



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 6FNK / pdb_00006fnk
Title : Crystal Structure of Ephrin B4 (EphB4) Receptor Protein Kinase with a pyrazolo[3,4-d]pyrimidine fragment of NVP-BHG712
Authors : Kudlinzki, D.; Troester, A.; Witt, K.; Linhard, V.L.; Saxena, K.; Schwalbe, H.
Deposited on : 2018-02-04
Resolution : 1.05 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

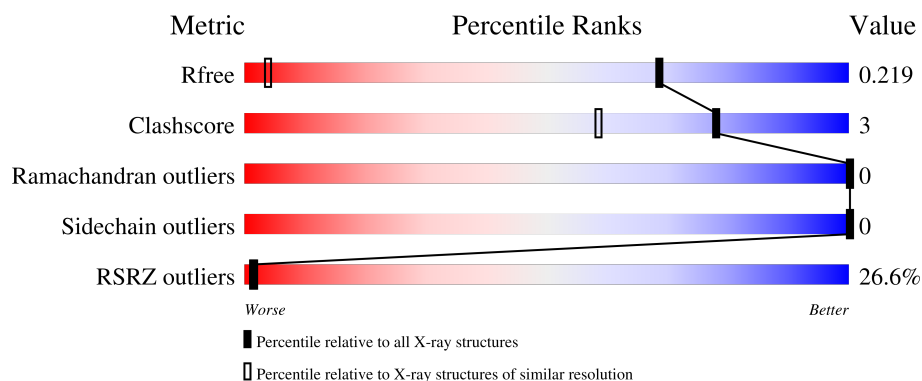
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1036 (1.06-1.02)
Clashscore	190562	1063 (1.06-1.02)
Ramachandran outliers	187476	1034 (1.06-1.02)
Sidechain outliers	187428	1035 (1.06-1.02)
RSRZ outliers	180081	1035 (1.06-1.02)

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	297	25% 85% 7% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2687 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.

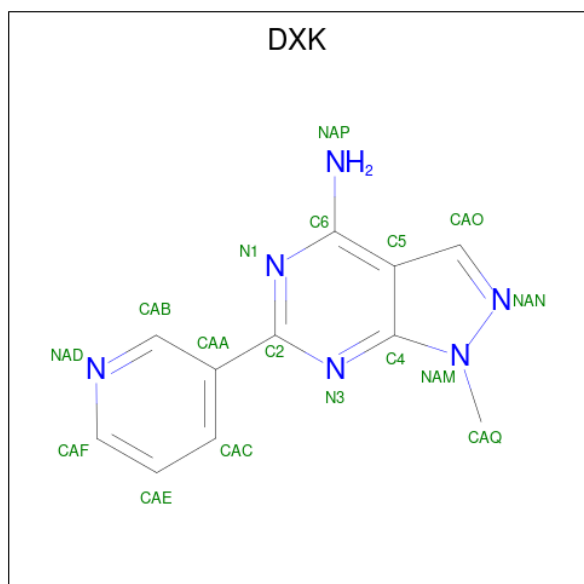
- Molecule 1 is a protein called Ephrin type-B receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2290	1446	407	418	19	0	13	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	GLY	-	expression tag	UNP P54760
A	597	MET	-	expression tag	UNP P54760
A	774	GLU	TYR	engineered mutation	UNP P54760
A	803	VAL	ALA	engineered mutation	UNP P54760
A	870	ILE	VAL	engineered mutation	UNP P54760

- Molecule 2 is 1-methyl-6-pyridin-3-yl-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: DXK) (formula: C₁₁H₁₀N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			17	11	6		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

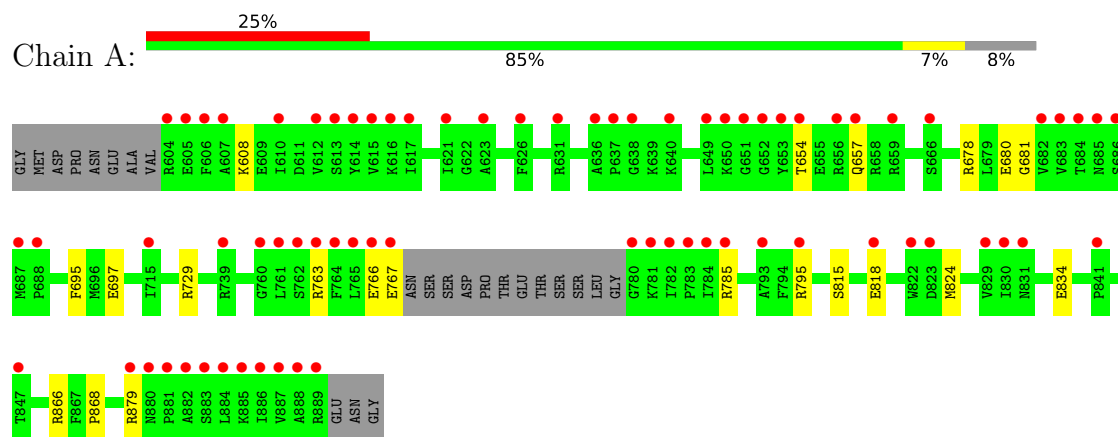
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	372	Total	O	0	0
			372	372		

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: Ephrin type-B receptor 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.52Å 53.58Å 61.34Å 90.00° 110.55° 90.00°	Depositor
Resolution (Å)	42.63 – 1.05 42.63 – 1.05	Depositor EDS
% Data completeness (in resolution range)	95.7 (42.63-1.05) 95.7 (42.63-1.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.05Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.220 0.199 , 0.219	Depositor DCC
R_{free} test set	2096 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2687	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% 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: EDO, DXK

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	0.42	0/2335	0.59	0/3146

There are no bond length outliers.

There are no bond angle outliers.

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	A	2290	0	2282	13	0
2	A	17	0	0	0	0
3	A	8	0	12	2	0
4	A	372	0	0	3	0
All	All	2687	0	2294	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 3.

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:A:695:PHE:CE2	1:A:697[B]:GLU:HG3	2.39	0.57
1:A:763:ARG:NH1	1:A:767:GLU:OE2	2.41	0.54
1:A:678:ARG:NH2	1:A:680:GLU:OE2	2.33	0.53
1:A:879:ARG:HD3	4:A:1127:HOH:O	2.12	0.49
1:A:815[A]:SER:O	1:A:818:GLU:HG2	2.13	0.48
1:A:766:GLU:HB3	1:A:795:ARG:CZ	2.44	0.48
1:A:654:THR:OG1	1:A:657:GLN:HG3	2.17	0.45
1:A:729:ARG:HD2	3:A:1003:EDO:H11	2.00	0.44
1:A:834:GLU:OE2	4:A:1101:HOH:O	2.20	0.44
1:A:608:LYS:HB3	1:A:681:GLY:HA2	2.01	0.42
1:A:785:ARG:NH2	1:A:824:MET:O	2.52	0.42
1:A:866:ARG:NH2	4:A:1108:HOH:O	2.35	0.42
1:A:868:PRO:HB3	3:A:1003:EDO:H11	2.01	0.42

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	A	283/297 (95%)	276 (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	A	250/256 (98%)	250 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	711	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 ⓘ

3 ligands are modelled in this entry.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DXK	A	1001	-	19,19,19	6.22	8 (42%)	24,27,27	2.96	9 (37%)
3	EDO	A	1003	-	3,3,3	0.24	0	2,2,2	1.12	0
3	EDO	A	1002	-	3,3,3	0.41	0	2,2,2	0.33	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
2	DXK	A	1001	-	-	0/4/4/4	0/3/3/3
3	EDO	A	1003	-	-	0/1/1/1	-
3	EDO	A	1002	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	DXK	NAM-NAN	-24.87	1.23	1.37
2	A	1001	DXK	C5-CAO	-6.65	1.34	1.42
2	A	1001	DXK	C5-C4	-4.77	1.33	1.40
2	A	1001	DXK	C5-C6	-4.14	1.36	1.42
2	A	1001	DXK	CAB-NAD	3.05	1.40	1.34
2	A	1001	DXK	CAA-C2	-2.93	1.40	1.48
2	A	1001	DXK	CAO-NAN	2.40	1.34	1.32
2	A	1001	DXK	CAF-NAD	2.27	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DXK	C5-C4-N3	-10.83	119.68	126.56
2	A	1001	DXK	C6-C5-C4	4.55	119.31	115.55
2	A	1001	DXK	N3-C2-N1	-3.64	119.14	125.13
2	A	1001	DXK	CAQ-NAM-C4	-3.31	125.97	128.30
2	A	1001	DXK	CAQ-NAM-NAN	2.76	123.46	120.05
2	A	1001	DXK	C4-N3-C2	2.40	121.55	115.92
2	A	1001	DXK	C5-CAO-NAN	-2.33	109.61	111.38
2	A	1001	DXK	CAA-C2-N1	2.19	121.02	117.40
2	A	1001	DXK	C6-N1-C2	2.09	119.89	117.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	EDO	2	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 ⓘ

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	274/297 (92%)	1.44	73 (26%) 1 1	7, 21, 54, 74	13 (4%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	LEU	6.6
1	A	653	TYR	6.5
1	A	761	LEU	6.2
1	A	780	GLY	6.0
1	A	822	TRP	5.5
1	A	606	PHE	5.2
1	A	654	THR	5.1
1	A	887	VAL	5.0
1	A	607	ALA	4.9
1	A	652	GLY	4.8
1	A	882	ALA	4.7
1	A	651	GLY	4.6
1	A	782	ILE	4.5
1	A	764	PHE	4.5
1	A	612	VAL	4.3
1	A	617	ILE	4.2
1	A	888	ALA	4.1
1	A	610	ILE	4.0
1	A	818	GLU	4.0
1	A	760	GLY	3.9
1	A	886	ILE	3.7
1	A	659	ARG	3.5
1	A	766	GLU	3.4
1	A	636	ALA	3.4
1	A	656	ARG	3.4
1	A	688	PRO	3.3
1	A	614	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	889	ARG	3.3
1	A	781	LYS	3.3
1	A	615	VAL	3.3
1	A	823[A]	ASP	3.1
1	A	767	GLU	3.0
1	A	881	PRO	3.0
1	A	762	SER	2.9
1	A	879	ARG	2.9
1	A	626	PHE	2.9
1	A	650	LYS	2.8
1	A	604	ARG	2.8
1	A	880	ASN	2.8
1	A	649	LEU	2.8
1	A	763	ARG	2.7
1	A	637	PRO	2.6
1	A	685	ASN	2.6
1	A	885	LYS	2.5
1	A	883	SER	2.5
1	A	793	ALA	2.4
1	A	783	PRO	2.4
1	A	631	ARG	2.4
1	A	684	THR	2.4
1	A	613	SER	2.4
1	A	715	ILE	2.4
1	A	686	SER	2.4
1	A	623	ALA	2.3
1	A	621	ILE	2.3
1	A	784	ILE	2.3
1	A	616	LYS	2.3
1	A	785	ARG	2.3
1	A	657	GLN	2.2
1	A	666	SER	2.2
1	A	830	ILE	2.2
1	A	831	ASN	2.2
1	A	605	GLU	2.2
1	A	638	GLY	2.2
1	A	640	LYS	2.2
1	A	829	VAL	2.1
1	A	687	MET	2.1
1	A	847	THR	2.1
1	A	683	VAL	2.1
1	A	841	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	795	ARG	2.1
1	A	884	LEU	2.0
1	A	682	VAL	2.0
1	A	739[A]	ARG	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](#)

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
2	DXK	A	1001	17/17	0.85	0.13	21,26,40,42	0
3	EDO	A	1003	4/4	0.86	0.17	15,25,33,37	0
3	EDO	A	1002	4/4	0.88	0.13	31,31,34,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.