Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 01:26 PM EDT

PDB ID	:	1TZI
Title	:	Crystal Structure of the Fab YADS2 Complexed with h-VEGF
Authors	:	Fellouse, F.A.; Wiesmann, C.; Sidhu, S.S.
Deposited on	:	2004-07-10
Resolution	:	2.80 Å(reported)

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

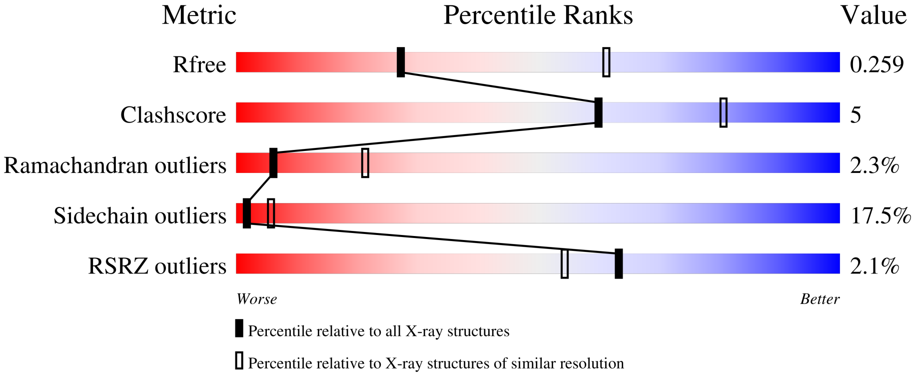
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

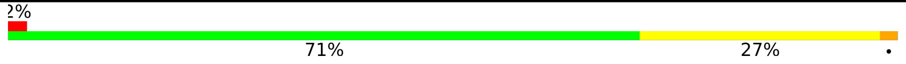
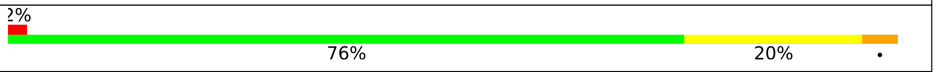
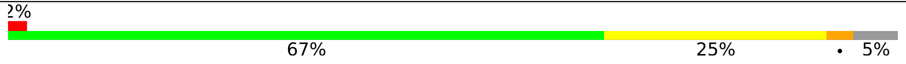
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	Quality of chain
1	A	214	
2	B	222	
3	V	102	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4077 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 Fab YADS2 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1645	1030	271	338	6	0	0	0

- Molecule 2 is a protein called Fab YADS2 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	222	1645	1040	271	328	6	0	0	0

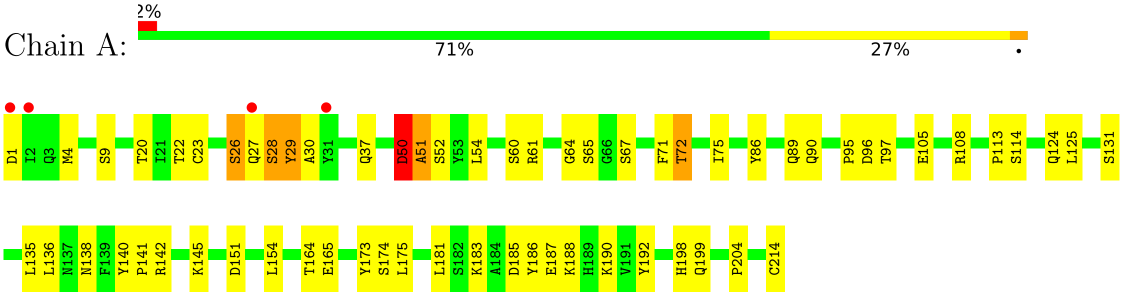
- Molecule 3 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	V	97	787	493	132	149	13	0	0	0

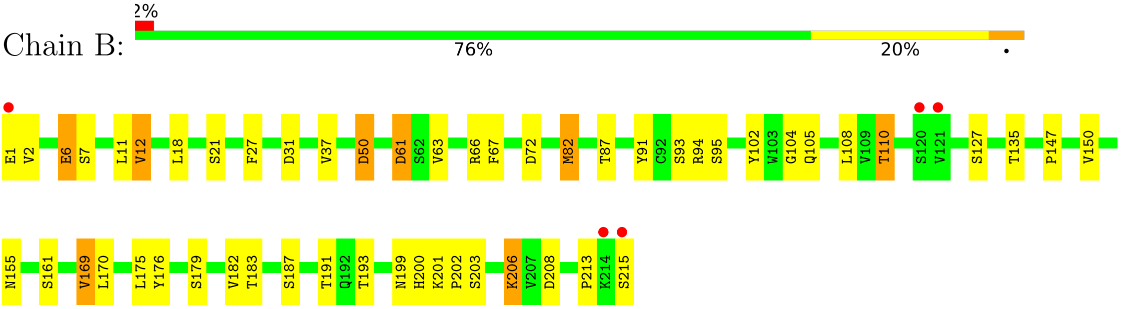
3 Residue-property plots ⓘ

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.

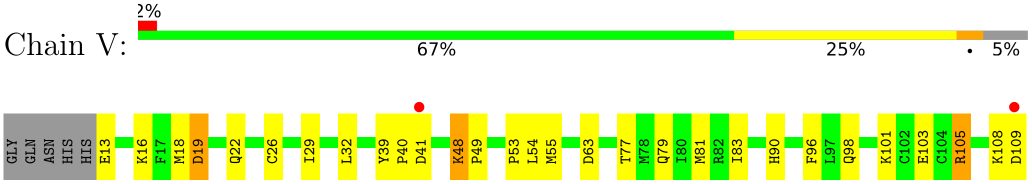
- Molecule 1: Fab YADS2 Light Chain



- Molecule 2: Fab YADS2 Heavy Chain



- Molecule 3: Vascular endothelial growth factor A



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	96.50Å 149.59Å 117.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.80) 97.6 (29.56-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.218 , 0.254 0.220 , 0.259	Depositor DCC
R_{free} test set	1024 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.949	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.2	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	0.94	EDS
Total number of atoms	4077	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.46	0/1682	0.77	3/2284 (0.1%)
2	B	0.54	0/1686	0.80	5/2302 (0.2%)
3	V	0.48	0/805	0.76	2/1084 (0.2%)
All	All	0.50	0/4173	0.78	10/5670 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	V	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	19	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	1	ASP	CB-CG-OD2	6.04	123.74	118.30
2	B	72	ASP	CB-CG-OD2	5.87	123.58	118.30
2	B	208	ASP	CB-CG-OD2	5.86	123.57	118.30
2	B	31	ASP	CB-CG-OD2	5.67	123.40	118.30
3	V	41	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	50	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	50	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	61	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	151	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	V	39	TYR	Peptide

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	1645	0	1582	18	0
2	B	1645	0	1598	14	0
3	V	787	0	751	5	0
All	All	4077	0	3931	37	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 (37) 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:200:HIS:HD2	2:B:203:SER:OG	1.66	0.78
2:B:147:PRO:O	2:B:200:HIS:HE1	1.89	0.56
2:B:6:GLU:OE1	2:B:104:GLY:HA3	2.06	0.55
2:B:200:HIS:CD2	2:B:203:SER:OG	2.55	0.54
1:A:95:PRO:C	1:A:97:THR:H	2.11	0.53
1:A:50:ASP:O	1:A:51:ALA:HB3	2.09	0.53
2:B:87:THR:HG23	2:B:110:THR:HA	1.90	0.52
1:A:65:SER:O	1:A:71:PHE:HA	2.11	0.51
1:A:136:LEU:HD12	1:A:136:LEU:N	2.25	0.51
2:B:2:VAL:HG11	2:B:102:TYR:CD1	2.46	0.51
1:A:138:ASN:HA	1:A:173:TYR:O	2.12	0.50
2:B:199:ASN:ND2	2:B:206:LYS:HG3	2.27	0.49
1:A:37:GLN:HG3	1:A:86:TYR:CE2	2.48	0.48
1:A:64:GLY:HA2	1:A:72:THR:O	2.13	0.48
2:B:201:LYS:N	2:B:202:PRO:CD	2.77	0.47
2:B:108:LEU:HD13	2:B:110:THR:HG22	1.97	0.46
2:B:67:PHE:CE1	2:B:82:MET:HB3	2.50	0.46
1:A:140:TYR:CG	1:A:141:PRO:HA	2.51	0.46
1:A:183:LYS:O	1:A:187:GLU:HG2	2.17	0.44
2:B:27:PHE:CE2	2:B:94:ARG:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLN:HE22	1:A:131:SER:CB	2.31	0.43
2:B:12:VAL:HG11	2:B:18:LEU:HG	2.01	0.42
1:A:61:ARG:O	1:A:75:ILE:HA	2.19	0.42
3:V:54:LEU:HD21	3:V:96:PHE:HB2	2.01	0.42
2:B:169:VAL:O	2:B:176:TYR:HA	2.20	0.42
1:A:50:ASP:O	1:A:51:ALA:CB	2.67	0.41
1:A:28:SER:O	1:A:29:TYR:O	2.39	0.41
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.55	0.41
1:A:186:TYR:CD1	1:A:192:TYR:CZ	3.09	0.41
3:V:32:LEU:HD23	3:V:53:PRO:HA	2.03	0.41
3:V:48:LYS:HG3	3:V:83:ILE:HD11	2.03	0.41
2:B:37:VAL:O	2:B:91:TYR:HB2	2.21	0.41
3:V:103:GLU:OE1	3:V:105:ARG:HD3	2.21	0.41
1:A:140:TYR:CD2	1:A:141:PRO:HA	2.56	0.40
1:A:95:PRO:C	1:A:97:THR:N	2.74	0.40
1:A:136:LEU:N	1:A:136:LEU:CD1	2.85	0.40
3:V:48:LYS:HA	3:V:49:PRO:HA	1.98	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	212/214 (99%)	187 (88%)	18 (8%)	7 (3%)	4	13
2	B	220/222 (99%)	206 (94%)	12 (6%)	2 (1%)	17	46
3	V	95/102 (93%)	85 (90%)	7 (7%)	3 (3%)	4	13
All	All	527/538 (98%)	478 (91%)	37 (7%)	12 (2%)	6	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	TYR
1	A	50	ASP
1	A	96	ASP
2	B	213	PRO
3	V	40	PRO
1	A	51	ALA
3	V	26	CYS
1	A	204	PRO
3	V	63	ASP
1	A	26	SER
1	A	30	ALA
2	B	155	ASN

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	186/186 (100%)	153 (82%)	33 (18%)	2	5
2	B	179/179 (100%)	149 (83%)	30 (17%)	2	6
3	V	92/96 (96%)	75 (82%)	17 (18%)	1	5
All	All	457/461 (99%)	377 (82%)	80 (18%)	2	6

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	9	SER
1	A	20	THR
1	A	22	THR
1	A	23	CYS
1	A	26	SER
1	A	27	GLN
1	A	28	SER
1	A	52	SER
1	A	54	LEU
1	A	60	SER

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Mol	Chain	Res	Type
1	A	67	SER
1	A	72	THR
1	A	89	GLN
1	A	90	GLN
1	A	105	GLU
1	A	108	ARG
1	A	114	SER
1	A	125	LEU
1	A	135	LEU
1	A	142	ARG
1	A	145	LYS
1	A	154	LEU
1	A	164	THR
1	A	165	GLU
1	A	174	SER
1	A	175	LEU
1	A	181	LEU
1	A	185	ASP
1	A	188	LYS
1	A	190	LYS
1	A	199	GLN
1	A	214	CYS
2	B	1	GLU
2	B	6	GLU
2	B	7	SER
2	B	11	LEU
2	B	12	VAL
2	B	21	SER
2	B	50	ASP
2	B	61	ASP
2	B	63	VAL
2	B	66	ARG
2	B	82	MET
2	B	93	SER
2	B	95	SER
2	B	105	GLN
2	B	110	THR
2	B	127	SER
2	B	135	THR
2	B	150	VAL
2	B	161	SER
2	B	169	VAL

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Mol	Chain	Res	Type
2	B	170	LEU
2	B	175	LEU
2	B	179	SER
2	B	182	VAL
2	B	183	THR
2	B	187	SER
2	B	191	THR
2	B	193	THR
2	B	206	LYS
2	B	215	SER
3	V	13	GLU
3	V	16	LYS
3	V	18	MET
3	V	19	ASP
3	V	22	GLN
3	V	29	ILE
3	V	48	LYS
3	V	55	MET
3	V	77	THR
3	V	79	GLN
3	V	81	MET
3	V	90	HIS
3	V	98	GLN
3	V	101	LYS
3	V	105	ARG
3	V	108	LYS
3	V	109	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	124	GLN
1	A	147	GLN
2	B	3	GLN
2	B	200	HIS
3	V	62	ASN
3	V	98	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	214/214 (100%)	-0.23	4 (1%)	66	59	26, 52, 72, 146	0
2	B	222/222 (100%)	-0.35	5 (2%)	60	51	18, 39, 61, 95	0
3	V	97/102 (95%)	-0.20	2 (2%)	63	54	32, 54, 89, 100	0
All	All	533/538 (99%)	-0.27	11 (2%)	63	54	18, 47, 74, 146	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	TYR	6.8
3	V	41	ASP	6.4
1	A	2	ILE	4.1
1	A	1	ASP	4.0
1	A	27	GLN	4.0
2	B	1	GLU	3.2
2	B	215	SER	3.1
3	V	109	ASP	2.5
2	B	120	SER	2.3
2	B	121	VAL	2.2
2	B	214	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides 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.