

wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 04:53 pm BST

PDB ID	:	8BF4
Title	:	Crystal structure of Mouse Plexin-B1 (20-535) in complex with VHH15 and
		VHH14
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Deposited on	:	2022-10-24
Resolution	:	2.15 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.15 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	Similar resolution
	(#Entries)	(#Entries, resolution range(A))
R _{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	$1560 \ (2.16-2.16)$
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	А	124	10% 72% 15%]	4%
1	D	124	85%	10%	6%
2	С	523	2% 82%	10%	8%
2	F	523	2% 82%	11%	• 6%
3	В	130	78%	15%	• 5%

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Mol	Chain	Length	Quality of chain		
			%		
3	Ε	130	78%	15%	• 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	F	604	Х	-	-	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11421 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	117	Total 876	$\begin{array}{c} \mathrm{C} \\ 548 \end{array}$	N 152	0 171	${ m S}{ m 5}$	0	0	0
1	А	107	Total 811	C 507	N 140	O 159	${f S}{5}$	0	0	0

• Molecule 1 is a protein called VHH14.

• Molecule 2 is a protein called Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	491	Total 3719	C 2347	N 650	0 701	S 21	0	1	0
2	С	483	Total 3661	C 2306	N 640	O 694	S 21	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	536	LYS	-	expression tag	UNP Q8CJH3
F	537	HIS	-	expression tag	UNP Q8CJH3
F	538	HIS	-	expression tag	UNP Q8CJH3
F	539	HIS	-	expression tag	UNP Q8CJH3
F	540	HIS	-	expression tag	UNP Q8CJH3
F	541	HIS	-	expression tag	UNP Q8CJH3
F	542	HIS	-	expression tag	UNP Q8CJH3
С	536	LYS	-	expression tag	UNP Q8CJH3
С	537	HIS	-	expression tag	UNP Q8CJH3
С	538	HIS	-	expression tag	UNP Q8CJH3
С	539	HIS	-	expression tag	UNP Q8CJH3
С	540	HIS	-	expression tag	UNP Q8CJH3
C	541	HIS	-	expression tag	UNP Q8CJH3
С	542	HIS	-	expression tag	UNP Q8CJH3

• Molecule 3 is a protein called VHH15.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	199	Total	С	Ν	0	S	0	0	0
J		122	927	576	162	183	6	0	0	
2	р	192	Total	С	Ν	0	S	0	0	0
5	D	123	932	579	163	184	6		U	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 14 & 8 & 1 & 5 \end{array}$	0	0
4	F	1	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0	0
4	F	1	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	С	1	Total C N O 14 8 1 5	0	0
4	С	1	Total C N O 14 8 1 5	0	0
4	С	1	Total C N O 14 8 1 5	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms		Atoms		ZeroOcc	AltConf
5	F	1	Total 1	Cl 1	0	0		

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	С	1	Total 4	${ m C} { m 2}$	O 2	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	27	Total O 27 27	0	0
7	F	168	Total O 168 168	0	0
7	Е	29	TotalO2929	0	0
7	А	20	TotalO2020	0	0
7	С	125	Total O 125 125	0	0
7	В	23	TotalO2323	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: VHH14







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	95.27Å 109.23Å 95.48Å	Deneriten
a, b, c, α , β , γ	90.00° 90.70° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	95.26 - 2.15	Depositor
Resolution (A)	$95.47 \ - \ 2.15$	EDS
% Data completeness	72.1 (95.26-2.15)	Depositor
(in resolution range)	70.3 (95.47 - 2.15)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.49 (at 2.14 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.211 , 0.228	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.212 , 0.227	DCC
R_{free} test set	2021 reflections $(2.63%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	34.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 37.3	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
	0.005 for l,k,-h	
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
	0.016 for l,-k,h	
F_o, F_c correlation	0.93	EDS
Total number of atoms	11421	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, NAG

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	Bo	ond lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/825	0.53	0/1114	
1	D	0.27	0/892	0.54	0/1206	
2	С	0.30	0/3749	0.57	1/5120~(0.0%)	
2	F	0.32	1/3815~(0.0%)	0.59	1/5216~(0.0%)	
3	В	0.28	0/950	0.53	0/1282	
3	Е	0.30	0/945	0.55	0/1275	
All	All	0.30	1/11176~(0.0%)	0.56	$2/15213 \ (0.0\%)$	

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
2	С	0	3
2	F	0	5
3	В	0	1
3	Е	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	F	174	SER	C-N	-5.45	1.21	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	436	GLY	N-CA-C	-5.38	99.64	113.10
2	F	175	ARG	N-CA-C	-5.25	96.83	111.00



There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	122	ARG	Sidechain
2	F	133	ARG	Sidechain
2	F	174	SER	Mainchain
2	F	175	ARG	Sidechain
2	F	384	SER	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	А	811	0	762	11	0
1	D	876	0	839	5	0
2	С	3661	0	3551	30	1
2	F	3719	0	3621	31	1
3	В	932	0	888	11	0
3	Е	927	0	883	10	0
4	С	42	0	39	1	0
4	F	56	0	52	2	0
5	F	1	0	0	0	0
6	С	4	0	6	0	0
7	А	20	0	0	0	0
7	В	23	0	0	0	0
7	С	125	0	0	3	0
7	D	27	0	0	0	0
7	Е	29	0	0	0	0
7	F	168	0	0	2	0
All	All	11421	0	10641	94	1

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.

The worst 5 of 94 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)	
3:B:91:THR:HG23	3:B:121:THR:HA	1.62	0.81	
2:C:384:SER:HB3	2:C:385:PRO:HD3	1.61	0.80	
1:A:91:THR:HG23	1:A:115:THR:HA	1.69	0.75	
2:F:448:GLN:NE2	2:F:470:THR:OG1	2.20	0.75	
2:F:487:ASP:OD1	2:F:490:SER:N	2.21	0.74	

All (1) 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)	
2:F:534:LEU:CD1	2:C:530:GLU:O[1_654]	2.12	0.08	

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	Perce	ntiles
1	А	101/124~(82%)	94 (93%)	7 (7%)	0	100	100
1	D	115/124~(93%)	112 (97%)	3(3%)	0	100	100
2	С	471/523~(90%)	454 (96%)	14 (3%)	3(1%)	25	18
2	F	486/523~(93%)	461 (95%)	21 (4%)	4 (1%)	19	12
3	В	121/130~(93%)	113 (93%)	8 (7%)	0	100	100
3	Ε	120/130~(92%)	118 (98%)	2(2%)	0	100	100
All	All	1414/1554 (91%)	1352 (96%)	55 (4%)	7~(0%)	29	22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	385	PRO
2	С	384	SER
2	F	174	SER
2	F	437	ARG

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Mol	Chain	Res	Type
2	С	437	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	83/96~(86%)	82~(99%)	1 (1%)	71 76
1	D	89/96~(93%)	86~(97%)	3~(3%)	37 35
2	С	397/430~(92%)	392~(99%)	5 (1%)	69 74
2	F	403/430~(94%)	395~(98%)	8 (2%)	55 59
3	В	97/104~(93%)	92~(95%)	5(5%)	23 19
3	Ε	97/104~(93%)	90~(93%)	7~(7%)	14 9
All	All	1166/1260~(92%)	1137 (98%)	29 (2%)	47 49

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Ε	46	GLU
3	В	96	CYS
3	Е	112	ASP
3	В	17	SER
3	Е	96	CYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such side chains are listed below:

Mol	Chain	Res	Type
2	С	331	GLN
2	С	494	HIS
2	F	448	GLN
2	F	465	HIS
3	Е	104	GLN



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	С	603	2	14,14,15	0.17	0	17,19,21	0.43	0
4	NAG	С	602	2	$14,\!14,\!15$	0.37	0	17,19,21	0.47	0
4	NAG	F	604	2	14,14,15	0.37	0	17,19,21	0.86	1(5%)
4	NAG	F	601	2	14,14,15	0.45	0	17,19,21	0.63	0
6	EDO	С	604	-	3,3,3	0.50	0	2,2,2	0.20	0
4	NAG	С	601	2	$14,\!14,\!15$	0.39	0	17,19,21	0.48	0
4	NAG	F	603	2	14,14,15	0.37	0	17,19,21	0.72	0
4	NAG	F	602	2	14,14,15	0.29	0	17,19,21	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	С	603	2	-	2/6/23/26	0/1/1/1
4	NAG	С	602	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	604	2	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	F	601	2	-	0/6/23/26	0/1/1/1
6	EDO	С	604	-	-	1/1/1/1	-
4	NAG	С	601	2	-	0/6/23/26	0/1/1/1
4	NAG	F	603	2	-	4/6/23/26	0/1/1/1
4	NAG	F	602	2	-	2/6/23/26	0/1/1/1

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There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	604	NAG	O5-C1-C2	2.45	115.15	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	604	NAG	C1

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	603	NAG	C8-C7-N2-C2
4	F	603	NAG	O7-C7-N2-C2
4	F	602	NAG	O5-C5-C6-O6
4	F	604	NAG	C8-C7-N2-C2
4	F	604	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	604	NAG	1	0
4	F	601	NAG	1	0
4	С	601	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

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, 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>	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	107/124~(86%)	0.57	13 (12%) 4 6	40, 62, 83, 91	0
1	D	117/124~(94%)	-0.02	0 100 100	35, 50, 69, 81	0
2	С	483/523~(92%)	0.07	11 (2%) 60 68	24, 42, 71, 103	0
2	F	491/523~(93%)	0.18	10 (2%) 65 72	24, 39, 78, 91	0
3	В	123/130~(94%)	0.29	2 (1%) 72 77	30, 54, 77, 89	0
3	Е	122/130~(93%)	0.00	1 (0%) 86 89	26, 42, 57, 69	0
All	All	1443/1554~(92%)	0.15	37 (2%) 56 64	24, 44, 77, 103	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	116	VAL	5.5
3	В	122	VAL	4.5
2	F	438	SER	4.1
2	F	177	VAL	3.8
2	F	504	LEU	3.3

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)

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, 95^{th} 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	$B-factors(A^2)$	Q<0.9
4	NAG	F	604	14/15	0.43	0.34	66,77,83,86	0
4	NAG	F	603	14/15	0.73	0.22	64,69,78,80	0
4	NAG	С	603	14/15	0.87	0.16	46,53,70,72	0
6	EDO	С	604	4/4	0.87	0.22	36,39,50,54	0
4	NAG	F	601	14/15	0.93	0.11	33,35,44,49	0
4	NAG	С	602	14/15	0.94	0.13	45,52,60,62	0
4	NAG	F	602	14/15	0.95	0.10	38,47,56,58	0
4	NAG	С	601	14/15	0.96	0.09	33,39,43,46	0
5	CL	F	605	1/1	0.97	0.08	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.

