

wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 03:49 PM EDT

PDB ID : 3V2A

Title: VEGFR-2/VEGF-A COMPLEX STRUCTURE

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Deposited on : 2011-12-12

Resolution : 3.20 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS : 2.36.1

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)

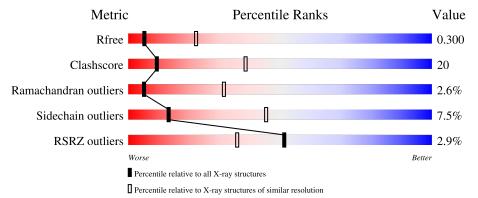
Validation Pipeline (wwPDB-VP) : 2.36.1

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 3.20 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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 <=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				Qual	ity of chain			
1	R	772	13%	10%			76%	_		
2	A	134	2%	45	5%		24%		29%	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2114 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 Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
1	R	185	Total 1369	C 879	N 216	O 264	S 10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	765	ARG	-	expression tag	UNP P35968
R	766	THR	-	expression tag	UNP P35968
R	767	HIS	-	expression tag	UNP P35968
R	768	HIS	-	expression tag	UNP P35968
R	769	HIS	-	expression tag	UNP P35968
R	770	HIS	-	expression tag	UNP P35968
R	771	HIS	-	expression tag	UNP P35968
R	772	HIS	-	expression tag	UNP P35968

• Molecule 2 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
2	Δ	95	Total	С	N	О	S	0	0	0
	Λ	90	745	468	122	143	12		U	U

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP P15692
A	-11	GLU	-	expression tag	UNP P15692
A	-10	PHE	-	expression tag	UNP P15692
A	-9	GLY	-	expression tag	UNP P15692
A	-8	SER	-	expression tag	UNP P15692
A	-7	HIS	-	expression tag	UNP P15692
A	-6	HIS	-	expression tag	UNP P15692
A	-5	HIS	-	expression tag	UNP P15692

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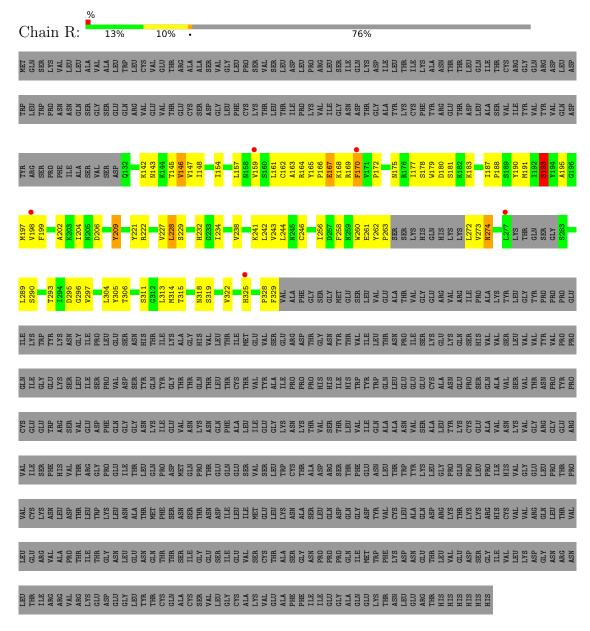
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P15692
A	-3	HIS	-	expression tag	UNP P15692
A	-2	HIS	-	expression tag	UNP P15692
A	-1	GLY	-	expression tag	UNP P15692
A	0	SER	-	expression tag	UNP P15692
A	115	ASN	-	expression tag	UNP P15692
A	116	CYS	-	expression tag	UNP P15692
A	117	ASP	-	expression tag	UNP P15692
A	118	LYS	_	expression tag	UNP P15692
A	119	PRO	-	expression tag	UNP P15692
A	120	ARG	-	expression tag	UNP P15692
A	121	ARG	_	expression tag	UNP P15692



3 Residue-property plots (i)

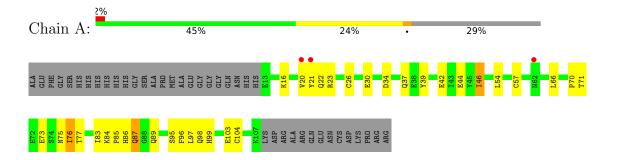
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Vascular endothelial growth factor receptor 2



• Molecule 2: Vascular endothelial growth factor A







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	80.97Å 80.97Å 332.06Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.61 - 3.20	Depositor
Resolution (A)	68.61 - 3.20	EDS
% Data completeness	98.7 (68.61-3.20)	Depositor
(in resolution range)	98.7 (68.61-3.20)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.16 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
D D.	0.244 , 0.300	Depositor
R, R_{free}	0.247 , 0.300	DCC
R_{free} test set	540 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 113.5	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2114	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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	$\mathbf{lengths}$	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	R	0.28	0/1397	0.49	0/1909	
2	A	0.30	0/763	0.46	0/1035	
All	All	0.29	0/2160	0.48	0/2944	

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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	R	1369	0	1272	61	0
2	A	745	0	676	22	0
All	All	2114	0	1948	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.

The worst 5 of 80 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:R:143:ASN:HA	1:R:190:TYR:CD2	2.05	0.91
1:R:179:TRP:CH2	1:R:181:SER:HA	2.18	0.79

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\begin{subarray}{c} \begin{subarray}{c} \begi$
2:A:73:GLU:HB3	2:A:97:LEU:HD11	1.66	0.75
1:R:261:GLU:HB3	1:R:306:THR:HB	1.67	0.74
1:R:274:ASN:HB3	1:R:290:SER:HA	1.69	0.74

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	d Favoured Allow		Outliers	Percentiles	
1	R	179/772 (23%)	144 (80%)	29 (16%)	6 (3%)	3	24
2	A	93/134 (69%)	83 (89%)	9 (10%)	1 (1%)	14	51
All	All	272/906 (30%)	227 (84%)	38 (14%)	7 (3%)	5	31

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	142	LYS
1	R	175	ASN
2	A	26	CYS
1	R	167	GLU
1	R	206	ASP

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	R	145/691 (21%)	135 (93%)	10 (7%)	15	49	
2	A	83/120 (69%)	76 (92%)	7 (8%)	11	39	
All	All	228/811 (28%)	211 (92%)	17 (8%)	13	45	

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	76	ILE
2	A	89	GLN
1	R	274	ASN
1	R	289	LEU
1	R	318	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	89	GLN
2	A	98	GLN
2	A	99	HIS
1	R	210	GLN
1	R	132	GLN

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 monosaccharides 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^{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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		>2	$OWAB(Å^2)$	Q < 0.9
1	R	185/772~(23%)	0.29	5 (2%)	54	39	86, 134, 176, 192	0
2	A	95/134 (70%)	0.43	3 (3%)	47	31	77, 106, 129, 153	0
All	All	280/906 (30%)	0.33	8 (2%)	51	36	77, 121, 174, 192	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	170	PHE	3.3
1	R	325	HIS	3.1
1	R	159	VAL	3.1
2	A	21	TYR	2.6
2	A	62	ASN	2.5

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 monosaccharides 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.

