



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:21 AM UTC

PDB ID : 4BKF / pdb_00004bkf
Title : crystal structure of the human EphA4 ectodomain in complex with human ephrinB3
Authors : Seiradake, E.; Schaupp, A.; del Toro Ruiz, D.; Kaufmann, R.; Mitakidis, N.; Harlos, K.; Aricescu, A.R.; Klein, R.; Jones, E.Y.
Deposited on : 2013-04-24
Resolution : 4.65 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
Xtrriage (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

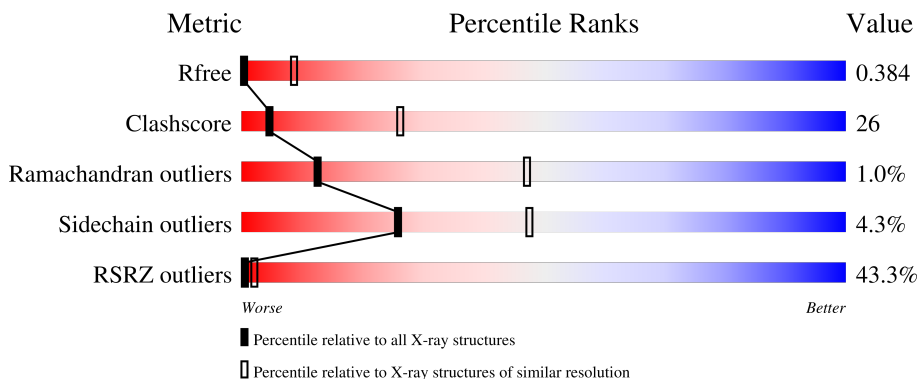
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.65 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	1016 (5.40-3.92)
Clashscore	190562	1000 (5.36-3.96)
Ramachandran outliers	187476	1075 (5.40-3.90)
Sidechain outliers	187428	1057 (5.40-3.90)
RSRZ outliers	180081	1011 (5.40-3.92)

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	568	
1	B	568	
2	C	183	
2	D	183	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10126 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-A RECEPTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	505	3931	2451	678	776	26	0	0	0
1	B	505	3931	2451	678	776	26	0	0	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P54764
A	-10	GLY	-	expression tag	UNP P54764
A	-9	ILE	-	expression tag	UNP P54764
A	-8	LEU	-	expression tag	UNP P54764
A	-7	PRO	-	expression tag	UNP P54764
A	-6	SER	-	expression tag	UNP P54764
A	-5	PRO	-	expression tag	UNP P54764
A	-4	GLY	-	expression tag	UNP P54764
A	-3	MET	-	expression tag	UNP P54764
A	-2	PRO	-	expression tag	UNP P54764
A	-1	ALA	-	expression tag	UNP P54764
A	0	LEU	-	expression tag	UNP P54764
A	1	LEU	-	expression tag	UNP P54764
A	2	SER	-	expression tag	UNP P54764
A	3	LEU	-	expression tag	UNP P54764
A	4	VAL	-	expression tag	UNP P54764
A	5	SER	-	expression tag	UNP P54764
A	6	LEU	-	expression tag	UNP P54764
A	7	LEU	-	expression tag	UNP P54764
A	8	SER	-	expression tag	UNP P54764
A	9	VAL	-	expression tag	UNP P54764
A	10	LEU	-	expression tag	UNP P54764
A	11	LEU	-	expression tag	UNP P54764
A	12	MET	-	expression tag	UNP P54764
A	13	GLY	-	expression tag	UNP P54764

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	-	expression tag	UNP P54764
A	15	VAL	-	expression tag	UNP P54764
A	16	ALA	-	expression tag	UNP P54764
A	17	GLU	-	expression tag	UNP P54764
A	18	THR	-	expression tag	UNP P54764
A	19	GLY	-	expression tag	UNP P54764
A	548	GLY	-	expression tag	UNP P54764
A	549	THR	-	expression tag	UNP P54764
A	550	LYS	-	expression tag	UNP P54764
A	551	HIS	-	expression tag	UNP P54764
A	552	HIS	-	expression tag	UNP P54764
A	553	HIS	-	expression tag	UNP P54764
A	554	HIS	-	expression tag	UNP P54764
A	555	HIS	-	expression tag	UNP P54764
A	556	HIS	-	expression tag	UNP P54764
A	28	THR	ALA	conflict	UNP P54764
B	-11	MET	-	expression tag	UNP P54764
B	-10	GLY	-	expression tag	UNP P54764
B	-9	ILE	-	expression tag	UNP P54764
B	-8	LEU	-	expression tag	UNP P54764
B	-7	PRO	-	expression tag	UNP P54764
B	-6	SER	-	expression tag	UNP P54764
B	-5	PRO	-	expression tag	UNP P54764
B	-4	GLY	-	expression tag	UNP P54764
B	-3	MET	-	expression tag	UNP P54764
B	-2	PRO	-	expression tag	UNP P54764
B	-1	ALA	-	expression tag	UNP P54764
B	0	LEU	-	expression tag	UNP P54764
B	1	LEU	-	expression tag	UNP P54764
B	2	SER	-	expression tag	UNP P54764
B	3	LEU	-	expression tag	UNP P54764
B	4	VAL	-	expression tag	UNP P54764
B	5	SER	-	expression tag	UNP P54764
B	6	LEU	-	expression tag	UNP P54764
B	7	LEU	-	expression tag	UNP P54764
B	8	SER	-	expression tag	UNP P54764
B	9	VAL	-	expression tag	UNP P54764
B	10	LEU	-	expression tag	UNP P54764
B	11	LEU	-	expression tag	UNP P54764
B	12	MET	-	expression tag	UNP P54764
B	13	GLY	-	expression tag	UNP P54764
B	14	CYS	-	expression tag	UNP P54764

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	VAL	-	expression tag	UNP P54764
B	16	ALA	-	expression tag	UNP P54764
B	17	GLU	-	expression tag	UNP P54764
B	18	THR	-	expression tag	UNP P54764
B	19	GLY	-	expression tag	UNP P54764
B	548	GLY	-	expression tag	UNP P54764
B	549	THR	-	expression tag	UNP P54764
B	550	LYS	-	expression tag	UNP P54764
B	551	HIS	-	expression tag	UNP P54764
B	552	HIS	-	expression tag	UNP P54764
B	553	HIS	-	expression tag	UNP P54764
B	554	HIS	-	expression tag	UNP P54764
B	555	HIS	-	expression tag	UNP P54764
B	556	HIS	-	expression tag	UNP P54764
B	28	THR	ALA	conflict	UNP P54764

- Molecule 2 is a protein called EPHRIN-B3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	141	1132	720	201	206	5	0	0	0
2	D	141	1132	720	201	206	5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	expression tag	UNP Q15768
C	-3	GLY	-	expression tag	UNP Q15768
C	-2	ILE	-	expression tag	UNP Q15768
C	-1	LEU	-	expression tag	UNP Q15768
C	0	PRO	-	expression tag	UNP Q15768
C	1	SER	-	expression tag	UNP Q15768
C	2	PRO	-	expression tag	UNP Q15768
C	3	GLY	-	expression tag	UNP Q15768
C	4	MET	-	expression tag	UNP Q15768
C	5	PRO	-	expression tag	UNP Q15768
C	6	ALA	-	expression tag	UNP Q15768
C	7	LEU	-	expression tag	UNP Q15768
C	8	LEU	-	expression tag	UNP Q15768
C	9	SER	-	expression tag	UNP Q15768
C	10	LEU	-	expression tag	UNP Q15768

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	VAL	-	expression tag	UNP Q15768
C	12	SER	-	expression tag	UNP Q15768
C	13	LEU	-	expression tag	UNP Q15768
C	14	LEU	-	expression tag	UNP Q15768
C	15	SER	-	expression tag	UNP Q15768
C	16	VAL	-	expression tag	UNP Q15768
C	17	LEU	-	expression tag	UNP Q15768
C	18	LEU	-	expression tag	UNP Q15768
C	19	MET	-	expression tag	UNP Q15768
C	20	GLY	-	expression tag	UNP Q15768
C	21	CYS	-	expression tag	UNP Q15768
C	22	VAL	-	expression tag	UNP Q15768
C	23	ALA	-	expression tag	UNP Q15768
C	24	GLU	-	expression tag	UNP Q15768
C	25	THR	-	expression tag	UNP Q15768
C	26	GLY	-	expression tag	UNP Q15768
C	170	GLY	-	expression tag	UNP Q15768
C	171	THR	-	expression tag	UNP Q15768
C	172	LYS	-	expression tag	UNP Q15768
C	173	HIS	-	expression tag	UNP Q15768
C	174	HIS	-	expression tag	UNP Q15768
C	175	HIS	-	expression tag	UNP Q15768
C	176	HIS	-	expression tag	UNP Q15768
C	177	HIS	-	expression tag	UNP Q15768
C	178	HIS	-	expression tag	UNP Q15768
C	75	SER	ASN	conflict	UNP Q15768
C	85	GLU	GLY	conflict	UNP Q15768
D	-4	MET	-	expression tag	UNP Q15768
D	-3	GLY	-	expression tag	UNP Q15768
D	-2	ILE	-	expression tag	UNP Q15768
D	-1	LEU	-	expression tag	UNP Q15768
D	0	PRO	-	expression tag	UNP Q15768
D	1	SER	-	expression tag	UNP Q15768
D	2	PRO	-	expression tag	UNP Q15768
D	3	GLY	-	expression tag	UNP Q15768
D	4	MET	-	expression tag	UNP Q15768
D	5	PRO	-	expression tag	UNP Q15768
D	6	ALA	-	expression tag	UNP Q15768
D	7	LEU	-	expression tag	UNP Q15768
D	8	LEU	-	expression tag	UNP Q15768
D	9	SER	-	expression tag	UNP Q15768
D	10	LEU	-	expression tag	UNP Q15768

Continued on next page...

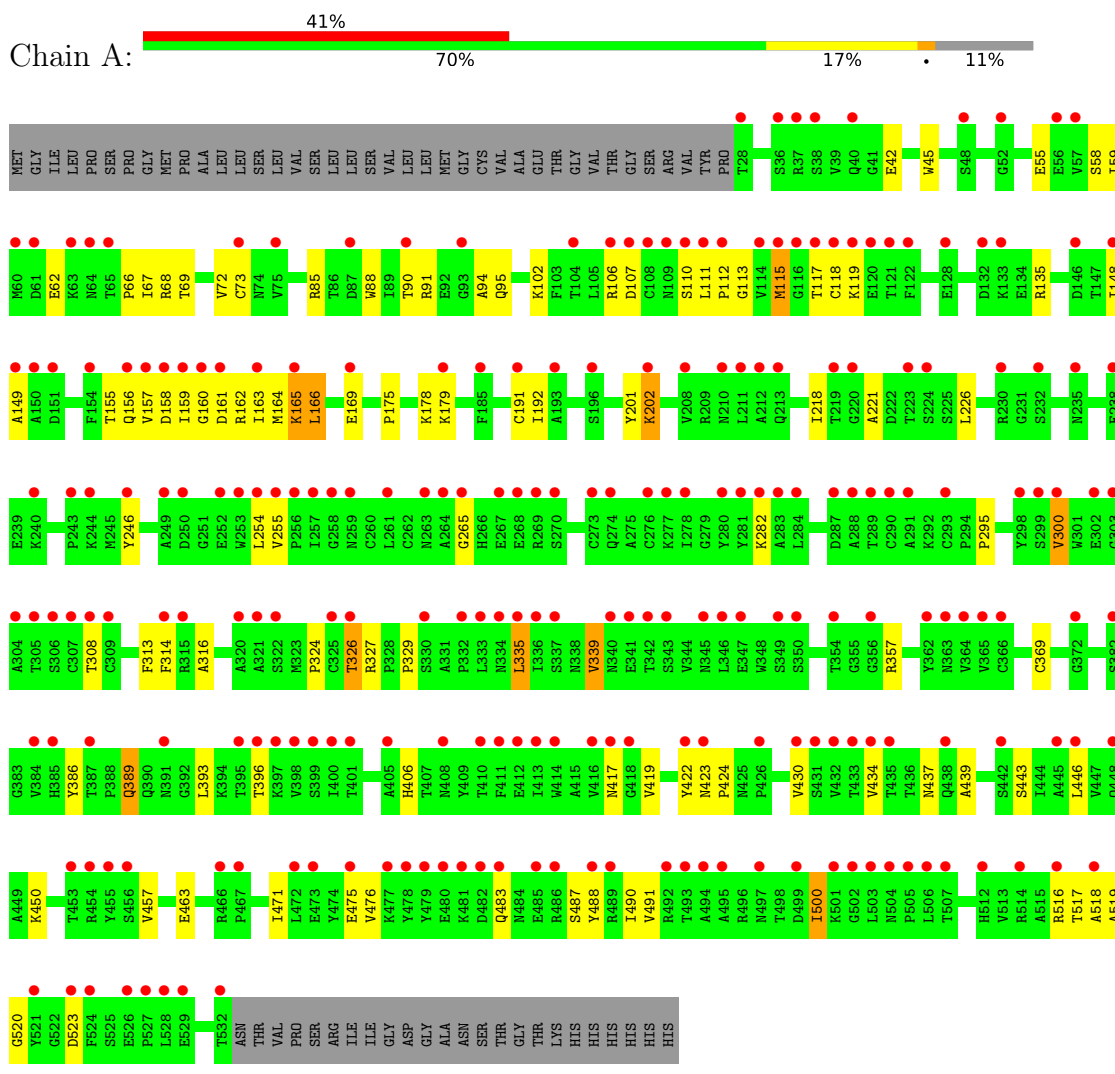
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	11	VAL	-	expression tag	UNP Q15768
D	12	SER	-	expression tag	UNP Q15768
D	13	LEU	-	expression tag	UNP Q15768
D	14	LEU	-	expression tag	UNP Q15768
D	15	SER	-	expression tag	UNP Q15768
D	16	VAL	-	expression tag	UNP Q15768
D	17	LEU	-	expression tag	UNP Q15768
D	18	LEU	-	expression tag	UNP Q15768
D	19	MET	-	expression tag	UNP Q15768
D	20	GLY	-	expression tag	UNP Q15768
D	21	CYS	-	expression tag	UNP Q15768
D	22	VAL	-	expression tag	UNP Q15768
D	23	ALA	-	expression tag	UNP Q15768
D	24	GLU	-	expression tag	UNP Q15768
D	25	THR	-	expression tag	UNP Q15768
D	26	GLY	-	expression tag	UNP Q15768
D	170	GLY	-	expression tag	UNP Q15768
D	171	THR	-	expression tag	UNP Q15768
D	172	LYS	-	expression tag	UNP Q15768
D	173	HIS	-	expression tag	UNP Q15768
D	174	HIS	-	expression tag	UNP Q15768
D	175	HIS	-	expression tag	UNP Q15768
D	176	HIS	-	expression tag	UNP Q15768
D	177	HIS	-	expression tag	UNP Q15768
D	178	HIS	-	expression tag	UNP Q15768
D	75	SER	ASN	conflict	UNP Q15768
D	85	GLU	GLY	conflict	UNP Q15768

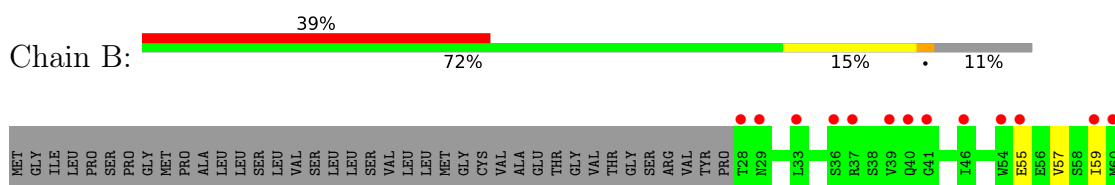
3 Residue-property plots

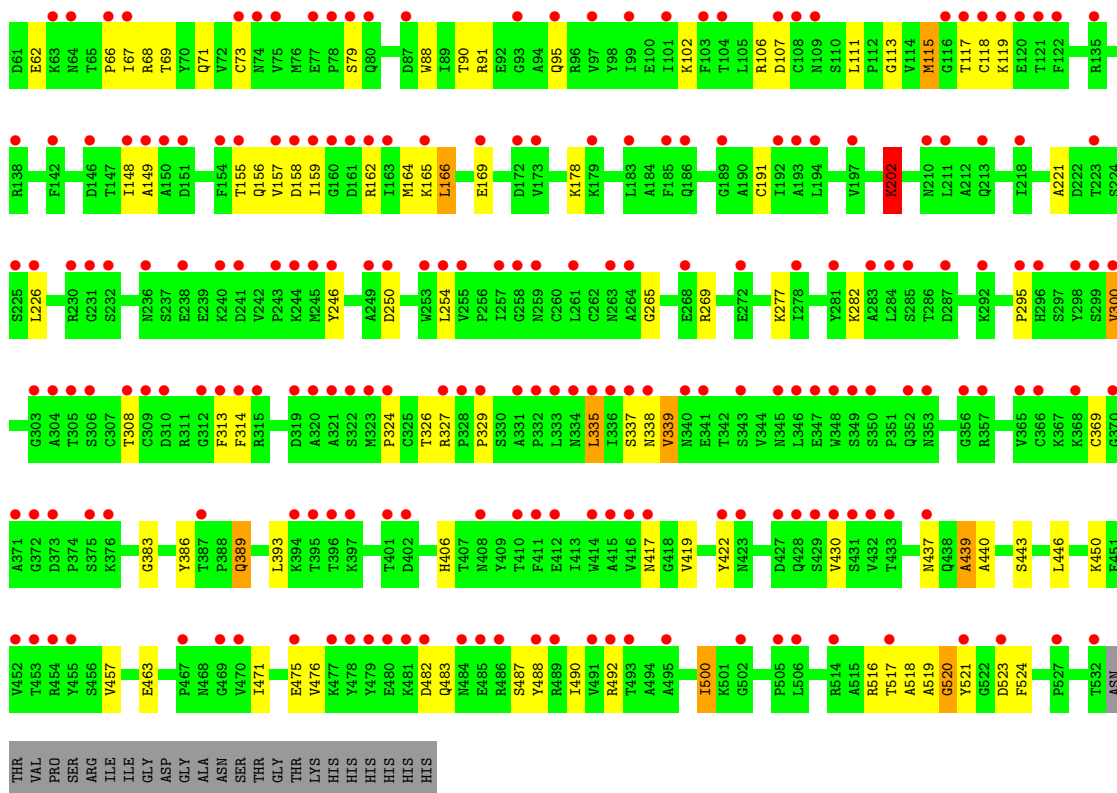
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: EPHRIN TYPE-A RECEPTOR 4

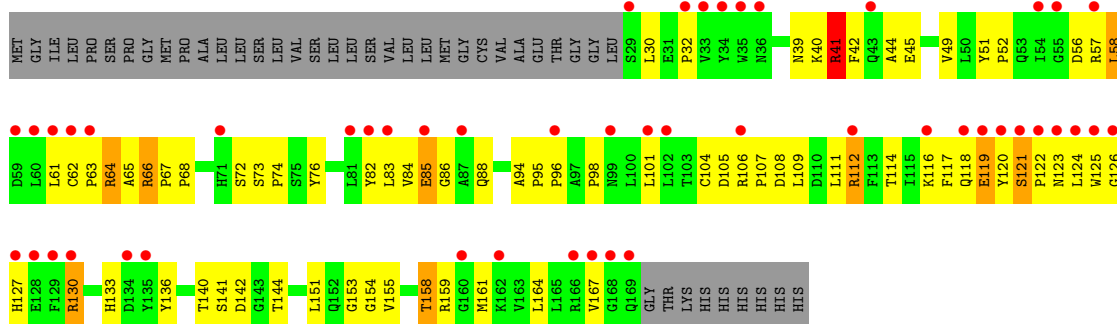


• Molecule 1: EPHRIN TYPE-A RECEPTOR 4

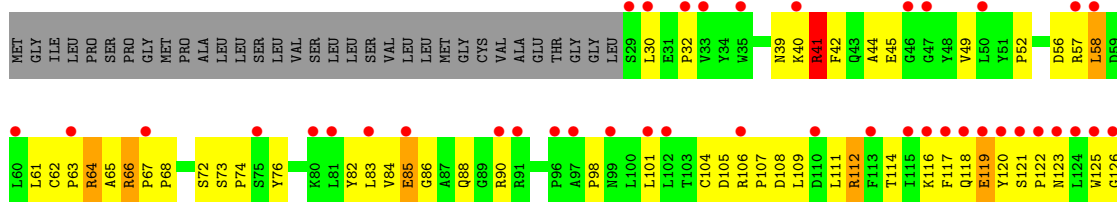


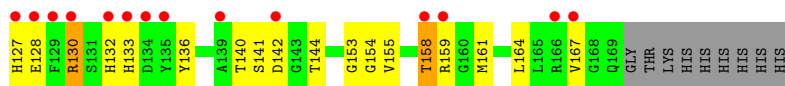


• Molecule 2: EPHRIN-B3



• Molecule 2: EPHRIN-B3





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	300.53Å 300.53Å 300.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.25 – 4.65 106.25 – 4.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (106.25-4.65) 99.8 (106.25-4.65)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 4.66Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.327 , 0.351 0.363 , 0.384	Depositor DCC
R_{free} test set	1298 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	209.6	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 420.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	10126	wwPDB-VP
Average B, all atoms (Å ²)	221.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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 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	0.96	2/4015 (0.0%)	1.24	10/5462 (0.2%)
1	B	0.84	1/4014 (0.0%)	1.02	7/5459 (0.1%)
2	C	0.41	0/1165	0.87	3/1582 (0.2%)
2	D	0.41	0/1165	0.87	3/1582 (0.2%)
All	All	0.82	3/10359 (0.0%)	1.08	23/14085 (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	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	THR	C-N	44.14	1.98	1.33
1	B	439	ALA	C-N	-34.95	0.61	1.33
1	A	439	ALA	C-N	11.17	1.65	1.33

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	THR	O-C-N	35.31	168.06	123.21
1	A	326	THR	CA-C-N	-23.34	83.68	121.03
1	A	326	THR	C-N-CA	-23.34	83.68	121.03
1	A	439	ALA	O-C-N	19.22	148.15	122.59
1	A	202	LYS	CA-C-N	-9.98	102.49	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	LYS	Mainchain
1	B	202	LYS	Mainchain
1	B	439	ALA	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	3931	0	3773	255	33
1	B	3931	0	3776	227	33
2	C	1132	0	1093	129	9
2	D	1132	0	1090	171	10
All	All	10126	0	9732	516	45

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 26.

The worst 5 of 516 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:159:ILE:HG23	2:D:127:HIS:CE1	1.21	1.68
1:A:159:ILE:CG2	2:D:127:HIS:HE1	1.04	1.60
1:B:314:PHE:HB3	1:B:422:TYR:CD2	1.36	1.59
1:B:157:VAL:CG1	2:C:126:GLY:H	1.05	1.57
1:A:59:ILE:HG21	2:D:122:PRO:CB	1.14	1.56

The worst 5 of 45 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:135:ARG:CZ	1:B:156:GLN:OE1[5_555]	0.38	1.82
2:C:51:TYR:CZ	2:D:64:ARG:NH2[9_555]	0.73	1.47
1:A:487:SER:OG	1:B:490:ILE:O[12_455]	1.05	1.15
1:A:135:ARG:NH1	1:B:156:GLN:OE1[5_555]	1.09	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:O	2:C:133:HIS:CE1[5_555]	1.21	0.99

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	503/568 (89%)	478 (95%)	25 (5%)	0	100	100
1	B	501/568 (88%)	477 (95%)	23 (5%)	1 (0%)	43	78
2	C	139/183 (76%)	120 (86%)	13 (9%)	6 (4%)	2	17
2	D	139/183 (76%)	120 (86%)	13 (9%)	6 (4%)	2	17
All	All	1282/1502 (85%)	1195 (93%)	74 (6%)	13 (1%)	12	47

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	440	ALA
2	C	64	ARG
2	D	64	ARG
2	C	45	GLU
2	C	153	GLY

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	437/490 (89%)	421 (96%)	16 (4%)	30	51
1	B	437/490 (89%)	421 (96%)	16 (4%)	30	51
2	C	121/155 (78%)	113 (93%)	8 (7%)	15	37
2	D	121/155 (78%)	113 (93%)	8 (7%)	15	37
All	All	1116/1290 (86%)	1068 (96%)	48 (4%)	26	47

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	476	VAL
2	C	112	ARG
1	B	483	GLN
2	C	41	ARG
2	C	121	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	123	ASN
2	D	127	HIS
2	D	169	GLN
2	C	169	GLN
1	B	338	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	326:THR	C	327:ARG	N	2.68
1	A	326:THR	C	327:ARG	N	1.98
1	A	439:ALA	C	440:ALA	N	1.65
1	B	439:ALA	C	440:ALA	N	0.61

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	505/568 (88%)	2.38	234 (46%) 0 2	87, 219, 291, 295	0
1	B	505/568 (88%)	2.18	222 (43%) 0 2	103, 224, 293, 294	0
2	C	141/183 (77%)	2.03	49 (34%) 1 4	145, 217, 296, 300	0
2	D	141/183 (77%)	1.96	55 (39%) 1 3	153, 227, 295, 298	0
All	All	1292/1502 (86%)	2.22	560 (43%) 0 2	87, 221, 293, 300	0

The worst 5 of 560 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	CYS	15.9
2	D	121	SER	14.1
1	A	287	ASP	13.7
1	B	430	VAL	13.6
1	B	160	GLY	13.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.