



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1SDD / pdb_00001sdd
Title : Crystal Structure of Bovine Factor Vai
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Deposited on : 2004-02-13
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

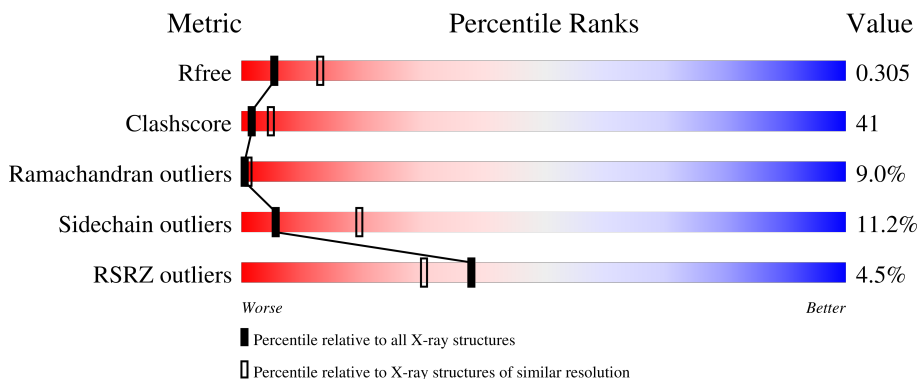
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	306	
2	B	647	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	2187	X	-	-	-
3	NAG	B	2189	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7271 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.

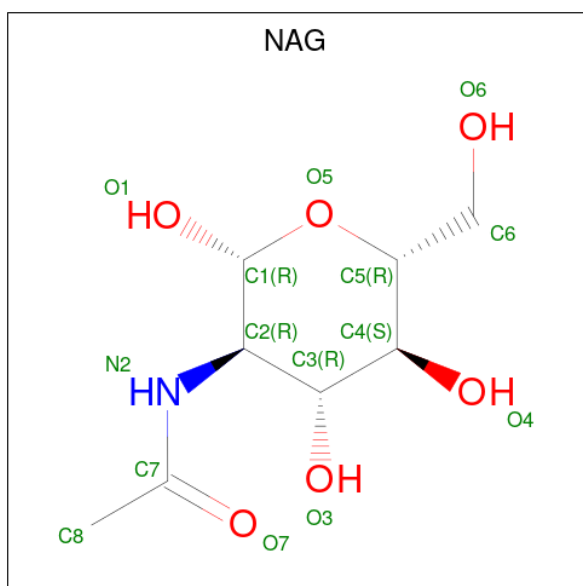
- Molecule 1 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2132	1366	356	398	12	0	0	0

- Molecule 2 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	601	4878	3127	840	888	23	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cu	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	142	Total	O	0	0
			142	142		

SER	TRP	ARG	ARG	ALA	SER	SER	GLU	VAL	LYS	N1760	H1765	A1766	I1767	M1770	I1771	N1773	M1773	L1774	Y1780	E1781	Q1782	E1783	W1784	V1785	R1786	L1787	H1788	L1789	L1790	M1791	L1792	G1793	G1794	D1797	I1798	V1801	H1802	F1803	H1804	G1805	Q1806	T1807	L1808	L1809	E1810	M1811	G1812	T1813	Q1814	Q1815	H1816	Q1817	L1818	G1819																																												
V1820	W1821	P1822	L1823	L1831	E1832	M1833	K1834	A1835	S1836	X1837	L1843	D1844	T1845	E1846	V1847	G1848	E1849	I1850	Q1851	R1852	A1853	G1854	M1855	Q1856	T1857	L1860	L1861	R1864	K1867	M1868	F1869	M1870	G1871	L1872	L1876	I1877	E1886	F1887	W1888	G1889	Y1890	W1891	E1892	P1893	K1894	L1895	A1896	D1897	L1898	M1899	M1900	Y1904	M1905	A1906	K1911	L1912	S1913	T1914	E1915	F1916	M1917	P1918	F1919	P1920	W1921	D1925	M1926	Q1927	K1928	L1931	I1935	Q1938	G1939	H1942	Y1943	L1944	K1945	P1946	T1950	E1951	D1959	R1960	W1963	R1964	I1965	F1966	K1967	G1968	M1969	S1970	M1973	V1974	E1988	I1991	D1992	P1993	R1998	Y1999
I2000	R2001	I2002	S2003	P2004	Y2008	M2009	K2010	P2011	A2012	L2013	R2014	L2015	E2016	L2017	Q2018	G2019	V2022	C2025	S2026	T2027	G2030	M2031	G2034	K2035	L2036	E2037	N2038	K2039	Q2040	I2041	S2044	S2045	F2046	K2047	K2048	S2049	W2050	W2051	G2052	N2053	Y2054	W2055	F2056	P2057	F2058	L2059	L2062	N2063	R2067	N2069																																																
A2070	W2071	Q2072	A2073	K2074	A2075	W2076	N2077	R2078	W2081	L2082	Q2083	L2084	D2085	L2086	L2087	K2088	L2089	K2090	K2091	L2092	T2093	V2096	T2097	Q2098	G2099	C2100	K2101	E2106	R2107	Y2108	V2109	K2110	S2111	Y2112	T2113	D2118	T2121	D2122	W2123	R2124	P2125	Y2126	R2127	E2128	R2132	N2140	N2141	W2142	W2143	R2144	G2145	H2146																																														
V2147	K2148	F2151	N2152	P2153	P2154	I2155	I2160	R2161	I2162	T2166	W2167	N2168	Q2169	S2170	I2171	A2172	L2173	R2174	L2175	F2178	G2179	C2180	D2181	M2182	TVR																																																																									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.37Å 86.56Å 229.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.80) 90.5 (30.00-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.296 0.248 , 0.305	Depositor DCC
R_{free} test set	918 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CA, NAG

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	0.40	0/2188	0.91	8/2960 (0.3%)
2	B	0.55	0/5012	1.02	31/6792 (0.5%)
All	All	0.51	0/7200	0.99	39/9752 (0.4%)

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
2	B	0	1

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	2014	ARG	N-CA-C	-9.03	93.53	108.34
2	B	1556	TYR	N-CA-C	-8.98	98.75	110.33
2	B	2143	VAL	N-CA-C	8.96	119.77	110.72
2	B	1837	LYS	CA-C-N	8.31	128.81	119.92
2	B	1837	LYS	C-N-CA	8.31	128.81	119.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1890	TYR	Sidechain

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	2132	0	2074	213	0
2	B	4878	0	4767	372	0
3	A	28	0	26	3	0
3	B	42	0	39	11	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	47	0	0	1	0
6	B	142	0	0	3	0
All	All	7271	0	6906	578	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 41.

The worst 5 of 578 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:1992:ASP:HB3	2:B:1993:PRO:HD3	1.13	1.13
2:B:2152:ASN:HB2	2:B:2153:PRO:HD3	1.22	1.10
2:B:1721:MET:HG3	2:B:1786:ARG:HH22	1.01	1.08
2:B:1914:THR:HB	2:B:1920:PRO:HD2	1.38	1.05
1:A:264:THR:HG21	2:B:1822:PRO:HG3	1.44	0.98

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	Favoured	Allowed	Outliers	Percentiles	
1	A	260/306 (85%)	178 (68%)	46 (18%)	36 (14%)	0	0
2	B	593/647 (92%)	479 (81%)	73 (12%)	41 (7%)	1	2
All	All	853/953 (90%)	657 (77%)	119 (14%)	77 (9%)	0	1

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	A	60	PRO
1	A	180	GLU
1	A	187	PHE
1	A	206	VAL

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	A	233/269 (87%)	205 (88%)	28 (12%)	5	17
2	B	526/570 (92%)	469 (89%)	57 (11%)	6	21
All	All	759/839 (90%)	674 (89%)	85 (11%)	6	19

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1887	PHE
2	B	2067	ARG
2	B	1895	LEU
2	B	1918	PRO
2	B	2112	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1815	GLN

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Mol	Chain	Res	Type
2	B	2168	ASN
2	B	1905	ASN
2	B	2076	ASN
2	B	1851	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
3	NAG	B	2188	2	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
3	NAG	A	2186	1	14,14,15	0.53	0	17,19,21	0.70	0
3	NAG	B	2187	2	14,14,15	0.61	0	17,19,21	0.79	0
3	NAG	B	2189	2	14,14,15	0.66	0	17,19,21	0.68	0
3	NAG	A	2185	1	14,14,15	0.67	0	17,19,21	0.70	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
3	NAG	B	2188	2	-	2/6/23/26	0/1/1/1
3	NAG	A	2186	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2187	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	2189	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	A	2185	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2188	NAG	C2-N2-C7	-2.21	119.94	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	2187	NAG	C1
3	B	2189	NAG	C1

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2185	NAG	C8-C7-N2-C2
3	A	2185	NAG	O7-C7-N2-C2
3	A	2186	NAG	C8-C7-N2-C2
3	A	2186	NAG	O7-C7-N2-C2
3	B	2187	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2188	NAG	4	0
3	B	2187	NAG	4	0
3	B	2189	NAG	3	0
3	A	2185	NAG	3	0

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 [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, 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	268/306 (87%)	0.94	25 (9%) 14 10	48, 89, 127, 136	0
2	B	601/647 (92%)	0.10	14 (2%) 61 51	26, 54, 91, 112	0
All	All	869/953 (91%)	0.36	39 (4%) 38 30	26, 64, 116, 136	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	5.6
2	B	1721	MET	4.4
1	A	217	ILE	3.7
1	A	188	ALA	3.5
1	A	54	THR	3.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	2185	14/15	0.28	0.14	127,128,129,130	0
3	NAG	B	2187	14/15	0.66	0.12	94,98,101,101	0
3	NAG	A	2186	14/15	0.80	0.12	86,88,90,91	0
3	NAG	B	2189	14/15	0.82	0.12	70,72,74,76	0
3	NAG	B	2188	14/15	0.88	0.10	73,74,76,78	0
4	CA	A	2184	1/1	0.92	0.07	68,68,68,68	0
5	CU	B	2190	1/1	0.96	0.09	65,65,65,65	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.