



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:40 PM GMT

PDB ID : 1SDD  
Title : Crystal Structure of Bovine Factor Vai  
Authors : Adams, T.E.; Hockin, M.F.; Mann, K.G.; Everse, S.J.  
Deposited on : 2004-02-13  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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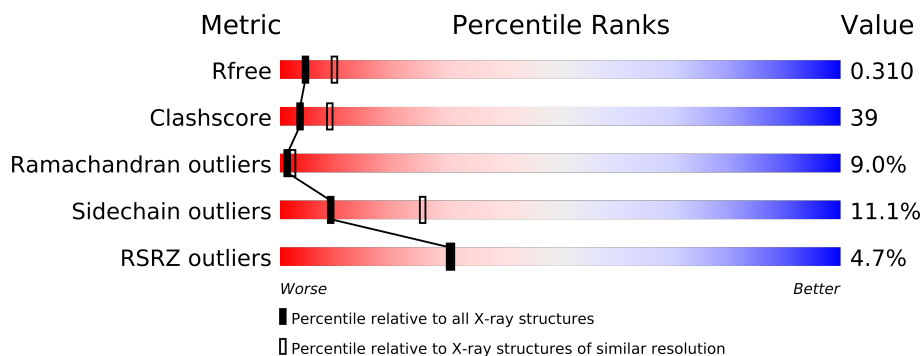
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	306	
2	B	647	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NDG	B	2187	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7271 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.

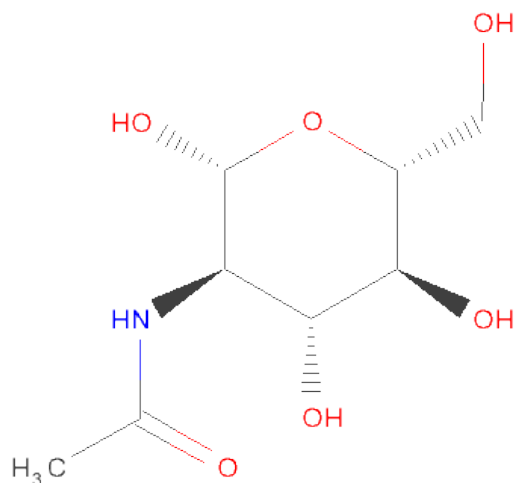
- Molecule 1 is a protein called Coagulation factor V.

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

- Molecule 2 is a protein called Coagulation factor V.

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



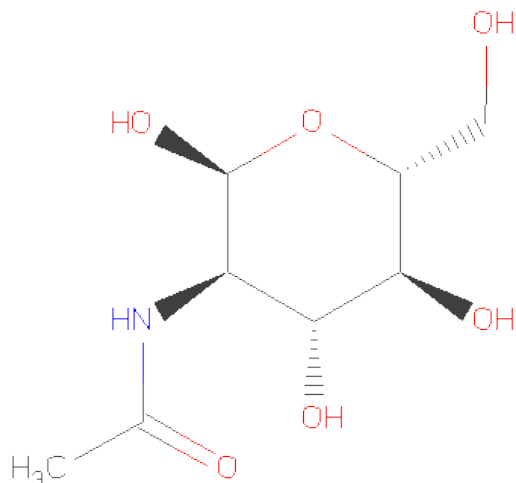
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

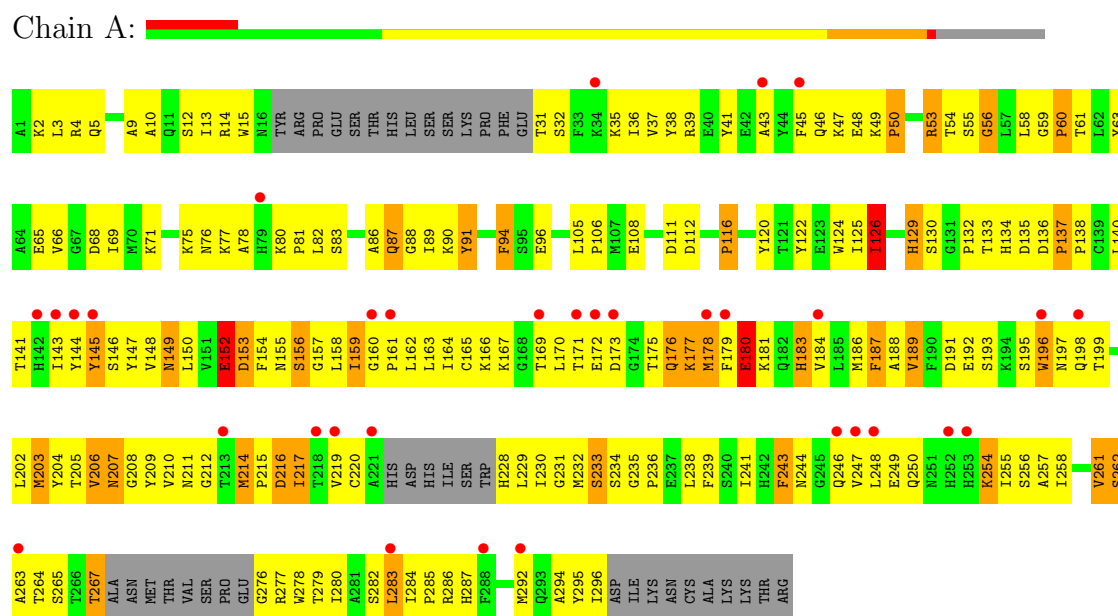
- Molecule 7 is water.

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

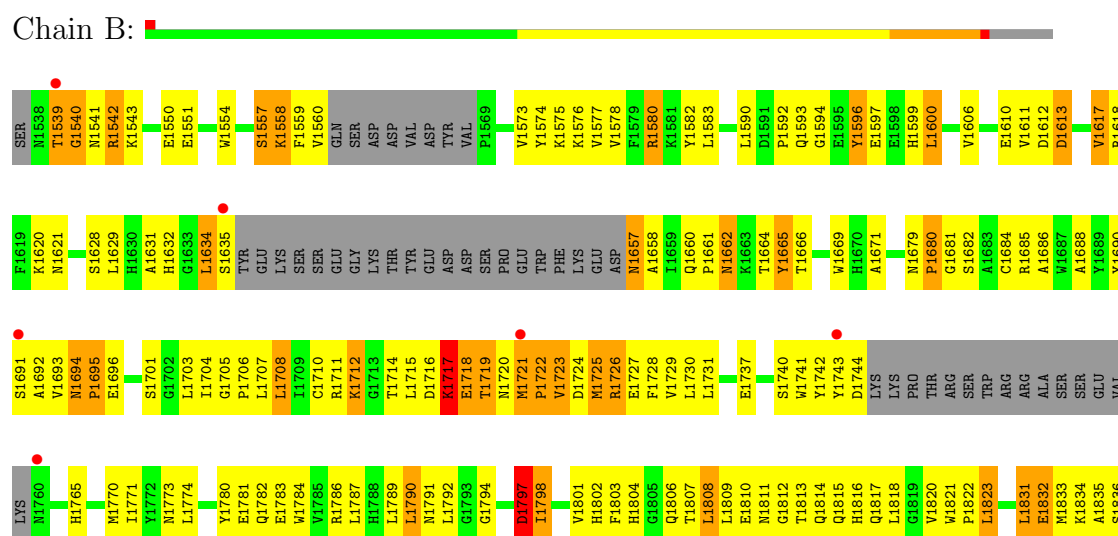
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Coagulation factor V



#### • Molecule 2: Coagulation factor V



L2171	K2088	E2016	P1920	K1837
A2172	I2089	L2017	M1921	
L2173	K2090	Q2018	M1926	L1843
R2174	K2091	G2019	Q1927	D1844
L2175	I2092		K1928	T1845
		V2022		E1846
F2178	V2096		L1931	V1847
G2179	T2097	C2025		G1848
G2180	Q2098	S2026	I1935	E1849
D2181	G2099	T2027		I1850
M2182	C2100		Q1938	Q1851
TYR	K2101	G2030	G1939	R1852
				A1853
	E2106	G2034		G1854
	R2107	K2035	H1942	M1855
	Y2108	I2036	Y1943	Q1856
	V2109	E2037	L1944	
	K2110	N2038	K1945	I1861
	S2111	K2039	P1946	
	Y2112	Q2040		R1864
	T2113		T1950	
		S2044	E1951	K1867
	D2118	S2045		M1868
		F2046	D1959	P1869
	T2121	K2047	R1960	M1870
	D2122	K2048		G1871
	W2123	S2049	W1963	L1872
	K2124	W2050	R1964	
	P2125	W2051	I1965	L1876
	Y2126	G2052	F1966	I1877
	R2127	N2053	K1967	
		Y2054	G1968	E1886
	M2132	W2055	M1969	F1887
			S1970	W1888
	N2140	F2058		G1889
	N2141		N1973	Y1890
	R2142	L2062	V1974	W1891
	V2143	N2063	M1975	E1892
	R2144			P1893
	G2145	K2067	E1988	K1894
	H2146	V2068		L1895
	V2147	N2069	I1991	A1896
	K2148	A2070	D1992	R1897
		W2071	P1993	L1898
		Q2072		M1899
	F2151	A2073	R1998	M1900
	N2152	K2074	Y1999	
	P2153	A2075	I2000	Y1904
	P2154	N2076	R2001	M1905
	I2155	N2077	I2002	A1906
		N2078	S2003	
	I2160	N2079	P2004	K1911
	R2161	Q2080		L1912
	T2162	W2081	Y2008	S1913
		L2082	N2009	T1914
	K2165	Q2083	K2010	T1915
	T2166	F2084	P2011	F1916
	W2167	D2085		M1917
	N2168	L2086	R2014	P1918
	Q2169	L2087	L2015	E1919
	S2170			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.37Å 86.56Å 229.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 28.63 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.80) 90.7 (28.63-2.81)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.252 , 0.296 0.243 , 0.310	Depositor DCC
$R_{free}$ test set	918 reflections (3.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28745 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities 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: CA, NDG, CU, 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	0.35	0/2188	0.60	0/2960
2	B	0.46	0/5012	0.70	2/6792 (0.0%)
All	All	0.43	0/7200	0.67	2/9752 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	1847	VAL	N-CA-C	-6.63	93.11	111.00
2	B	2014	ARG	N-CA-C	-6.47	93.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1890	TYR	Sidechain

### 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	2132	0	2074	198	0
2	B	4878	0	4767	357	0
3	A	28	0	26	3	0
3	B	14	0	13	4	0
4	B	28	0	26	6	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	47	0	0	1	0
7	B	142	0	0	3	0
All	All	7271	0	6906	548	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 39.

The worst 5 of 548 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 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	260/306 (85%)	178 (68%)	46 (18%)	36 (14%)	0 1
2	B	593/647 (92%)	479 (81%)	73 (12%)	41 (7%)	2 4
All	All	853/953 (90%)	657 (77%)	119 (14%)	77 (9%)	1 2

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 ⓘ

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%)	208 (89%)	25 (11%)	10	26
2	B	526/570 (92%)	467 (89%)	59 (11%)	9	25
All	All	759/839 (90%)	675 (89%)	84 (11%)	9	25

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1707	LEU
2	B	1808	LEU
2	B	2140	ASN
2	B	1711	ARG
2	B	1720	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1804	HIS
2	B	1817	GLN
2	B	2083	GLN
2	B	1814	GLN
2	B	1851	GLN

### 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 ⓘ

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	A	2185	1	12,14,15	0.50	0	15,19,21	0.66	0
3	NAG	A	2186	1	12,14,15	0.51	0	15,19,21	0.63	0
4	NDG	B	2187	2	12,14,15	0.51	0	15,19,21	0.65	0
3	NAG	B	2188	2	12,14,15	0.47	0	15,19,21	0.73	0
4	NDG	B	2189	2	12,14,15	0.42	0	15,19,21	0.75	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	A	2185	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2186	1	-	0/6/23/26	0/1/1/1
4	NDG	B	2187	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2188	2	-	0/6/23/26	0/1/1/1
4	NDG	B	2189	2	-	0/6/23/26	0/1/1/1

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, 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	268/306 (87%)	0.70	32 (11%) 5 4	48, 89, 127, 136	0
2	B	601/647 (92%)	-0.14	9 (1%) 70 71	26, 54, 91, 112	0
All	All	869/953 (91%)	0.12	41 (4%) 30 30	26, 64, 116, 136	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	MET	4.5
1	A	218	THR	4.0
1	A	34	LYS	3.9
1	A	145	TYR	3.6
2	B	1760	ASN	3.6

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NDG	B	2187	14/15	0.38	14.21	94,98,101,101	0
3	NAG	A	2185	14/15	0.36	0.29	127,128,129,130	0
4	NDG	B	2189	14/15	0.17	-0.40	70,72,74,76	0
5	CU	B	2190	1/1	0.19	-0.56	65,65,65,65	0
3	NAG	B	2188	14/15	0.14	-1.29	73,74,76,78	0
6	CA	A	2184	1/1	0.09	-1.58	68,68,68,68	0
3	NAG	A	2186	14/15	0.15	-1.63	86,88,90,91	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.