

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 04:36 pm BST

PDB ID	:	2WO1
Title	:	Crystal Structure of the EphA4 Ligand Binding Domain
Authors	:	Bowden, T.A.; Aricescu, A.R.; Nettleship, J.E.; Siebold, C.; Rahman-Huq, N.;
		Owens, R.J.; Stuart, D.I.; Jones, E.Y.
Deposited on	:	2009-07-21
Resolution	:	1.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

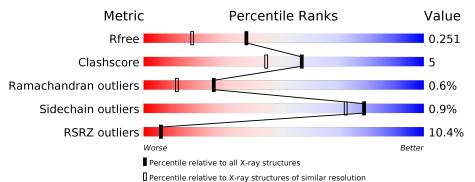
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.85 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	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625(1.86-1.86)
Ramachandran outliers	138981	2592(1.86-1.86)
Sidechain outliers	138945	2592(1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	А	185	9%	11%	·
1	В	185	84%	10% •	• 5%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3253 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	Λ	180	Total	С	Ν	Ο	S	0	n	0
	100	1476	931	254	283	8	0	2	0	
1	р	176	Total	С	Ν	Ο	S	0	Б	0
I D	170	1460	924	246	282	8	0	5	0	

• Molecule 1 is a protein called EPHRIN TYPE-A RECEPTOR.

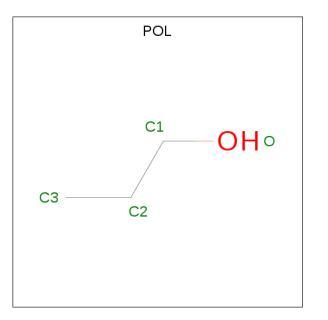
Chain	Residue	Modelled	Actual	Comment	Reference
А	27	GLU	-	expression tag	UNP P54764
A	28	THR	-	expression tag	UNP P54764
А	29	GLY	-	expression tag	UNP P54764
А	203	ARG	-	expression tag	UNP P54764
A	204	THR	-	expression tag	UNP P54764
A	205	LYS	-	expression tag	UNP P54764
А	206	HIS	-	expression tag	UNP P54764
A	207	HIS	_	expression tag	UNP P54764
А	208	HIS	-	expression tag	UNP P54764
A	209	HIS	_	expression tag	UNP P54764
A	210	HIS	-	expression tag	UNP P54764
А	211	HIS	-	expression tag	UNP P54764
В	27	GLU	-	expression tag	UNP P54764
В	28	THR	-	expression tag	UNP P54764
В	29	GLY	-	expression tag	UNP P54764
В	203	ARG	-	expression tag	UNP P54764
В	204	THR	-	expression tag	UNP P54764
В	205	LYS	_	expression tag	UNP P54764
В	206	HIS	-	expression tag	UNP P54764
В	207	HIS	-	expression tag	UNP P54764
В	208	HIS	-	expression tag	UNP P54764
В	209	HIS	-	expression tag	UNP P54764
В	210	HIS	-	expression tag	UNP P54764
В	211	HIS	-	expression tag	UNP P54764

There are 24 discrepancies between the modelled and reference sequences:





• Molecule 2 is N-PROPANOL (three-letter code: POL) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O	0	Ο
		*	4 3 1	0	0
2	А	1	Total C O	0	0
	11	L	4 3 1	0	0
2	А	1	Total C O	0	0
2	11	T	$4 \ 3 \ 1$	0	0
2	В	1	Total C O	0	0
2	D	T	$4 \ 3 \ 1$	0	0
2	B	1	Total C O	0	0
	1	$4 \ 3 \ 1$	0		

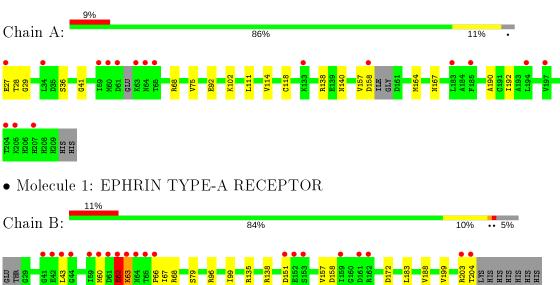
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	153	Total O 153 153	0	0
3	В	144	Total O 144 144	0	0



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-A RECEPTOR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	48.74Å 73.23Å 54.42Å	Depositor
a, b, c, α , β , γ	90.00° 98.35° 90.00°	Depositor
Resolution (Å)	23.75 - 1.85	Depositor
Resolution (A)	22.90 - 1.85	EDS
% Data completeness	98.2 (23.75-1.85)	Depositor
(in resolution range)	98.2 (22.90-1.85)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.93 (at 1.85 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
D D	0.187 , 0.234	Depositor
R, R_{free}	0.215 , 0.251	DCC
R_{free} test set	1595 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	26.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 42.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3253	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.56% 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: POL

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	А	0.53	0/1511	0.66	0/2042	
1	В	0.50	0/1490	0.66	0/2016	
All	All	0.52	0/3001	0.66	0/4058	

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	А	1476	0	1431	18	0
1	В	1460	0	1427	16	0
2	А	12	0	24	3	0
2	В	8	0	16	1	0
3	А	153	0	0	0	0
3	В	144	0	0	1	0
All	All	3253	0	2898	29	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 5.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance (m \AA)$	overlap (Å)
1:A:36:SER:OG	2:A:1210:POL:H32	1.82	0.80
1:B:96:ARG:HG2	2:B:1206:POL:H32	1.74	0.67
1:A:102:LYS:HE2	2:A:1212:POL:H32	1.79	0.65
1:A:114:VAL:HB	1:A:118:CYS:HB2	1.87	0.57
1:B:62:GLU:CD	1:B:67:ILE:HD11	2.25	0.57
1:A:92:GLU:OE1	1:B:138:ARG:NH1	2.37	0.53
1:B:157:VAL:HG23	3:B:2118:HOH:O	2.09	0.51
1:A:138:ARG:NH2	1:A:140:ASN:OD1	2.44	0.50
1:A:75:VAL:HG21	1:A:111:LEU:HD13	1.94	0.50
1:A:92:GLU:CD	1:B:138:ARG:NH1	2.66	0.49
1:A:158:ASP:HB2	1:A:164:MET:HG2	1.94	0.49
1:A:102:LYS:CE	2:A:1212:POL:H32	2.44	0.48
1:B:43:LEU:HD12	1:B:68:ARG:HD3	1.95	0.48
1:B:96:ARG:NH1	1:B:172:ASP:OD2	2.45	0.48
1:B:99:ILE:HG12	1:B:183[B]:LEU:HD21	1.95	0.47
1:A:157:VAL:HG22	1:A:158:ASP:H	1.80	0.46
1:B:62:GLU:O	1:B:63:LYS:CB	2.64	0.46
1:A:41:GLY:O	1:A:68:ARG:NH1	2.48	0.46
1:A:157:VAL:HG22	1:A:158:ASP:N	2.32	0.45
1:A:27:GLU:HG3	1:B:188:VAL:HG11	1.98	0.45
1:A:28:THR:HG23	1:B:79:SER:HA	2.00	0.44
1:A:27:GLU:HG3	1:B:188:VAL:CG1	2.48	0.43
1:A:28:THR:OG1	1:A:29:GLY:N	2.51	0.43
1:B:203:ARG:O	1:B:204:THR:HG22	2.18	0.43
1:A:190:ALA:HB3	1:A:192:ILE:HD11	2.00	0.43
1:B:157:VAL:HG22	1:B:158:ASP:N	2.34	0.42
1:A:102:LYS:HA	1:A:167:ASN:O	2.19	0.42
1:B:60:MET:HA	1:B:66:PRO:HA	2.04	0.40
1:B:183[A]:LEU:HD11	1:B:199:VAL:HG21	2.02	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	176/185~(95%)	167~(95%)	9~(5%)	0	100	100
1	В	179/185~(97%)	168 (94%)	9~(5%)	2(1%)	14	4
All	All	355/370~(96%)	335~(94%)	18 (5%)	2(1%)	25	12

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	63	LYS
1	В	62	GLU

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	А	164/166~(99%)	164~(100%)	0	100 100		
1	В	162/166~(98%)	159~(98%)	3~(2%)	57 43		
All	All	326/332~(98%)	323~(99%)	3~(1%)	78 72		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	62	GLU
1	В	135	ARG
1	В	151	ASP

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 (i)

5 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).

Mal	Mol Type Chain		nain Res Lin		Link G Bond lengths			Bond angles		
	туре	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POL	А	1211	-	3,3,3	0.35	0	2,2,2	0.21	0
2	POL	В	1205	-	3,3,3	0.25	0	2,2,2	0.26	0
2	POL	А	1210	-	3,3,3	0.40	0	$2,\!2,\!2$	0.18	0
2	POL	А	1212	-	3,3,3	0.38	0	2,2,2	0.17	0
2	POL	В	1206	-	3,3,3	0.26	0	2,2,2	0.25	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	POL	А	1211	-	-	0/1/1/1	-
2	POL	В	1205	-	-	0/1/1/1	-
2	POL	А	1210	-	-	1/1/1/1	-
2	POL	А	1212	-	-	0/1/1/1	-
2	POL	В	1206	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1210	POL	O-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1210	POL	1	0
2	А	1212	POL	2	0
2	В	1206	POL	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, 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		$OWAB(A^2)$	Q<0.9	
1	А	180/185~(97%)	0.64	17~(9%)	8	8	17, 26, 51, 69	0
1	В	176/185~(95%)	0.70	20 (11%)	5	5	19, 30, 61, 84	0
All	All	356/370~(96%)	0.67	37 (10%)	6	6	17, 29, 55, 84	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	60	MET	7.1
1	В	59	ILE	6.7
1	А	61	ASP	6.0
1	В	64	ASN	5.2
1	В	65	THR	5.1
1	В	41	GLY	4.7
1	В	63	LYS	4.7
1	В	161	ASP	4.6
1	В	42	GLU	4.6
1	В	204	THR	4.1
1	В	66	PRO	4.1
1	В	61	ASP	4.1
1	А	64	ASN	3.9
1	В	152	GLU	3.8
1	В	159	ILE	3.8
1	А	207	HIS	3.6
1	А	63	LYS	3.6
1	В	62	GLU	3.3
1	А	65	THR	3.2
1	В	203	ARG	3.1
1	В	153	SER	3.0
1	А	158	ASP	2.8
1	А	27	GLU	2.7
1	A	197	VAL	2.6

Continued on next page...



Mol	Chain	Res	Type	RSRZ
1	В	44	GLY	2.6
1	В	151	ASP	2.6
1	А	60	MET	2.3
1	А	194	LEU	2.3
1	В	43	LEU	2.3
1	А	34	LEU	2.2
1	А	204	THR	2.2
1	А	205	LYS	2.2
1	В	162	ARG	2.1
1	А	59	ILE	2.1
1	А	183	LEU	2.1
1	А	185	PHE	2.0
1	А	133	LYS	2.0

Continued from previous page...

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 carbohydrates 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	POL	А	1212	4/4	0.84	0.21	42,42,42,42	0
2	POL	А	1211	4/4	0.86	0.34	55, 56, 56, 56	0
2	POL	В	1205	4/4	0.88	0.16	$31,\!34,\!34,\!35$	0
2	POL	В	1206	4/4	0.90	0.27	33,33,34,34	0
2	POL	А	1210	4/4	0.93	0.24	$30,\!34,\!34,\!35$	0

6.5 Other polymers (i)

There are no such residues in this entry.

