Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:48 pm BST

PDB ID	:	3ZFY
Title	:	Crystal structure of EphB3
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Deposited on	:	2012-12-12
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

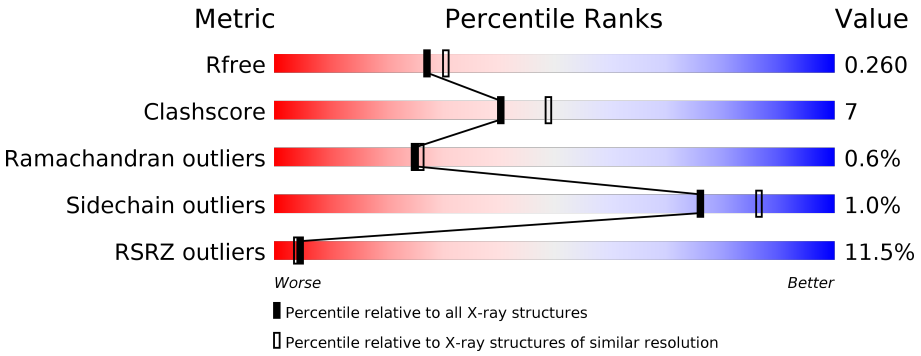
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	A	298	9% 73% 14% 13%
1	B	298	11% 71% 15% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4117 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			2015	1287	339	372	17			
1	B	255	Total	C	N	O	S	0	1	0
			1974	1259	332	366	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	613	GLY	-	expression tag	UNP P54753
A	614	SER	-	expression tag	UNP P54753
A	615	SER	-	expression tag	UNP P54753
A	899	PRO	ALA	conflict	UNP P54753
B	613	GLY	-	expression tag	UNP P54753
B	614	SER	-	expression tag	UNP P54753
B	615	SER	-	expression tag	UNP P54753
B	899	PRO	ALA	conflict	UNP P54753

- Molecule 2 is water.

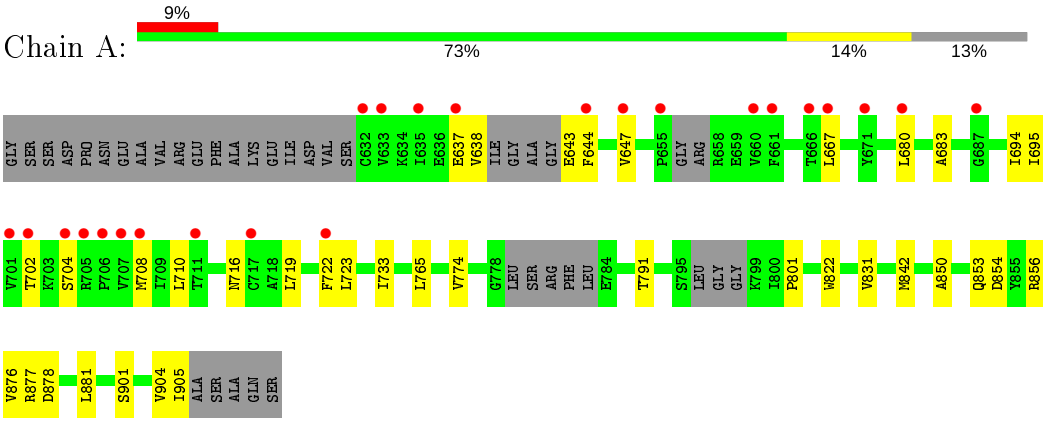
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	67	Total	O	0	0
			67	67		
2	B	61	Total	O	0	0
			61	61		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

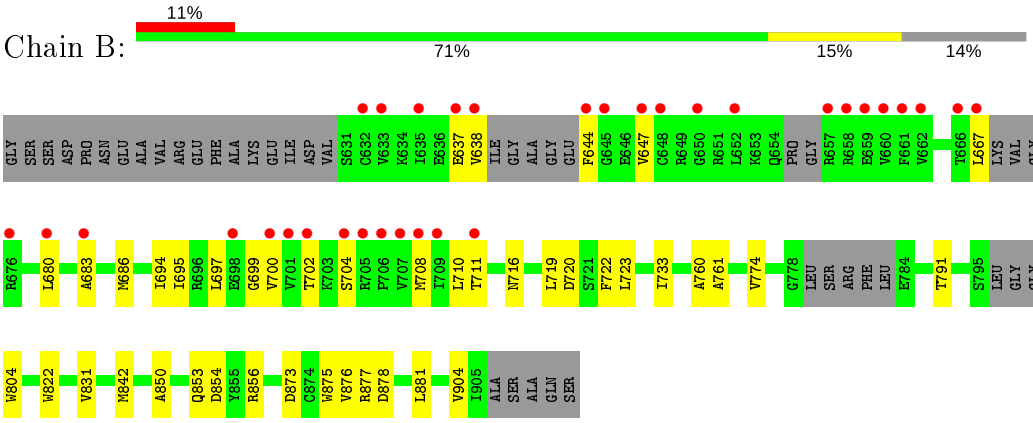
- Molecule 1: EPHRIN TYPE-B RECEPTOR 3

Chain A:



- Molecule 1: EPHRIN TYPE-B RECEPTOR 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	46.99Å 56.49Å 61.35Å 93.02° 90.65° 90.03°	Depositor
Resolution (Å)	61.26 – 2.20 37.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (61.26-2.20) 92.3 (37.49-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.252 0.230 , 0.260	Depositor DCC
R_{free} test set	1515 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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	A	0.47	0/2059	0.68	4/2797 (0.1%)
1	B	0.49	0/2012	0.67	2/2733 (0.1%)
All	All	0.48	0/4071	0.67	6/5530 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	696	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	856	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	856	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	873	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	873	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	856	ARG	NE-CZ-NH2	-5.14	117.73	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	A	2015	0	1939	24	0
1	B	1974	0	1888	32	0
2	A	67	0	0	4	0
2	B	61	0	0	4	0
All	All	4117	0	3827	56	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 7.

All (56) 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:B:876:VAL:HG13	2:B:2052:HOH:O	1.82	0.79
1:A:876:VAL:HG13	2:A:2055:HOH:O	1.85	0.75
1:B:686:MET:HE3	1:B:695:ILE:HG22	1.77	0.65
1:A:877[B]:ARG:HD2	2:A:2036:HOH:O	1.97	0.64
1:B:644:PHE:O	1:B:667:LEU:HD12	1.96	0.64
1:B:686:MET:HE2	1:B:711:THR:HG22	1.80	0.61
1:B:697:LEU:HD12	1:B:710:LEU:O	2.01	0.61
1:B:686:MET:CE	1:B:695:ILE:HG22	2.31	0.61
1:A:697:LEU:HD12	1:A:710:LEU:O	2.02	0.60
1:A:643:GLU:HG3	1:A:644:PHE:CD2	2.38	0.59
1:A:876:VAL:HG11	1:A:881:LEU:HB2	1.87	0.57
1:B:719:LEU:HD21	1:B:831:VAL:HG22	1.87	0.55
1:A:638:VAL:O	1:A:638:VAL:HG13	2.05	0.55
1:A:719:LEU:HD21	1:A:831:VAL:HG22	1.89	0.53
1:A:853:GLN:O	1:A:854:ASP:HB2	2.09	0.53
1:B:876:VAL:HG11	1:B:881:LEU:HB2	1.90	0.52
1:A:904:VAL:HG21	2:A:2050:HOH:O	2.10	0.52
1:B:686:MET:CE	1:B:711:THR:HG22	2.40	0.52
1:B:853:GLN:O	1:B:854:ASP:HB2	2.10	0.50
1:B:904:VAL:CG1	2:B:2050:HOH:O	2.59	0.50
1:B:686:MET:CE	1:B:711:THR:CG2	2.89	0.50
1:B:723:LEU:CD1	1:B:831:VAL:HA	2.42	0.49
1:A:644:PHE:O	1:A:667:LEU:HD12	2.12	0.49
1:A:695:ILE:HD13	1:A:765:LEU:HD12	1.95	0.49
1:A:700:VAL:HG12	1:A:702:THR:HG23	1.95	0.48
1:B:904:VAL:HG12	2:B:2050:HOH:O	2.14	0.48
1:B:716:ASN:HB3	1:B:722:PHE:CD1	2.49	0.47
1:A:694:ILE:HD13	1:A:774:VAL:HB	1.96	0.47
1:B:876:VAL:HG12	1:B:878:ASP:N	2.28	0.47
1:A:723:LEU:CD1	1:A:831:VAL:HA	2.45	0.47
1:A:901:SER:O	1:A:904:VAL:HG12	2.15	0.47
1:B:686:MET:HE1	1:B:711:THR:CG2	2.45	0.47
1:B:694:ILE:HD13	1:B:774:VAL:HB	1.96	0.46
1:B:842:MET:HE1	1:B:850:ALA:CB	2.46	0.46
1:A:716:ASN:HB3	1:A:722:PHE:CD1	2.51	0.45
1:A:733:ILE:HA	1:A:733:ILE:HD13	1.84	0.44
1:B:680:LEU:O	1:B:683:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ILE:HG23	2:A:2049:HOH:O	2.17	0.44
1:A:842:MET:HE1	1:A:850:ALA:CB	2.48	0.44
1:B:822:TRP:CE3	1:B:875:TRP:HA	2.53	0.44
1:B:733:ILE:HA	1:B:733:ILE:HD13	1.86	0.44
1:A:680:LEU:O	1:A:683:ALA:HB3	2.18	0.43
1:A:876:VAL:HG12	1:A:878:ASP:N	2.33	0.43
1:A:822:TRP:CE3	1:A:875:TRP:HA	2.53	0.43
1:B:877[A]:ARG:HD3	2:B:2046:HOH:O	2.18	0.43
1:B:686:MET:HE1	1:B:711:THR:HG21	2.00	0.42
1:B:699:GLY:C	1:B:700:VAL:HG23	2.39	0.42
1:A:700:VAL:HG13	1:A:708:MET:O	2.20	0.42
1:B:644:PHE:HB3	1:B:667:LEU:CD1	2.49	0.42
1:B:700:VAL:HG13	1:B:708:MET:O	2.20	0.41
1:B:700:VAL:HG12	1:B:702:THR:HG23	2.02	0.41
1:B:720:ASP:HB3	1:B:761:ALA:HB3	2.02	0.41
1:B:638:VAL:O	1:B:638:VAL:HG13	2.21	0.40
1:B:791:THR:O	1:B:801:PRO:HA	2.21	0.40
1:A:791:THR:O	1:A:801:PRO:HA	2.21	0.40
1:B:760:ALA:HB2	1:B:804:TRP:CD1	2.57	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	A	251/298 (84%)	240 (96%)	9 (4%)	2 (1%)	19	19
1	B	244/298 (82%)	231 (95%)	12 (5%)	1 (0%)	34	37
All	All	495/596 (83%)	471 (95%)	21 (4%)	3 (1%)	25	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	GLU
1	A	637	GLU
1	A	647	VAL

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	214/261 (82%)	212 (99%)	2 (1%)	78 88
1	B	209/261 (80%)	207 (99%)	2 (1%)	76 86
All	All	423/522 (81%)	419 (99%)	4 (1%)	76 88

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

Mol	Chain	Res	Type
1	A	696	ARG
1	A	704	SER
1	B	647	VAL
1	B	704	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	A	260/298 (87%)	0.46	26 (10%)	7	6	13, 32, 98, 122	0
1	B	255/298 (85%)	0.49	33 (12%)	3	3	12, 30, 108, 133	0
All	All	515/596 (86%)	0.48	59 (11%)	4	4	12, 31, 101, 133	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	633	VAL	6.3
1	B	667	LEU	6.2
1	A	705	ARG	6.2
1	A	706	PRO	5.8
1	B	635	ILE	5.6
1	B	633	VAL	5.2
1	B	647	VAL	5.1
1	B	700	VAL	5.0
1	B	650	GLY	5.0
1	B	652	LEU	4.9
1	B	704	SER	4.9
1	A	637	GLU	4.9
1	B	706	PRO	4.3
1	B	637	GLU	3.9
1	A	666	THR	3.6
1	B	661	PHE	3.6
1	A	660	VAL	3.5
1	A	707	VAL	3.5
1	B	666	THR	3.4
1	B	645	GLY	3.4
1	B	701	VAL	3.4
1	B	705	ARG	3.3
1	B	683	ALA	3.2
1	B	638	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	707	VAL	3.2
1	B	680	LEU	3.1
1	B	662	VAL	3.0
1	B	648	CYS	3.0
1	B	698	GLU	3.0
1	B	676	ARG	2.9
1	A	655	PRO	2.9
1	A	635	ILE	2.8
1	A	647	VAL	2.7
1	A	632	CYS	2.7
1	A	667	LEU	2.7
1	A	700	VAL	2.7
1	B	660	VAL	2.7
1	A	708	MET	2.5
1	B	709	ILE	2.5
1	B	708	MET	2.4
1	B	644	PHE	2.4
1	A	702	THR	2.3
1	A	671	TYR	2.3
1	A	680	LEU	2.3
1	A	701	VAL	2.3
1	A	687	GLY	2.3
1	A	704	SER	2.3
1	A	722	PHE	2.3
1	B	657	ARG	2.3
1	A	661	PHE	2.2
1	B	659	GLU	2.2
1	B	658	ARG	2.2
1	B	702	THR	2.2
1	A	711	THR	2.2
1	B	711	THR	2.1
1	A	696	ARG	2.1
1	A	717	CYS	2.1
1	B	632	CYS	2.0
1	A	644	PHE	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

There are no carbohydrates 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.