Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2022 – 04:16 pm BST

PDB ID	:	7P5U
Title	:	Neuropilin-b1 in a complex with a VEGFB-derived peptide
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Deposited on	:	2021-07-14
Resolution	:	1.60 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:

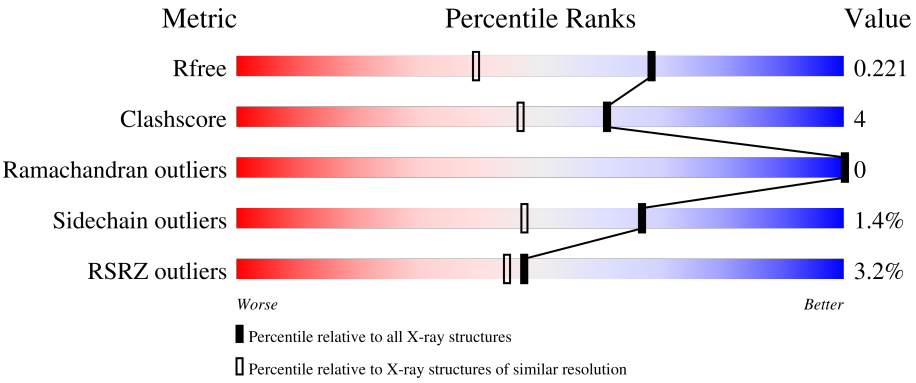
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	AAA	158	3% 88% 9% .
1	BBB	158	2% 95% . .
2	CCC	13	15% 23% 77%
2	EEE	13	8% 15% 8% 77%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2772 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 Neuropilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	153	Total	C	N	O	S	0	5	0
			1247	798	204	239	6			
1	BBB	158	Total	C	N	O	S	0	4	0
			1282	818	215	243	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	270	GLY	-	expression tag	UNP O14786
AAA	271	HIS	-	expression tag	UNP O14786
AAA	272	MET	-	expression tag	UNP O14786
BBB	270	GLY	-	expression tag	UNP O14786
BBB	271	HIS	-	expression tag	UNP O14786
BBB	272	MET	-	expression tag	UNP O14786

- Molecule 2 is a protein called MGC0122.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	CCC	3	Total	C	N	O	0	0	0
			28	16	7	5			
2	EEE	3	Total	C	N	O	0	0	0
			28	16	7	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	87	Total	O	0	0
			87	87		
3	BBB	96	Total	O	0	0
			96	96		
3	CCC	2	Total	O	0	0
			2	2		

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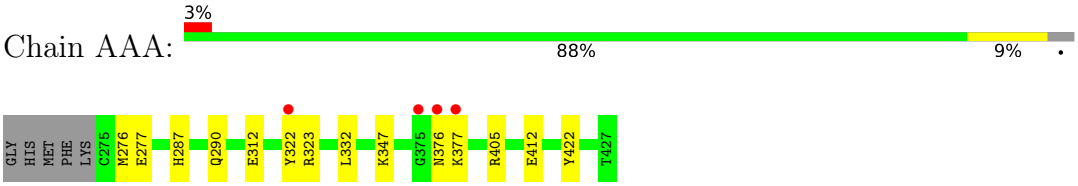
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	EEE	2	Total O 2 2	0	0

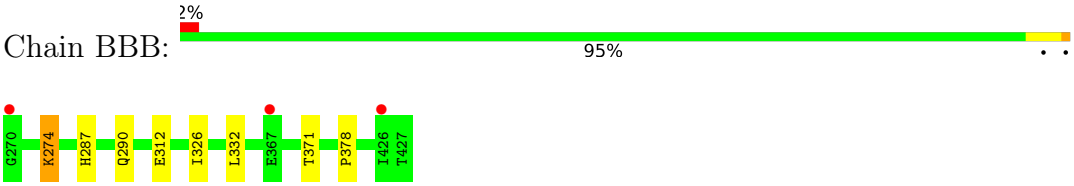
3 Residue-property plots (i)

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: Neuropilin-1



• Molecule 1: Neuropilin-1



• Molecule 2: MGC0122

• Molecule 2: MGC0122

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.50Å 74.35Å 91.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.68 – 1.60 57.68 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (57.68-1.60) 99.4 (57.68-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.214 0.199 , 0.221	Depositor DCC
R_{free} test set	2189 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2772	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	AAA	0.95	2/1292 (0.2%)	1.06	1/1751 (0.1%)
1	BBB	0.78	1/1325 (0.1%)	0.91	0/1793
2	CCC	0.68	0/28	0.94	0/35
2	EEE	0.82	0/28	1.12	0/35
All	All	0.87	3/2673 (0.1%)	0.99	1/3614 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	312	GLU	CD-OE2	-6.00	1.19	1.25
1	AAA	412	GLU	CD-OE2	-5.72	1.19	1.25
1	AAA	412	GLU	CD-OE1	-5.28	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	405	ARG	NE-CZ-NH1	-5.66	117.47	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AAA	1247	0	1235	14	0
1	BBB	1282	0	1269	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	28	0	30	0	0
2	EEE	28	0	30	0	0
3	AAA	87	0	0	1	0
3	BBB	96	0	0	1	0
3	CCC	2	0	0	0	0
3	EEE	2	0	0	0	0
All	All	2772	0	2564	23	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 4.

All (23) 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:BBB:371:THR:HG23	3:BBB:544:HOH:O	1.53	1.06
1:BBB:371:THR:HG21	1:BBB:378:PRO:HG3	1.63	0.80
1:BBB:371:THR:HG21	1:BBB:378:PRO:CG	2.20	0.71
1:BBB:371:THR:HG21	1:BBB:378:PRO:HB3	1.76	0.68
1:BBB:371:THR:HG21	1:BBB:378:PRO:CB	2.25	0.67
1:AAA:322[B]:TYR:HE1	1:AAA:323:ARG:CZ	2.09	0.66
1:AAA:322[B]:TYR:CE1	1:AAA:323:ARG:NE	2.67	0.62
1:BBB:371:THR:CG2	1:BBB:378:PRO:HB3	2.33	0.58
1:AAA:322[B]:TYR:CE1	1:AAA:323:ARG:CZ	2.87	0.57
1:AAA:276[B]:MET:HG2	1:AAA:422:TYR:HB3	1.89	0.53
1:AAA:287:HIS:H	1:AAA:290:GLN:NE2	2.07	0.52
1:BBB:287:HIS:H	1:BBB:290:GLN:NE2	2.07	0.52
1:AAA:312[B]:GLU:HG3	1:AAA:347:LYS:CG	2.44	0.48
1:AAA:322[B]:TYR:HE1	1:AAA:323:ARG:NE	2.10	0.47
1:BBB:332:LEU:N	1:BBB:332:LEU:HD23	2.31	0.46
1:BBB:274:LYS:HB3	1:BBB:274:LYS:NZ	2.31	0.45
1:AAA:312[B]:GLU:HG3	1:AAA:347:LYS:HG2	2.01	0.42
1:AAA:322[B]:TYR:HE1	1:AAA:323:ARG:NH2	2.17	0.42
1:AAA:322[B]:TYR:CE1	1:AAA:323:ARG:HG2	2.54	0.42
1:AAA:332:LEU:N	1:AAA:332:LEU:HD23	2.35	0.42
1:AAA:376:ASN:ND2	3:AAA:505:HOH:O	2.53	0.42
1:AAA:322[B]:TYR:CD1	1:AAA:323:ARG:HG2	2.55	0.41
1:AAA:277:GLU:O	1:AAA:422:TYR:HA	2.21	0.40

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	AAA	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
1	BBB	160/158 (101%)	156 (98%)	4 (2%)	0	100	100
2	CCC	1/13 (8%)	0	1 (100%)	0	100	100
2	EEE	1/13 (8%)	1 (100%)	0	0	100	100
All	All	318/342 (93%)	311 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	139/138 (101%)	138 (99%)	1 (1%)	84	73
1	BBB	142/138 (103%)	140 (99%)	2 (1%)	67	47
2	CCC	3/11 (27%)	3 (100%)	0	100	100
2	EEE	3/11 (27%)	2 (67%)	1 (33%)	0	0
All	All	287/298 (96%)	283 (99%)	4 (1%)	67	47

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	377	LYS
1	BBB	274	LYS

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Mol	Chain	Res	Type
1	BBB	326	ILE
2	EEE	1	GLN

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 monosaccharides 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, 95^{th} 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	AAA	153/158 (96%)	-0.07	4 (2%) 56 53	11, 18, 36, 66	0
1	BBB	158/158 (100%)	-0.12	3 (1%) 66 65	10, 16, 35, 56	0
2	CCC	3/13 (23%)	2.87	2 (66%) 0 0	26, 26, 55, 76	0
2	EEE	3/13 (23%)	0.88	1 (33%) 0 0	20, 20, 41, 57	0
All	All	317/342 (92%)	-0.06	10 (3%) 47 44	10, 18, 37, 76	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	375	GLY	6.7
2	CCC	2	PRO	5.4
1	AAA	376	ASN	4.1
1	BBB	270	GLY	4.0
2	CCC	1	GLN	3.4
1	BBB	426	ILE	3.2
1	AAA	322[A]	TYR	2.7
2	EEE	1	GLN	2.4
1	AAA	377	LYS	2.2
1	BBB	367	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.