



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2024 – 05:37 PM EDT

PDB ID : 1KGY
Title : Crystal Structure of the EphB2-ephrinB2 complex
Authors : Himanen, J.P.; Rajashankar, K.R.; Lackmann, M.; Cowan, C.A.; Henkemeyer, M.; Nikolov, D.B.
Deposited on : 2001-11-28
Resolution : 2.70 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	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

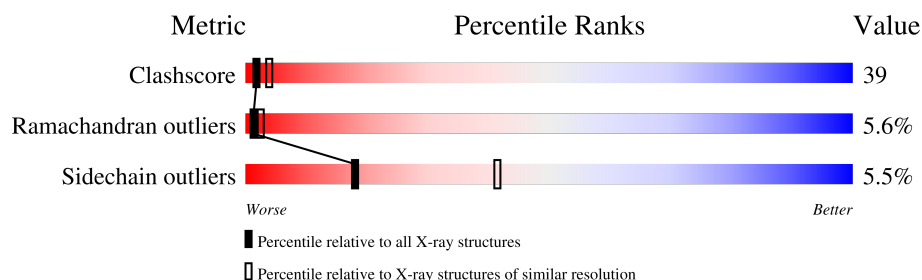
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	43% 50% 7% .
1	B	181	56% 37% 6% .
1	C	181	52% 39% 7% .
1	D	181	39% 54% 7% .
2	E	138	42% 51% 7% .
2	F	138	57% 36% 7%
2	G	138	48% 47% 5%
2	H	138	43% 51% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10260 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1463	925	252	274	12			
1	B	181	Total	C	N	O	S	0	0	0
			1463	925	252	274	12			
1	C	181	Total	C	N	O	S	0	0	0
			1463	925	252	274	12			
1	D	181	Total	C	N	O	S	0	0	0
			1463	925	252	274	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	VAL	conflict	UNP P54763
B	227	ALA	VAL	conflict	UNP P54763
C	427	ALA	VAL	conflict	UNP P54763
D	627	ALA	VAL	conflict	UNP P54763

- Molecule 2 is a protein called EPHRIN-B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	138	Total	C	N	O	S	0	0	0
			1102	706	179	210	7			
2	F	138	Total	C	N	O	S	0	0	0
			1102	706	179	210	7			
2	G	138	Total	C	N	O	S	0	0	0
			1102	706	179	210	7			
2	H	138	Total	C	N	O	S	0	0	0
			1102	706	179	210	7			

There are 4 discrepancies between the modelled and reference sequences:

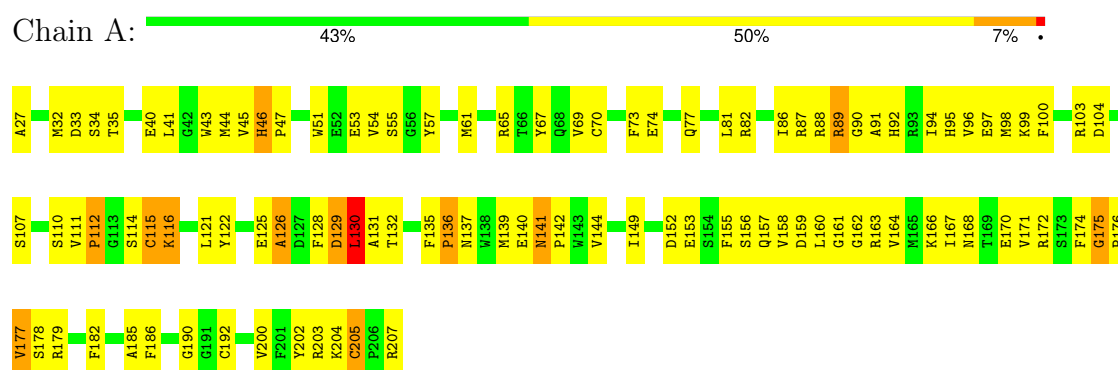
Chain	Residue	Modelled	Actual	Comment	Reference
E	1049	GLY	GLN	conflict	UNP P52800
F	1249	GLY	GLN	conflict	UNP P52800
G	1449	GLY	GLN	conflict	UNP P52800
H	1649	GLY	GLN	conflict	UNP P52800

3 Residue-property plots

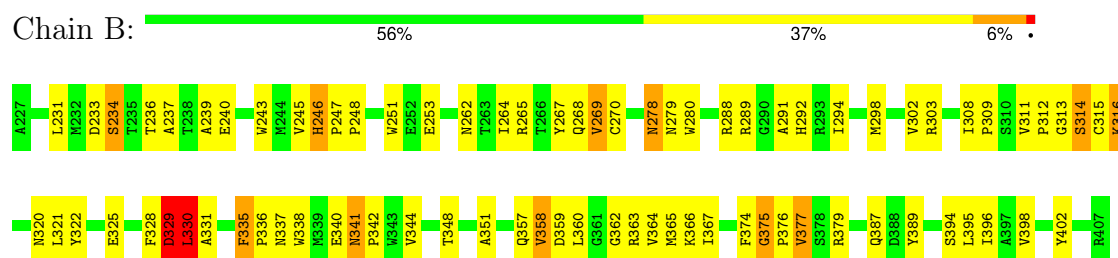
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

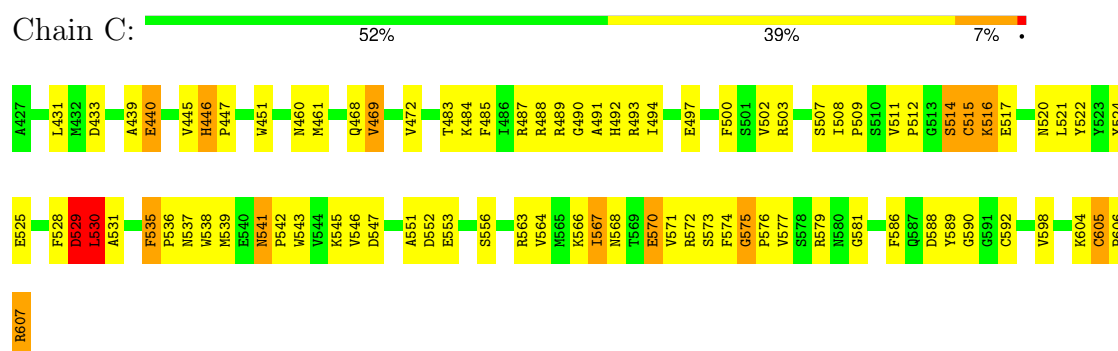
• Molecule 1: EPHRIN TYPE-B RECEPTOR 2



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• Molecule 1: EPHRIN TYPE-B RECEPTOR 2

D1708	Q1709	D1710	V1711	K1712	F1713	T1714	I1715	K1716	F1717	Q1718	E1719	F1720	S1721	P1722	N1723	L1724	W1725		E1728	F1729	Q1730	K1731	N1732		Y1736	I1737	I1738		N1742	G1743	S1744	L1745	E1746	G1747	L1748		Q1751	E1752		V1755		T1758	R1759	A1760	M1761	K1762	I1763		K1766	V1767	G1768
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.00Å 78.00Å 78.00Å 69.00° 75.00° 69.00°	Depositor
Resolution (Å)	25.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10260	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/1502	0.74	0/2035
1	B	0.46	0/1502	0.72	0/2035
1	C	0.44	0/1502	0.74	0/2035
1	D	0.41	0/1502	0.69	0/2035
2	E	0.42	0/1125	0.75	0/1519
2	F	0.42	0/1125	0.74	0/1519
2	G	0.47	0/1125	0.79	0/1519
2	H	0.43	0/1125	0.75	0/1519
All	All	0.43	0/10508	0.74	0/14216

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 [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	1463	0	1389	206	0
1	B	1463	0	1389	93	0
1	C	1463	0	1389	87	0
1	D	1463	0	1389	112	0
2	E	1102	0	1096	137	0
2	F	1102	0	1096	67	0
2	G	1102	0	1096	78	0
2	H	1102	0	1096	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10260	0	9940	790	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 39.

The worst 5 of 790 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:128:PHE:CZ	2:H:1639:ASN:HB3	1.84	1.12
1:A:128:PHE:HB3	2:H:1637:TYR:CD2	1.86	1.10
1:A:89:ARG:HA	2:H:1671:LYS:CG	1.83	1.09
1:A:89:ARG:N	2:H:1671:LYS:NZ	2.02	1.08
1:A:135:PHE:CE2	2:H:1634:GLU:OE2	2.08	1.06

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	179/181 (99%)	144 (80%)	22 (12%)	13 (7%)	1	1
1	B	179/181 (99%)	135 (75%)	32 (18%)	12 (7%)	1	1
1	C	179/181 (99%)	144 (80%)	24 (13%)	11 (6%)	1	2
1	D	179/181 (99%)	138 (77%)	31 (17%)	10 (6%)	1	2
2	E	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	2	4
2	F	136/138 (99%)	110 (81%)	23 (17%)	3 (2%)	5	15
2	G	136/138 (99%)	112 (82%)	17 (12%)	7 (5%)	1	3
2	H	136/138 (99%)	110 (81%)	18 (13%)	8 (6%)	1	2
All	All	1260/1276 (99%)	1005 (80%)	185 (15%)	70 (6%)	1	2

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	130	LEU
1	A	175	GLY
1	B	309	PRO
1	B	375	GLY

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	160/160 (100%)	155 (97%)	5 (3%)	35	64
1	B	160/160 (100%)	153 (96%)	7 (4%)	24	51
1	C	160/160 (100%)	152 (95%)	8 (5%)	20	46
1	D	160/160 (100%)	146 (91%)	14 (9%)	8	20
2	E	124/124 (100%)	118 (95%)	6 (5%)	21	48
2	F	124/124 (100%)	115 (93%)	9 (7%)	11	29
2	G	124/124 (100%)	115 (93%)	9 (7%)	11	29
2	H	124/124 (100%)	120 (97%)	4 (3%)	34	63
All	All	1136/1136 (100%)	1074 (94%)	62 (6%)	18	41

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	741	ASN
2	G	1552	GLU
2	E	1071	LYS
2	G	1545	LEU
2	H	1742	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	1118	GLN
2	F	1309	GLN
2	E	1123	ASN
2	F	1256	GLN
2	F	1342	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](#)

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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.