



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:25 AM GMT

PDB ID : 2X11
Title : CRYSTAL STRUCTURE OF THE COMPLETE EPHA2 ECTODOMAIN IN
COMPLEX WITH EPHRIN A5 RECEPTOR BINDING DOMAIN
Authors : Seiradake, E.; Harlos, K.; Sutton, G.; Aricescu, A.R.; Jones, E.Y.
Deposited on : 2009-12-21
Resolution : 4.83 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

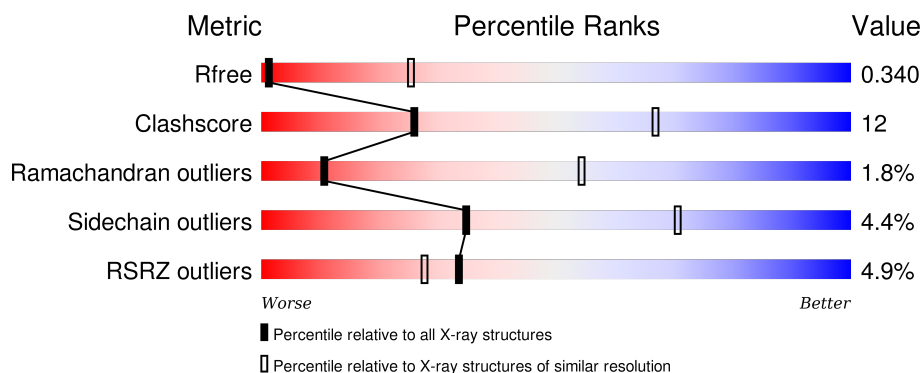
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.83 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}	91344	1117 (6.00-3.60)
Clashscore	102246	1017 (6.00-3.66)
Ramachandran outliers	100387	1156 (6.00-3.60)
Sidechain outliers	100360	1134 (6.00-3.60)
RSRZ outliers	91569	1120 (6.00-3.60)

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. 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	545	
2	B	177	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4889 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	2	0
			3738	2358	628	724	28			

- Molecule 2 is a protein called EPHRIN-A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	1
			1151	736	199	208	8			

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	173.63Å 59.63Å 112.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.48 – 4.83 49.15 – 4.83	Depositor EDS
% Data completeness (in resolution range)	93.7 (40.48-4.83) 99.8 (49.15-4.83)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 4.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.312 , 0.314 0.316 , 0.340	Depositor DCC
R_{free} test set	273 reflections (4.55%)	DCC
Wilson B-factor (Å ²)	180.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 171.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 6016 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4889	wwPDB-VP
Average B, all atoms (Å ²)	247.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	0/3834	0.42	0/5226
2	B	0.27	0/1190	0.43	0/1612
All	All	0.23	0/5024	0.42	0/6838

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	3738	0	3490	88	0
2	B	1151	0	1068	44	0
All	All	4889	0	4558	117	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 12.

All (117) 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)
2:B:126:THR:HG21	2:B:131:GLY:HA3	1.24	1.11
1:A:159:ARG:HA	2:B:130:LEU:CD1	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:HA	2:B:130:LEU:HD13	1.45	0.98
1:A:92:GLU:HB3	1:A:218:SER:HB2	1.51	0.93
1:A:156:PHE:O	2:B:130:LEU:HD21	1.70	0.91
2:B:154:ARG:HB2	2:B:154:ARG:HH11	1.37	0.90
2:B:87:ASN:OD1	2:B:99:LYS:HB3	1.80	0.81
1:A:293:CYS:HB3	1:A:297:THR:HG21	1.63	0.78
1:A:237:PRO:HD2	1:A:238:PRO:HD3	1.67	0.76
1:A:68:SER:HB2	2:B:127:PRO:HB2	1.69	0.75
2:B:126:THR:HG22	2:B:128:PHE:H	1.53	0.74
1:A:190:ALA:HB3	2:B:128:PHE:HD2	1.53	0.73
2:B:35:ARG:HG2	2:B:61:TYR:HB2	1.69	0.73
1:A:156:PHE:HA	2:B:130:LEU:HG	1.71	0.72
1:A:295:GLU:HB2	1:A:324:PRO:HB3	1.71	0.72
1:A:370:TRP:HB3	1:A:373:SER:HB3	1.71	0.71
1:A:103:ARG:HB3	1:A:188:CYS:HB3	1.76	0.65
2:B:141:PHE:CE2	2:B:160:LYS:HG3	2.32	0.65
2:B:126:THR:HG21	2:B:131:GLY:CA	2.16	0.64
1:A:215:ILE:N	1:A:215:ILE:HD13	2.11	0.64
2:B:88:PHE:O	2:B:91:TYR:N	2.32	0.62
1:A:237:PRO:CD	1:A:238:PRO:HD3	2.29	0.61
1:A:269:VAL:HB	1:A:274:GLN:HG3	1.82	0.61
2:B:80:ARG:HB3	2:B:147:ILE:HD12	1.83	0.59
1:A:335:LEU:HD22	1:A:412:VAL:HG12	1.84	0.59
1:A:153:SER:O	1:A:156:PHE:HB2	2.02	0.59
1:A:246:HIS:ND1	1:A:255:VAL:HG23	2.18	0.59
2:B:151:ASN:HB3	2:B:154:ARG:HH22	1.68	0.58
1:A:411:THR:HG22	1:A:429:THR:HG22	1.86	0.57
1:A:460:PRO:N	1:A:461:PRO:HD2	2.19	0.57
1:A:58:ILE:HG21	2:B:102:LYS:NZ	2.20	0.56
1:A:159:ARG:HA	2:B:130:LEU:HD11	1.83	0.56
1:A:99:LYS:HB2	1:A:193:SER:HB3	1.85	0.56
1:A:448:SER:O	1:A:449:THR:HB	2.05	0.56
1:A:380:GLU:O	1:A:383:VAL:HG22	2.05	0.56
2:B:154:ARG:HB2	2:B:154:ARG:NH1	2.15	0.56
1:A:223:LEU:HD21	1:A:254:LEU:HD12	1.87	0.56
2:B:58:ILE:O	2:B:59:ASN:HB2	2.06	0.55
1:A:482:TYR:CD2	1:A:482:TYR:N	2.74	0.55
2:B:102:LYS:NZ	2:B:102:LYS:HB3	2.21	0.55
1:A:473:TYR:CE2	1:A:483:ASN:HB2	2.41	0.55
1:A:508:GLN:HA	1:A:518:GLY:HA2	1.88	0.55
1:A:344:VAL:CG2	1:A:399:VAL:HB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:CA	2:B:130:LEU:CD1	2.76	0.54
1:A:102:VAL:HG21	1:A:147:PRO:HG3	1.90	0.53
1:A:245:MET:HB3	1:A:253:TRP:CE3	2.44	0.53
2:B:97:THR:O	2:B:99:LYS:HD3	2.08	0.52
1:A:293:CYS:HB3	1:A:297:THR:CG2	2.38	0.52
2:B:122:PHE:CE1	2:B:161:VAL:HG11	2.45	0.51
1:A:152:VAL:O	1:A:155:ASP:HB2	2.10	0.51
1:A:70:CYS:HB2	2:B:127:PRO:HG3	1.93	0.51
1:A:474:ARG:HG2	1:A:475:LYS:N	2.27	0.50
2:B:101:PHE:CD1	2:B:101:PHE:N	2.79	0.50
1:A:108:PHE:HZ	1:A:188:CYS:SG	2.34	0.50
2:B:126:THR:CG2	2:B:131:GLY:HA3	2.17	0.50
1:A:123:TYR:HB3	1:A:142:ILE:HD11	1.94	0.49
1:A:85:TRP:CZ2	1:A:177:GLY:HA3	2.47	0.49
1:A:444:LEU:HD11	1:A:524:PHE:HB3	1.95	0.49
1:A:449:THR:OG1	1:A:499:PRO:HA	2.13	0.49
1:A:440:PRO:HA	1:A:458:ILE:HG23	1.94	0.49
1:A:471:VAL:O	1:A:484:VAL:HA	2.13	0.48
1:A:344:VAL:HG22	1:A:402:LEU:HD11	1.96	0.48
1:A:328:PRO:HG2	1:A:422:VAL:HG11	1.96	0.48
1:A:190:ALA:HB3	2:B:128:PHE:CD2	2.42	0.48
1:A:112:ALA:C	1:A:114:SER:H	2.17	0.47
1:A:237:PRO:HG2	1:A:261:LEU:HD12	1.97	0.47
1:A:236:VAL:HA	1:A:237:PRO:HD3	1.58	0.47
2:B:83:LEU:HD22	2:B:144:SER:HB3	1.97	0.46
1:A:313:PHE:HB3	1:A:325:CYS:HB3	1.96	0.46
1:A:327:ARG:O	1:A:355:GLY:HA3	2.16	0.46
1:A:468:LYS:O	1:A:510:LEU:HB2	2.16	0.46
1:A:392:LEU:HD21	1:A:397:VAL:HG11	1.97	0.46
2:B:103:ARG:HG3	2:B:104:TRP:CE2	2.51	0.46
1:A:70:CYS:HB2	2:B:127:PRO:CA	2.46	0.45
1:A:456:TRP:HZ3	1:A:492:VAL:HG22	1.80	0.45
2:B:73:VAL:HA	2:B:74:PRO:HD3	1.82	0.45
2:B:128:PHE:CD1	2:B:129:SER:O	2.70	0.45
1:A:220:ALA:N	1:A:221:PRO:HD2	2.31	0.45
1:A:447:ARG:HG3	1:A:527:LEU:CD1	2.47	0.45
1:A:294:PRO:HG3	1:A:321:ALA:O	2.17	0.45
1:A:188:CYS:SG	2:B:127:PRO:HA	2.57	0.45
1:A:369:CYS:O	1:A:371:PRO:HD3	2.18	0.44
1:A:440:PRO:HA	1:A:458:ILE:CG2	2.47	0.44
1:A:348:TRP:CZ3	1:A:397:VAL:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ALA:HB1	1:A:305:THR:HG22	1.99	0.43
1:A:344:VAL:HG23	1:A:399:VAL:HB	1.99	0.43
1:A:74:SER:HB2	1:A:77:GLN:NE2	2.33	0.43
1:A:96:ILE:O	1:A:167:GLU:HA	2.18	0.43
1:A:348:TRP:CH2	1:A:397:VAL:HG22	2.53	0.43
2:B:108:ARG:HB2	2:B:116:LEU:HD12	2.00	0.42
1:A:46:HIS:HA	1:A:47:PRO:C	2.39	0.42
1:A:337:ALA:HB1	1:A:432:VAL:CG2	2.49	0.42
1:A:215:ILE:CD1	1:A:215:ILE:N	2.74	0.42
1:A:262:CYS:O	1:A:282:LYS:NZ	2.52	0.42
1:A:281:PHE:CD1	1:A:281:PHE:C	2.93	0.42
1:A:189:VAL:HG12	1:A:190:ALA:N	2.33	0.42
1:A:472:THR:HG23	1:A:482:TYR:HD1	1.85	0.42
2:B:68:HIS:HE1	2:B:111:SER:O	2.03	0.42
2:B:116:LEU:HD23	2:B:117:LYS:N	2.35	0.42
1:A:92:GLU:HB3	1:A:218:SER:CB	2.36	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.78	0.42
1:A:130:TYR:HB3	1:A:133:ASN:HB2	2.01	0.42
1:A:44:LEU:HD23	1:A:44:LEU:C	2.40	0.42
1:A:70:CYS:HB2	2:B:127:PRO:CG	2.51	0.41
2:B:147:ILE:N	2:B:148:PRO:HD2	2.35	0.41
2:B:88:PHE:O	2:B:89:ASP:C	2.59	0.41
2:B:141:PHE:N	2:B:141:PHE:CD1	2.88	0.41
1:A:466:VAL:HG12	1:A:509:ALA:HB1	2.03	0.41
1:A:387:GLU:HG3	1:A:388:PRO:HD2	2.02	0.41
2:B:126:THR:HA	2:B:127:PRO:HD3	1.74	0.41
1:A:80:TRP:NE1	1:A:136:LYS:HE3	2.35	0.41
1:A:192:LEU:HD21	2:B:128:PHE:CE2	2.56	0.40
1:A:99:LYS:HA	1:A:164:ASN:O	2.21	0.40
2:B:122:PHE:CZ	2:B:161:VAL:HG11	2.57	0.40
1:A:448:SER:HA	1:A:527:LEU:HD22	2.04	0.40
1:A:146:ALA:HA	1:A:147:PRO:HD3	1.92	0.40
1:A:403:GLU:HA	1:A:404:PRO:HD3	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	476/545 (87%)	436 (92%)	37 (8%)	3 (1%)	30	74
2	B	137/177 (77%)	123 (90%)	6 (4%)	8 (6%)	2	27
All	All	613/722 (85%)	559 (91%)	43 (7%)	11 (2%)	11	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	112	PRO
2	B	154	ARG
2	B	113	ASN
1	A	480	ASN
2	B	33	ALA
2	B	88	PHE
2	B	150	ASP
2	B	152	GLY
1	A	237	PRO
1	A	294	PRO
2	B	74	PRO

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	402/464 (87%)	382 (95%)	20 (5%)	30	67
2	B	127/159 (80%)	124 (98%)	3 (2%)	57	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	529/623 (85%)	506 (96%)	23 (4%)	35	71

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	150	ILE
1	A	157	GLU
1	A	174	THR
1	A	188	CYS
1	A	191	LEU
1	A	192	LEU
1	A	204	LEU
1	A	215	ILE
1	A	349	THR
1	A	379	CYS
1	A	387	GLU
1	A	392	LEU
1	A	397	VAL
1	A	411	THR
1	A	441	LYS
1	A	442	VAL
1	A	462	GLN
1	A	484	VAL
1	A	494	LEU
2	B	52	TYR
2	B	101	PHE
2	B	154	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	333	HIS
2	B	48	GLN
2	B	68	HIS

5.3.3 RNA ⓘ

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](#)

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 ⓘ

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	488/545 (89%)	0.32	25 (5%) 32 26	184, 250, 285, 314	0
2	B	139/177 (78%)	0.27	6 (4%) 39 32	253, 269, 293, 298	0
All	All	627/722 (86%)	0.31	31 (4%) 33 28	184, 259, 287, 314	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	ALA	4.7
1	A	405	HIS	4.2
1	A	371	PRO	3.8
1	A	469	TYR	3.6
1	A	470	GLU	3.6
1	A	486	ARG	3.4
1	A	412	VAL	3.3
1	A	414	ALA	3.3
1	A	362	TYR	2.9
1	A	432	VAL	2.8
2	B	105	GLU	2.6
1	A	344	VAL	2.6
1	A	479	SER	2.5
1	A	489	GLY	2.5
1	A	463	GLN	2.5
2	B	102	LYS	2.4
1	A	348	TRP	2.4
2	B	48	GLN	2.4
1	A	413	GLU	2.3
1	A	505	VAL	2.3
2	B	77	LYS	2.3
1	A	484	VAL	2.2
2	B	104	TRP	2.2
1	A	481	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	139	GLU	2.1
1	A	471	VAL	2.1
1	A	402	LEU	2.1
1	A	485	ARG	2.1
1	A	516	GLY	2.1
1	A	374	GLY	2.0
1	A	410	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 [i](#)

There are no carbohydrates 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.