP P70207
D	709	HIS	-	expression tag	UNP P70207
D	710	HIS	-	expression tag	UNP P70207
D	711	HIS	-	expression tag	UNP P70207
D	712	HIS	-	expression tag	UNP P70207
E	32	GLU	-	expression tag	UNP P70207
E	704	GLY	-	expression tag	UNP P70207
E	705	THR	-	expression tag	UNP P70207
E	706	LYS	-	expression tag	UNP P70207
E	707	HIS	-	expression tag	UNP P70207
E	708	HIS	-	expression tag	UNP P70207
E	709	HIS	-	expression tag	UNP P70207
E	710	HIS	-	expression tag	UNP P70207
E	711	HIS	-	expression tag	UNP P70207
E	712	HIS	-	expression tag	UNP P70207
F	32	GLU	-	expression tag	UNP P70207
F	704	GLY	-	expression tag	UNP P70207
F	705	THR	-	expression tag	UNP P70207
F	706	LYS	-	expression tag	UNP P70207
F	707	HIS	-	expression tag	UNP P70207
F	708	HIS	-	expression tag	UNP P70207
F	709	HIS	-	expression tag	UNP P70207
F	710	HIS	-	expression tag	UNP P70207
F	711	HIS	-	expression tag	UNP P70207

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Chain	Residue	Modelled	Actual	Comment	Reference
F	712	HIS	-	expression tag	UNP P70207

- Molecule 2 is a protein called Semaphorin-3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	484	Total	C	N	O	S	0	0	0
			3882	2474	669	720	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	18	GLU	-	expression tag	UNP O08665
G	19	THR	-	expression tag	UNP O08665
G	20	GLY	-	expression tag	UNP O08665
G	475	VAL	ILE	SEE REMARK 999	UNP O08665

- Molecule 3 is a protein called Neuropilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	117	Total	C	N	O	S	0	0	0
			944	611	152	176	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	19	GLU	-	expression tag	UNP P97333
H	20	THR	-	expression tag	UNP P97333
H	21	GLY	-	expression tag	UNP P97333
H	587	ARG	-	expression tag	UNP P97333
H	588	THR	-	expression tag	UNP P97333
H	589	LYS	-	expression tag	UNP P97333
H	590	HIS	-	expression tag	UNP P97333
H	591	HIS	-	expression tag	UNP P97333
H	592	HIS	-	expression tag	UNP P97333
H	593	HIS	-	expression tag	UNP P97333
H	594	HIS	-	expression tag	UNP P97333
H	595	HIS	-	expression tag	UNP P97333

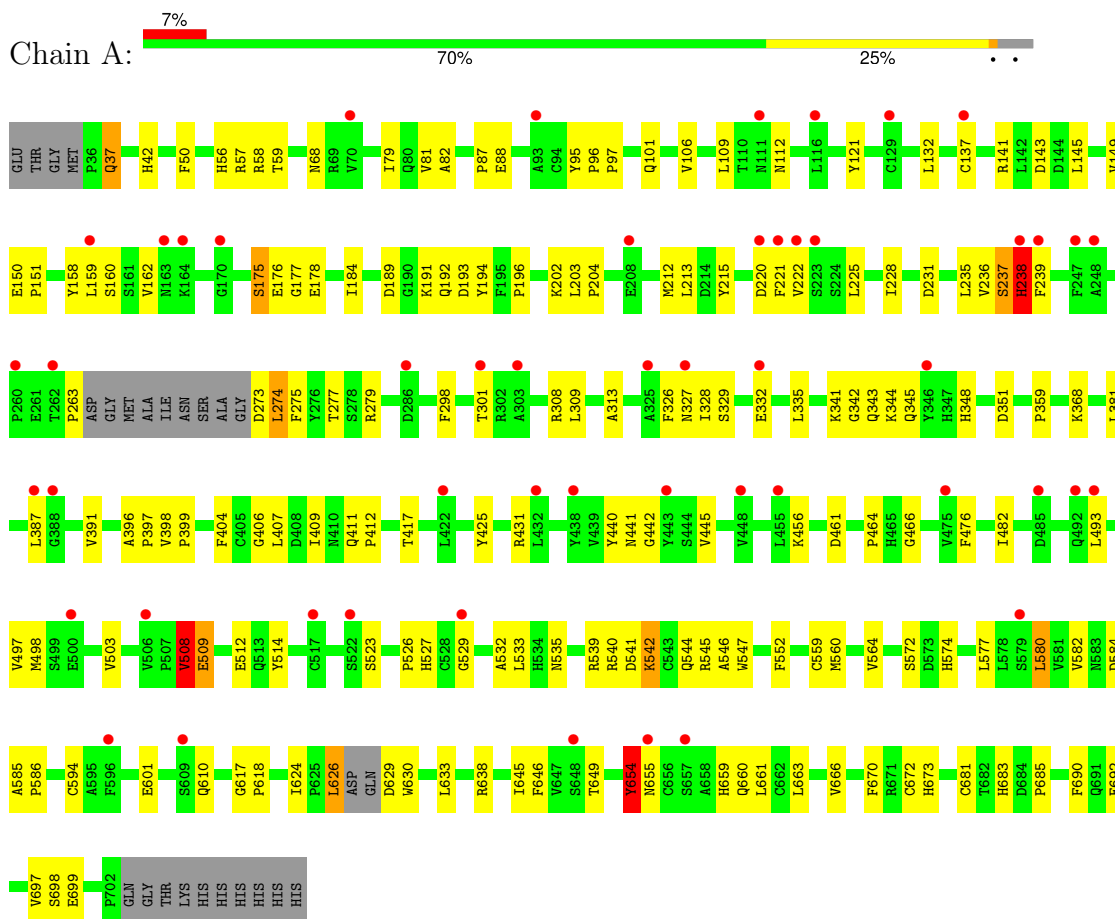
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Ca 1	0	0

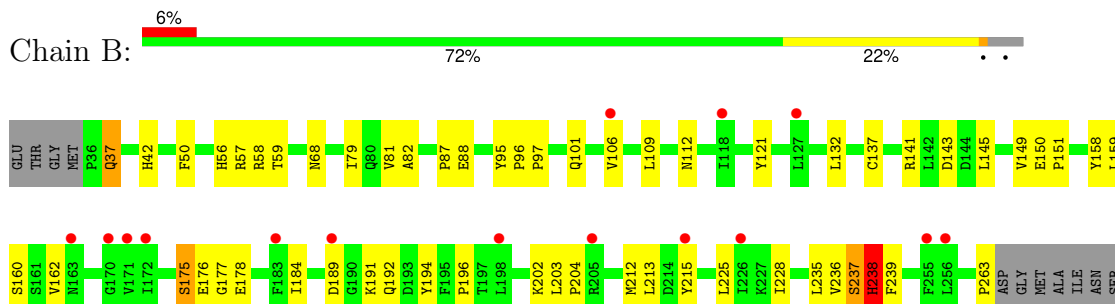
3 Residue-property plots

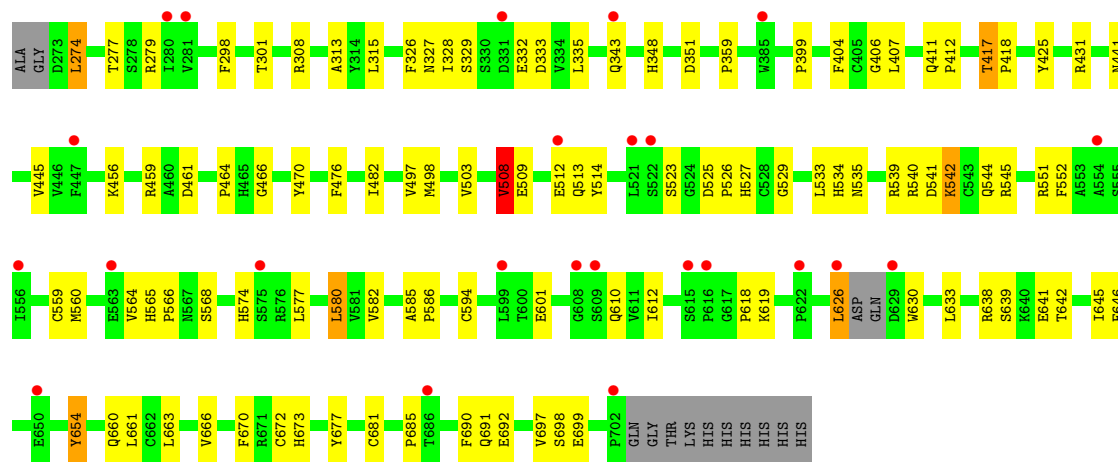
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-A2

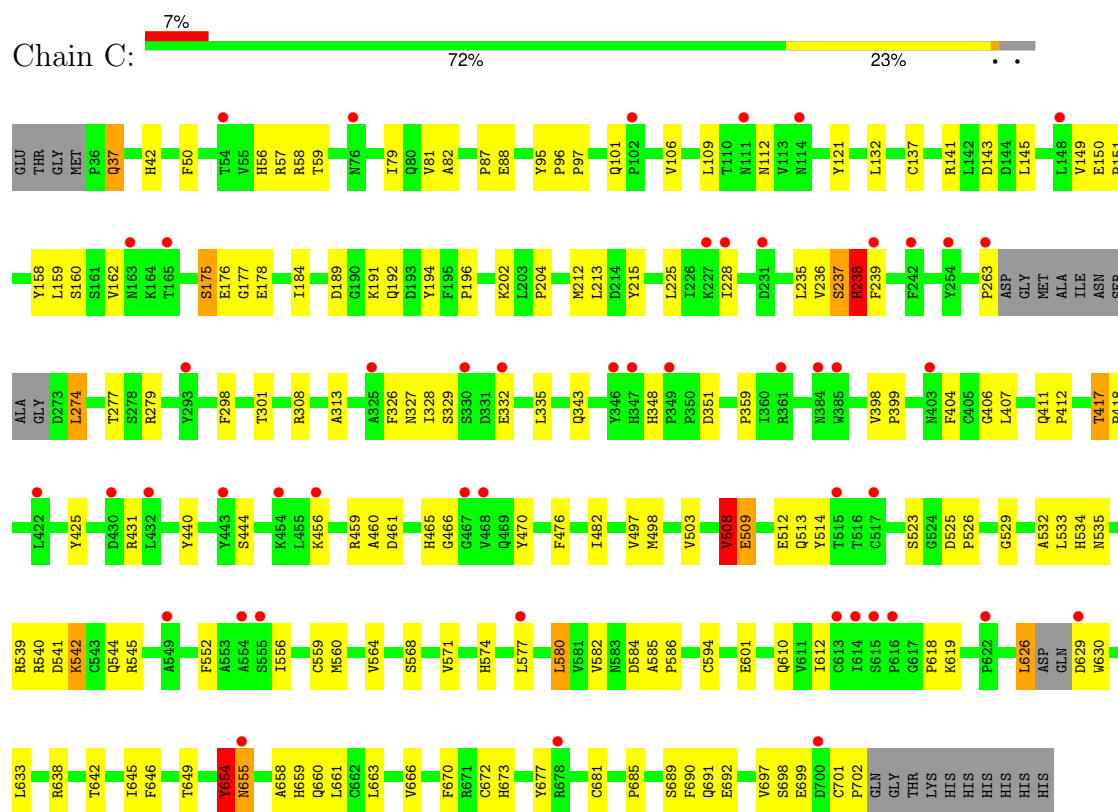


• Molecule 1: Plexin-A2

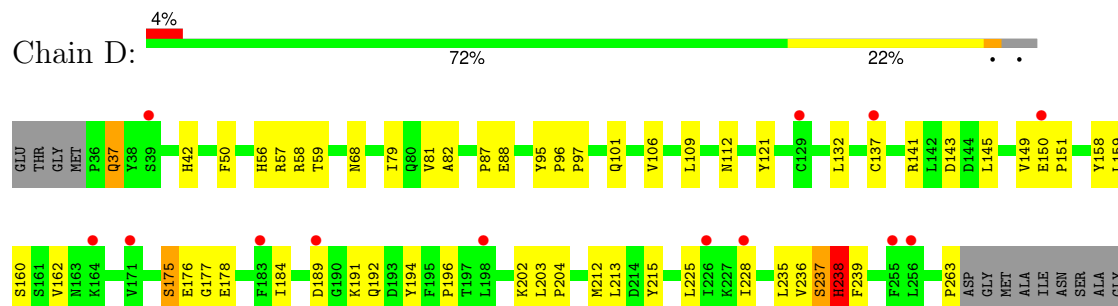




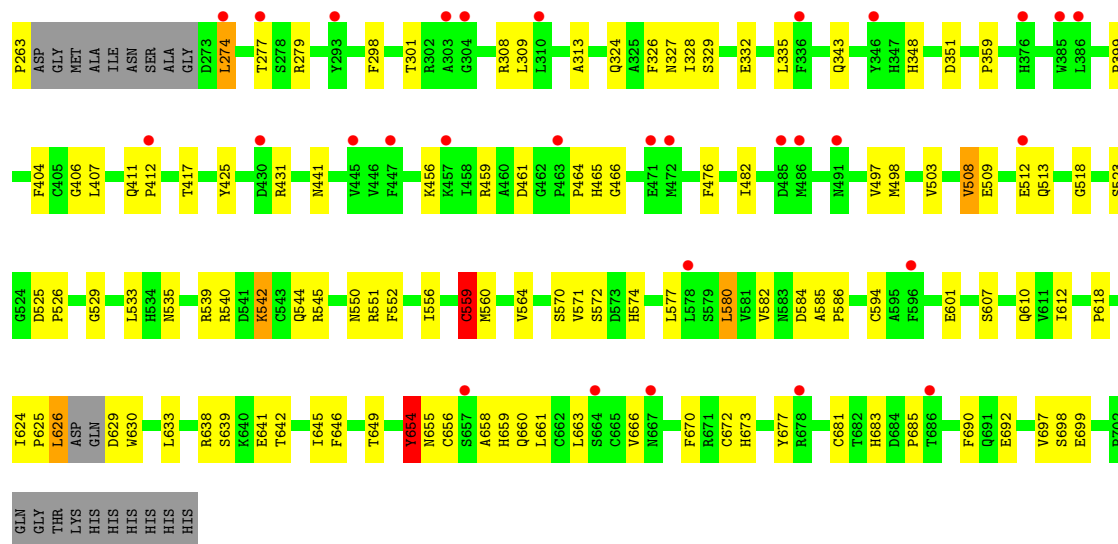
• Molecule 1: Plexin-A2



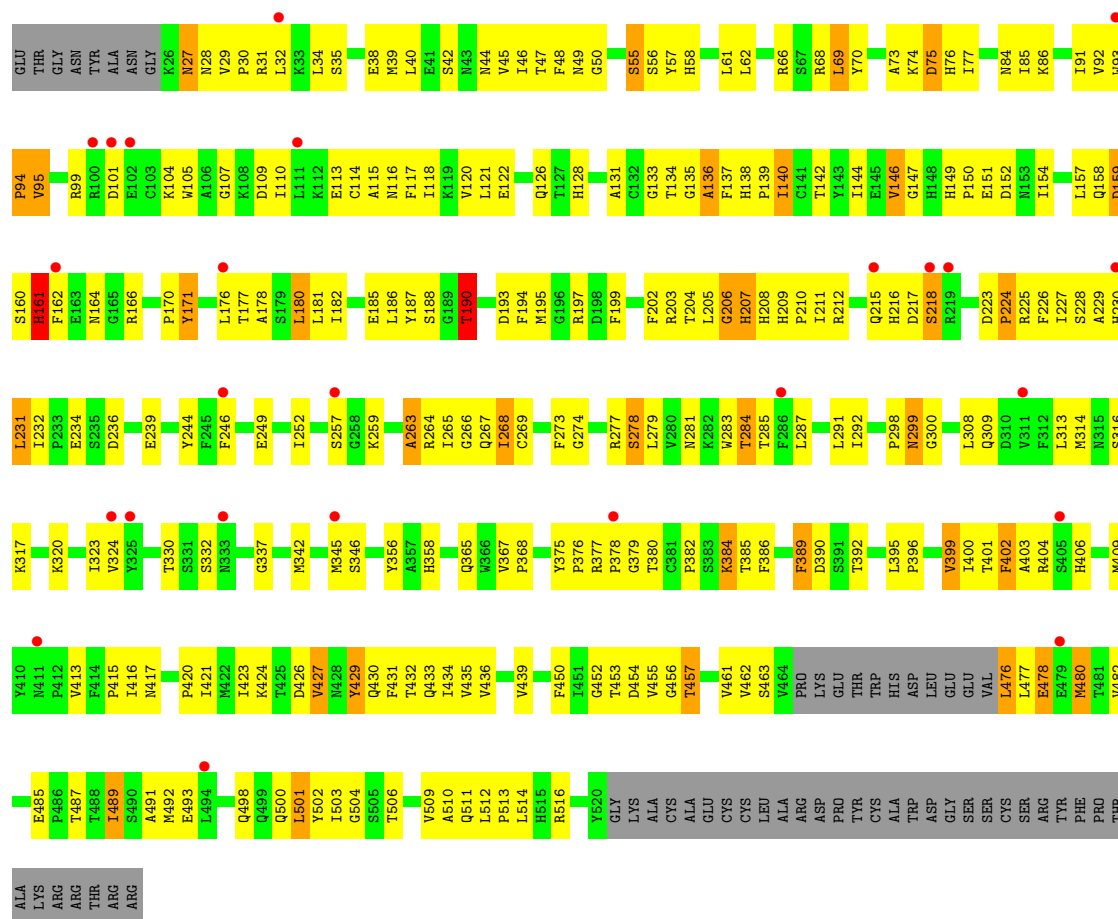
• Molecule 1: Plexin-A2



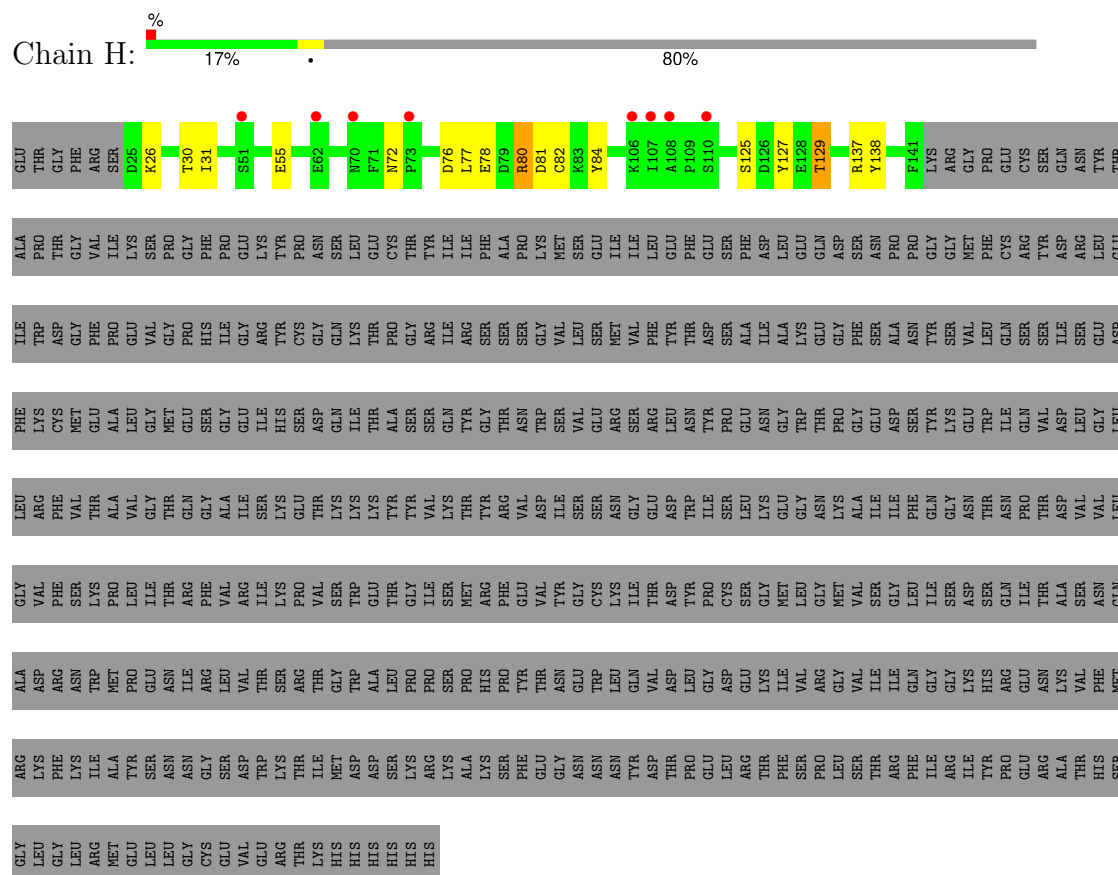




• Molecule 2: Semaphorin-3A



• Molecule 3: Neuropilin-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.63Å 293.60Å 252.18Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	125.51 – 7.00 125.51 – 7.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (125.51-7.00) 95.5 (125.51-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 6.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.285 , 0.285 0.281 , 0.286	Depositor DCC
R_{free} test set	1022 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	293.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 478.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	35655	wwPDB-VP
Average B, all atoms (Å ²)	323.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.77	6/5260 (0.1%)	0.79	14/7138 (0.2%)
1	B	0.41	7/5260 (0.1%)	0.87	12/7138 (0.2%)
1	C	0.62	8/5260 (0.2%)	1.00	10/7138 (0.1%)
1	D	0.69	7/5261 (0.1%)	0.98	13/7141 (0.2%)
1	E	0.40	6/5261 (0.1%)	1.07	15/7141 (0.2%)
1	F	0.50	6/5261 (0.1%)	0.87	16/7141 (0.2%)
2	G	0.61	0/3988	1.04	20/5411 (0.4%)
3	H	0.70	0/977	0.80	1/1325 (0.1%)
All	All	0.59	40/36528 (0.1%)	0.94	101/49573 (0.2%)

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	1
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	2
2	G	0	2
3	H	0	1
All	All	0	12

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	508	VAL	C-N	46.75	1.91	1.33
1	C	508	VAL	C-N	-34.26	0.85	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	559	CYS	C-N	31.58	1.79	1.33
1	F	508	VAL	C-N	23.45	1.63	1.33
1	D	654	TYR	C-N	-20.15	1.05	1.33

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	654	TYR	O-C-N	-53.52	51.41	122.59
1	D	654	TYR	O-C-N	-49.21	57.14	122.59
1	E	654	TYR	O-C-N	-41.76	72.32	123.27
1	E	654	TYR	CA-C-N	29.11	174.09	121.70
1	E	654	TYR	C-N-CA	29.11	174.09	121.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	654	TYR	Mainchain
1	B	508	VAL	Mainchain
1	C	508	VAL	Mainchain
1	C	654	TYR	Mainchain
1	D	508	VAL	Mainchain

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	5138	0	4989	294	34
1	B	5138	0	4991	186	18
1	C	5138	0	4990	238	0
1	D	5138	0	4989	197	0
1	E	5138	0	4993	165	29
1	F	5138	0	4995	180	23
2	G	3882	0	3747	302	11
3	H	944	0	875	43	5
4	H	1	0	0	0	0
All	All	35655	0	34569	1291	63

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 18.

The worst 5 of 1291 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:344:LYS:CD	3:H:80:ARG:HH11	1.00	1.58
1:A:344:LYS:HD3	3:H:80:ARG:CD	1.23	1.57
1:A:222:VAL:CG2	2:G:166:ARG:HH12	1.17	1.54
1:D:577:LEU:HD11	1:F:607:SER:CB	1.44	1.47
1:E:324:GLN:NE2	1:F:518:GLY:HA3	1.23	1.47

The worst 5 of 63 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:690:PHE:CE1	1:F:540:ARG:NE[3_455]	0.68	1.52
1:A:690:PHE:CE2	1:F:540:ARG:CG[3_455]	0.78	1.42
1:B:541:ASP:N	1:E:690:PHE:CE2[3_455]	0.79	1.41
1:A:577:LEU:CD1	1:E:610:GLN:OE1[3_455]	0.87	1.33
1:B:540:ARG:C	1:E:690:PHE:CZ[3_455]	0.87	1.33

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	648/681 (95%)	628 (97%)	18 (3%)	2 (0%)	36	72
1	B	648/681 (95%)	629 (97%)	16 (2%)	3 (0%)	24	63
1	C	648/681 (95%)	627 (97%)	17 (3%)	4 (1%)	21	59
1	D	650/681 (95%)	630 (97%)	16 (2%)	4 (1%)	21	59
1	E	650/681 (95%)	632 (97%)	15 (2%)	3 (0%)	24	63
1	F	650/681 (95%)	631 (97%)	17 (3%)	2 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	480/538 (89%)	408 (85%)	55 (12%)	17 (4%)	3	20
3	H	115/577 (20%)	106 (92%)	7 (6%)	2 (2%)	7	36
All	All	4489/5201 (86%)	4291 (96%)	161 (4%)	37 (1%)	16	54

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	655	ASN
2	G	161	HIS
2	G	207	HIS
2	G	257	SER
3	H	81	ASP

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	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	B	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	C	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	D	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	E	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	F	578/597 (97%)	566 (98%)	12 (2%)	47	65
2	G	428/472 (91%)	400 (94%)	28 (6%)	15	37
3	H	102/506 (20%)	98 (96%)	4 (4%)	28	49
All	All	3998/4560 (88%)	3894 (97%)	104 (3%)	40	62

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	542	LYS
1	F	626	LEU

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Mol	Chain	Res	Type
2	G	501	LEU
1	E	626	LEU
1	F	301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	89	GLN
2	G	370	GLN
2	G	158	GLN
2	G	216	HIS
2	G	411	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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	D	3
1	A	2
1	C	2
1	B	1
1	F	1
1	E	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	559:CYS	C	560:MET	N	2.86
1	B	559:CYS	C	560:MET	N	2.56
1	C	559:CYS	C	560:MET	N	2.24
1	A	508:VAL	C	509:GLU	N	1.91
1	D	559:CYS	C	560:MET	N	1.79

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	656/681 (96%)	0.62	51 (7%)	19	25	287, 291, 313, 313	0
1	B	656/681 (96%)	0.50	39 (5%)	28	32	290, 308, 308, 308	0
1	C	656/681 (96%)	0.55	49 (7%)	20	26	278, 322, 327, 327	0
1	D	656/681 (96%)	0.28	29 (4%)	39	39	294, 342, 342, 342	0
1	E	656/681 (96%)	0.50	45 (6%)	23	28	304, 341, 351, 351	0
1	F	656/681 (96%)	0.56	57 (8%)	16	23	305, 348, 370, 370	0
2	G	484/538 (89%)	0.44	25 (5%)	33	35	340, 340, 340, 340	0
3	H	117/577 (20%)	0.33	8 (6%)	23	29	370, 370, 370, 370	0
All	All	4537/5201 (87%)	0.49	303 (6%)	24	29	278, 322, 348, 370	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	107	ILE	7.4
1	F	165	THR	6.9
1	E	320	GLU	6.1
1	D	303	ALA	6.0
1	E	244	ILE	5.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	H	601	1/1	0.91	0.16	369,369,369,369	0

6.5 Other polymers

There are no such residues in this entry.