



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 10:31 pm GMT

PDB ID : 3V6B  
Title : VEGFR-2/VEGF-E complex structure  
Authors : Brozzo, M.S.; Leppanen, V.-M.; Winkler, F.K.; Kisko, K.; Ballmer-Hofer, K.  
Deposited on : 2011-12-19  
Resolution : 3.21 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](mailto: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 : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

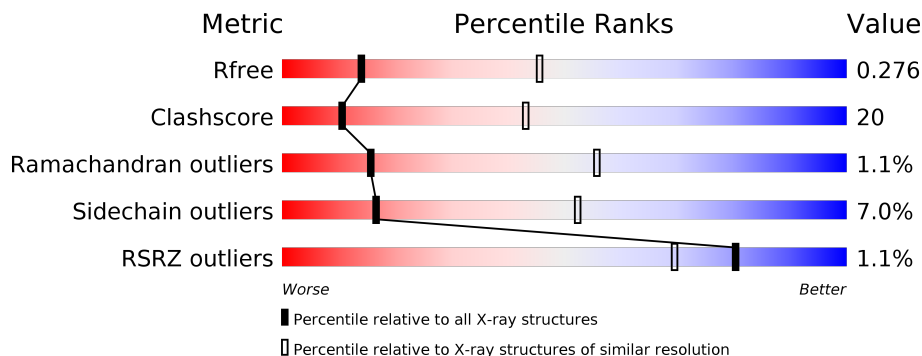
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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))
$R_{free}$	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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  $\geq 3$ , 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	137	
2	R	424	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2093 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 VEGF-E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	94	692	420	124	137	11	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLU	-	EXPRESSION TAG	UNP Q2F842
A	-12	LEU	-	EXPRESSION TAG	UNP Q2F842
A	-11	SER	-	EXPRESSION TAG	UNP Q2F842
A	-10	THR	-	EXPRESSION TAG	UNP Q2F842
A	-9	SER	-	EXPRESSION TAG	UNP Q2F842
A	-8	LEU	-	EXPRESSION TAG	UNP Q2F842
A	-7	TYR	-	EXPRESSION TAG	UNP Q2F842
A	-6	LYS	-	EXPRESSION TAG	UNP Q2F842
A	-5	LYS	-	EXPRESSION TAG	UNP Q2F842
A	-4	ALA	-	EXPRESSION TAG	UNP Q2F842
A	-3	GLY	-	EXPRESSION TAG	UNP Q2F842
A	-2	PHE	-	EXPRESSION TAG	UNP Q2F842
A	-1	HIS	-	EXPRESSION TAG	UNP Q2F842
A	0	HIS	-	EXPRESSION TAG	UNP Q2F842
A	1	HIS	-	EXPRESSION TAG	UNP Q2F842
A	2	HIS	-	EXPRESSION TAG	UNP Q2F842
A	3	HIS	-	EXPRESSION TAG	UNP Q2F842
A	4	HIS	-	EXPRESSION TAG	UNP Q2F842
A	5	GLU	-	EXPRESSION TAG	UNP Q2F842
A	6	ASN	-	EXPRESSION TAG	UNP Q2F842
A	7	LEU	-	EXPRESSION TAG	UNP Q2F842
A	8	TYR	-	EXPRESSION TAG	UNP Q2F842
A	9	PHE	-	EXPRESSION TAG	UNP Q2F842
A	10	GLN	-	EXPRESSION TAG	UNP Q2F842

- Molecule 2 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	187	Total	C	N	O	S	0	0	0
			1401	894	230	268	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	131	HIS	-	EXPRESSION TAG	UNP P35968
R	547	ARG	VAL	CONFLICT	UNP P35968
R	549	HIS	-	EXPRESSION TAG	UNP P35968
R	550	HIS	-	EXPRESSION TAG	UNP P35968
R	551	HIS	-	EXPRESSION TAG	UNP P35968
R	552	HIS	-	EXPRESSION TAG	UNP P35968
R	553	HIS	-	EXPRESSION TAG	UNP P35968
R	554	HIS	-	EXPRESSION TAG	UNP P35968



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.88Å 79.88Å 340.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.79 – 3.21 67.79 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (67.79-3.21) 99.4 (67.79-3.20)	Depositor EDS
$R_{merge}$	0.94	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.237 , 0.276 0.238 , 0.276	Depositor DCC
$R_{free}$ test set	543 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 104.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.32	0/705	0.51	0/958
2	R	0.27	0/1428	0.48	0/1946
All	All	0.29	0/2133	0.49	0/2904

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	692	0	648	10	0
2	R	1401	0	1323	73	0
All	All	2093	0	1971	80	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 20.

All (80) 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:R:140:GLU:HG3	2:R:222:ARG:HH12	1.29	0.94
2:R:234:ILE:HD12	2:R:322:VAL:HG22	1.64	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:302:GLN:HG3	2:R:323:ARG:HA	1.66	0.77
2:R:188:PRO:HG2	2:R:191:MET:SD	2.24	0.77
2:R:140:GLU:HG3	2:R:222:ARG:NH1	1.99	0.77
2:R:138:ILE:HD13	2:R:216:VAL:HG13	1.67	0.75
2:R:306:THR:HA	2:R:319:SER:HB3	1.68	0.74
2:R:210:GLN:HE21	2:R:210:GLN:H	1.35	0.73
2:R:164:ARG:HG2	2:R:167:GLU:HG2	1.75	0.69
2:R:241:LYS:HD3	2:R:295:ASP:HA	1.75	0.68
1:A:80:LEU:HD12	1:A:94:LEU:HD12	1.75	0.68
1:A:81:LEU:CD1	2:R:215:ILE:HG21	2.25	0.66
1:A:81:LEU:HD12	2:R:215:ILE:HD13	1.79	0.65
2:R:236:LEU:HD22	2:R:240:GLU:OE1	1.97	0.64
2:R:304:LEU:HD11	2:R:319:SER:HB2	1.81	0.62
2:R:241:LYS:HG3	2:R:242:LEU:N	2.16	0.60
1:A:27:LYS:HG2	1:A:29:ARG:HE	1.67	0.60
2:R:248:ALA:HB3	2:R:288:PHE:HB2	1.84	0.59
2:R:143:ASN:HA	2:R:190:TYR:HD2	1.67	0.59
1:A:81:LEU:HD13	2:R:215:ILE:HG21	1.85	0.58
2:R:138:ILE:HG13	2:R:189:SER:HB2	1.86	0.58
2:R:222:ARG:HB2	2:R:251:GLU:HG2	1.86	0.58
2:R:228:LEU:HD12	2:R:228:LEU:H	1.69	0.56
2:R:163:ALA:O	2:R:167:GLU:HA	2.05	0.56
2:R:210:GLN:NE2	2:R:210:GLN:H	2.04	0.56
2:R:200:CYS:O	2:R:210:GLN:HB2	2.07	0.54
2:R:149:PRO:HG2	2:R:214:TYR:CE1	2.42	0.54
1:A:16:GLY:O	1:A:20:VAL:HG23	2.07	0.54
2:R:148:ILE:HD12	2:R:148:ILE:N	2.22	0.54
1:A:84:SER:O	1:A:85:GLY:C	2.46	0.54
2:R:210:GLN:N	2:R:210:GLN:HE21	2.03	0.53
2:R:197:MET:CE	2:R:213:MET:HG3	2.38	0.53
2:R:227:VAL:HA	2:R:318:ASN:HD22	1.74	0.53
2:R:199:PHE:CE2	2:R:210:GLN:HG3	2.44	0.53
2:R:187:ILE:HG13	2:R:188:PRO:HD2	1.92	0.51
2:R:302:GLN:HE22	2:R:323:ARG:NH1	2.08	0.51
1:A:27:LYS:HE2	1:A:29:ARG:NH2	2.25	0.51
2:R:261:GLU:OE2	2:R:261:GLU:HA	2.11	0.50
2:R:204:ILE:HD12	2:R:204:ILE:N	2.26	0.49
2:R:302:GLN:CD	2:R:323:ARG:HD2	2.33	0.48
2:R:306:THR:CA	2:R:319:SER:HB3	2.39	0.48
2:R:188:PRO:HG2	2:R:191:MET:HG3	1.96	0.47
2:R:138:ILE:HG21	2:R:218:VAL:HG13	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:210:GLN:NE2	2:R:210:GLN:N	2.62	0.46
2:R:140:GLU:CG	2:R:222:ARG:HH12	2.15	0.46
2:R:188:PRO:HG2	2:R:191:MET:CG	2.45	0.46
2:R:136:VAL:HG12	2:R:146:VAL:HG21	1.98	0.46
2:R:204:ILE:HD13	2:R:209:TYR:HE2	1.81	0.46
2:R:302:GLN:HA	2:R:322:VAL:O	2.15	0.46
2:R:187:ILE:CG1	2:R:188:PRO:HD2	2.47	0.45
2:R:199:PHE:CD2	2:R:210:GLN:HG3	2.51	0.45
2:R:251:GLU:HG3	2:R:254:VAL:CG2	2.45	0.45
2:R:302:GLN:HE22	2:R:323:ARG:HH11	1.65	0.45
1:A:38:THR:C	1:A:40:PRO:HD3	2.37	0.45
2:R:302:GLN:NE2	2:R:323:ARG:HD2	2.32	0.45
2:R:223:ILE:HA	2:R:250:THR:HG22	1.99	0.44
2:R:289:LEU:HG	2:R:290:SER:N	2.31	0.44
2:R:164:ARG:HA	2:R:165:TYR:HA	1.72	0.44
2:R:164:ARG:HB3	2:R:165:TYR:CD2	2.52	0.44
2:R:142:LYS:C	2:R:144:LYS:H	2.21	0.44
2:R:161:LEU:HD12	2:R:199:PHE:C	2.38	0.44
2:R:323:ARG:HE	2:R:325:HIS:CD2	2.36	0.44
2:R:149:PRO:HG2	2:R:214:TYR:CZ	2.53	0.43
2:R:138:ILE:CG2	2:R:218:VAL:HG13	2.48	0.43
2:R:170:PHE:N	2:R:170:PHE:CD2	2.87	0.43
2:R:163:ALA:C	2:R:164:ARG:HG3	2.39	0.42
2:R:272:LEU:O	2:R:273:VAL:HG23	2.20	0.42
2:R:240:GLU:O	2:R:297:VAL:HG13	2.19	0.42
2:R:132:GLN:HE21	2:R:133:HIS:H	1.67	0.42
1:A:33:VAL:HG12	1:A:34:PRO:O	2.20	0.42
2:R:286:LYS:HE2	2:R:288:PHE:CZ	2.55	0.41
2:R:250:THR:HG21	2:R:256:ILE:HD11	2.02	0.41
2:R:313:LEU:HD12	2:R:314:MET:N	2.35	0.41
2:R:241:LYS:HG3	2:R:242:LEU:H	1.84	0.41
2:R:143:ASN:HA	2:R:190:TYR:CD2	2.53	0.41
2:R:197:MET:HE3	2:R:213:MET:HG3	2.02	0.41
2:R:242:LEU:HD23	2:R:242:LEU:C	2.41	0.41
2:R:237:SER:HA	2:R:325:HIS:O	2.21	0.41
2:R:142:LYS:O	2:R:143:ASN:HB3	2.21	0.40
2:R:250:THR:HB	2:R:254:VAL:HG21	2.03	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	92/137 (67%)	82 (89%)	9 (10%)	1 (1%)	16	56
2	R	181/424 (43%)	163 (90%)	16 (9%)	2 (1%)	16	56
All	All	273/561 (49%)	245 (90%)	25 (9%)	3 (1%)	16	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLY
2	R	251	GLU
2	R	232	HIS

### 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	80/126 (64%)	74 (92%)	6 (8%)	15	49
2	R	150/379 (40%)	140 (93%)	10 (7%)	18	54
All	All	230/505 (46%)	214 (93%)	16 (7%)	16	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	26	CYS
1	A	29	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	44	SER
1	A	92	GLN
1	A	95	SER
2	R	145	THR
2	R	156	ASN
2	R	157	LEU
2	R	185	PHE
2	R	209	TYR
2	R	210	GLN
2	R	228	LEU
2	R	232	HIS
2	R	289	LEU
2	R	299	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
2	R	132	GLN
2	R	141	ASN
2	R	210	GLN
2	R	302	GLN
2	R	318	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 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	94/137 (68%)	0.08	0	100 100	76, 100, 125, 140	0
2	R	187/424 (44%)	0.09	3 (1%)	72 59	74, 125, 159, 176	0
All	All	281/561 (50%)	0.09	3 (1%)	80 69	74, 115, 156, 176	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	244	LEU	2.7
2	R	152	GLY	2.1
2	R	329	PHE	2.1

### 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 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.