



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:22 AM GMT

PDB ID : 4IF8
Title : Structure Of Vaspin
Authors : Kuettner, E.B.; Strater, N.; Heiker, J.T.; Kloting, N.; Kovacs, P.; Schultz, S.;
Kern, M.; Stumvoll, M.; Bluher, M.; Beck-Sickinger, A.G.
Deposited on : 2012-12-14
Resolution : 2.08 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

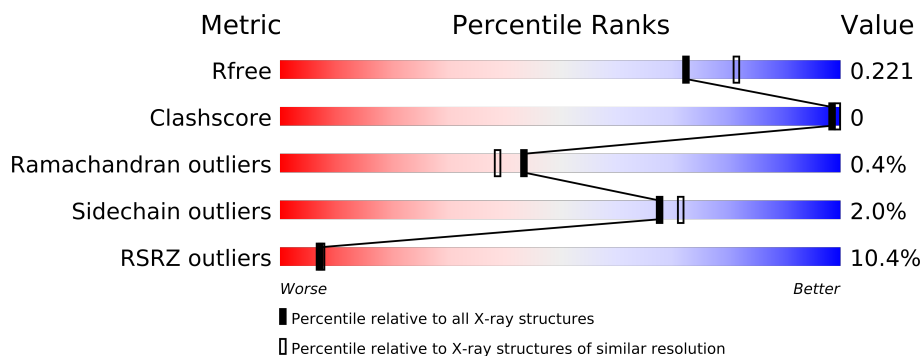
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.08 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}	66092	3396 (2.10-2.06)
Clashscore	79885	4085 (2.10-2.06)
Ramachandran outliers	78287	4045 (2.10-2.06)
Sidechain outliers	78261	4046 (2.10-2.06)
RSRZ outliers	66119	3397 (2.10-2.06)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	414	
1	B	414	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	501	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6275 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Serpin A12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	7	0
			3008	1938	509	547	14			
1	B	361	Total	C	N	O	S	0	1	0
			2946	1905	498	531	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q8IW75
A	2	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	3	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	4	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	5	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	6	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	7	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	8	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	9	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	10	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	11	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	12	SER	-	EXPRESSION TAG	UNP Q8IW75
A	13	SER	-	EXPRESSION TAG	UNP Q8IW75
A	14	GLY	-	EXPRESSION TAG	UNP Q8IW75
A	15	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	16	ILE	-	EXPRESSION TAG	UNP Q8IW75
A	17	GLU	-	EXPRESSION TAG	UNP Q8IW75
A	18	GLY	-	EXPRESSION TAG	UNP Q8IW75
A	19	ARG	-	EXPRESSION TAG	UNP Q8IW75
A	20	HIS	-	EXPRESSION TAG	UNP Q8IW75
A	21	MET	-	EXPRESSION TAG	UNP Q8IW75
B	1	GLY	-	EXPRESSION TAG	UNP Q8IW75
B	2	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	3	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	4	HIS	-	EXPRESSION TAG	UNP Q8IW75

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	6	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	7	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	8	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	9	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	10	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	11	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	12	SER	-	EXPRESSION TAG	UNP Q8IW75
B	13	SER	-	EXPRESSION TAG	UNP Q8IW75
B	14	GLY	-	EXPRESSION TAG	UNP Q8IW75
B	15	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	16	ILE	-	EXPRESSION TAG	UNP Q8IW75
B	17	GLU	-	EXPRESSION TAG	UNP Q8IW75
B	18	GLY	-	EXPRESSION TAG	UNP Q8IW75
B	19	ARG	-	EXPRESSION TAG	UNP Q8IW75
B	20	HIS	-	EXPRESSION TAG	UNP Q8IW75
B	21	MET	-	EXPRESSION TAG	UNP Q8IW75

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total 214	O 214	0	0
3	B	97	Total 97	O 97	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.55Å 152.10Å 61.45Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	29.80 – 2.08 29.82 – 2.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.80-2.08) 100.0 (29.82-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.08Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.197 , 0.221 0.201 , 0.221	Depositor DCC
R_{free} test set	1069 reflections (1.49%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 72715 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6275	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.53	0/3105	0.67	0/4176
1	B	0.44	0/3012	0.61	0/4053
All	All	0.49	0/6117	0.64	0/8229

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3008	0	0	1	0
1	B	2946	0	0	2	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	214	0	0	1	0
3	B	97	0	0	0	0
All	All	6275	0	0	3	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

All (3) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:ARG:NH2	3:A:692:HOH:O	2.48	0.46
1:B:166:ASN:ND2	1:B:172:MET:SD	2.93	0.41

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	370/414 (89%)	361 (98%)	7 (2%)	2 (0%)	38	32
1	B	356/414 (86%)	343 (96%)	12 (3%)	1 (0%)	50	48
All	All	726/828 (88%)	704 (97%)	19 (3%)	3 (0%)	43	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	HIS
1	A	267	ASN
1	B	267	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	339/369 (92%)	334 (98%)	5 (2%)	76	81
1	B	328/369 (89%)	320 (98%)	8 (2%)	61	64
All	All	667/738 (90%)	654 (98%)	13 (2%)	68	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	MET
1	A	161	GLU
1	A	294	ARG
1	A	344	HIS
1	A	401	SER
1	B	168	GLN
1	B	188	LYS
1	B	211	ARG
1	B	243	ARG
1	B	260	LEU
1	B	269	THR
1	B	289	VAL
1	B	385	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	501	-	4,4,4	0.66	0	6,6,6	0.35	0
2	SO4	B	501	-	4,4,4	0.19	0	6,6,6	0.08	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	367/414 (88%)	-0.03	10 (2%)	52 56	18, 34, 63, 92	0
1	B	361/414 (87%)	0.68	65 (18%)	2 2	23, 59, 122, 143	0
All	All	728/828 (87%)	0.33	75 (10%)	7 8	18, 43, 118, 143	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	PHE	8.0
1	B	382	LEU	7.3
1	B	221	ASN	5.4
1	B	232	LYS	5.0
1	B	251	TYR	5.0
1	A	378	MET	5.0
1	B	222	VAL	4.8
1	B	37	GLN	4.8
1	B	246	ILE	4.6
1	B	230	LEU	4.6
1	B	218	PHE	4.5
1	B	244	SER	4.5
1	B	215	LYS	4.2
1	B	298	LEU	4.1
1	B	290	ASP	3.9
1	B	301	ARG	3.9
1	B	303	VAL	3.8
1	B	254	LYS	3.8
1	B	305	ASP	3.6
1	B	36	VAL	3.6
1	B	392	LEU	3.6
1	B	128	GLN	3.5
1	A	232	LYS	3.2
1	A	233	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	247	TYR	3.2
1	B	285	LYS	3.2
1	B	236	VAL	3.1
1	B	237	LYS	3.1
1	B	297	THR	3.0
1	B	234	SER	3.0
1	B	253	ASP	3.0
1	B	306	VAL	2.8
1	A	126	LYS	2.8
1	B	35	GLU	2.8
1	B	277	GLU	2.8
1	B	235	SER	2.7
1	B	302	ARG	2.7
1	B	412	ILE	2.6
1	B	216	HIS	2.6
1	A	399	ILE	2.6
1	B	217	GLU	2.5
1	B	223	THR	2.5
1	B	270	ALA	2.5
1	B	224	LYS	2.5
1	B	219	ASP	2.5
1	A	402	VAL	2.5
1	B	365	THR	2.4
1	B	233	ASN	2.4
1	B	78	SER	2.4
1	B	220	PRO	2.4
1	B	66	TYR	2.4
1	B	394	ILE	2.4
1	B	282	HIS	2.4
1	B	129	ASP	2.3
1	A	289	VAL	2.3
1	B	255	LEU	2.3
1	B	271	ILE	2.3
1	B	299	LEU	2.3
1	B	391	LEU	2.2
1	B	225	GLU	2.2
1	B	256	SER	2.2
1	B	383	VAL	2.2
1	B	209	PHE	2.2
1	A	208	ILE	2.2
1	B	65	PHE	2.2
1	B	77	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	126	LYS	2.1
1	B	229	PHE	2.1
1	B	403	LEU	2.1
1	A	79	ILE	2.1
1	A	394	ILE	2.1
1	B	79	ILE	2.1
1	B	363	ARG	2.1
1	B	82	ALA	2.0
1	B	289	VAL	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	501	5/5	0.36	3.52	66,70,71,71	5
2	SO4	A	501	5/5	0.10	-0.06	60,63,65,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.