



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:12 am 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

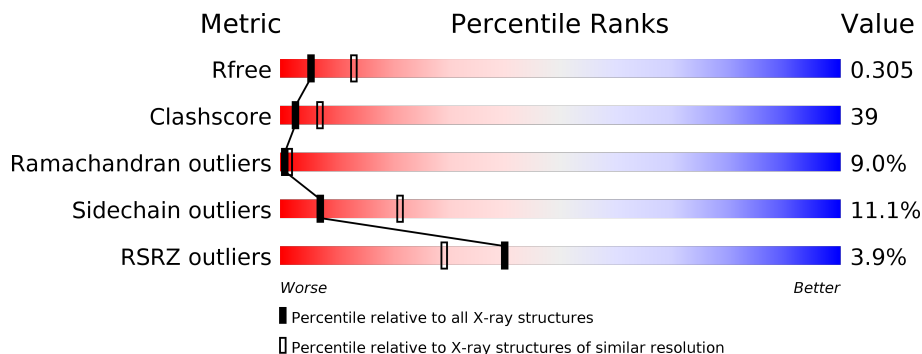
1 Overall quality at a glance

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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>9%</div> <div>26% 49% 11% • 12%</div> </div>
2	B	647	<div> <div>%</div> <div>41% 41% 10% • 7%</div> </div>

2 Entry composition [i](#)

There are 7 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.

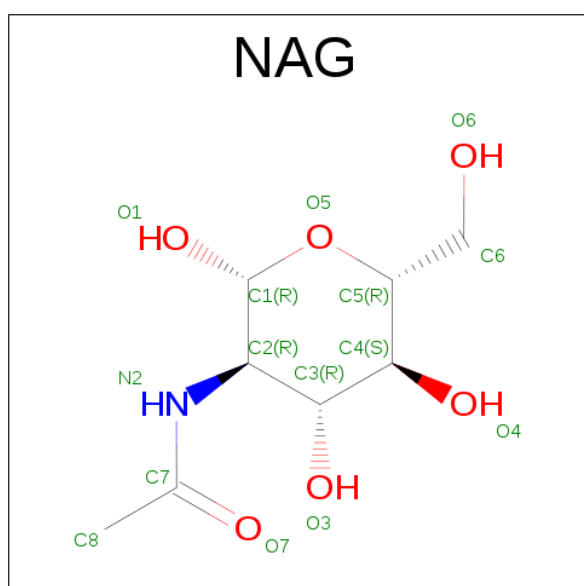
- Molecule 1 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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: $C_8H_{15}NO_6$).



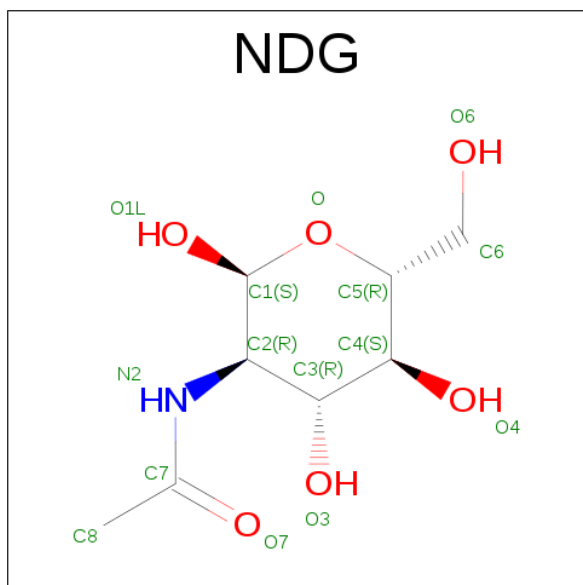
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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: C₈H₁₅NO₆).



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		

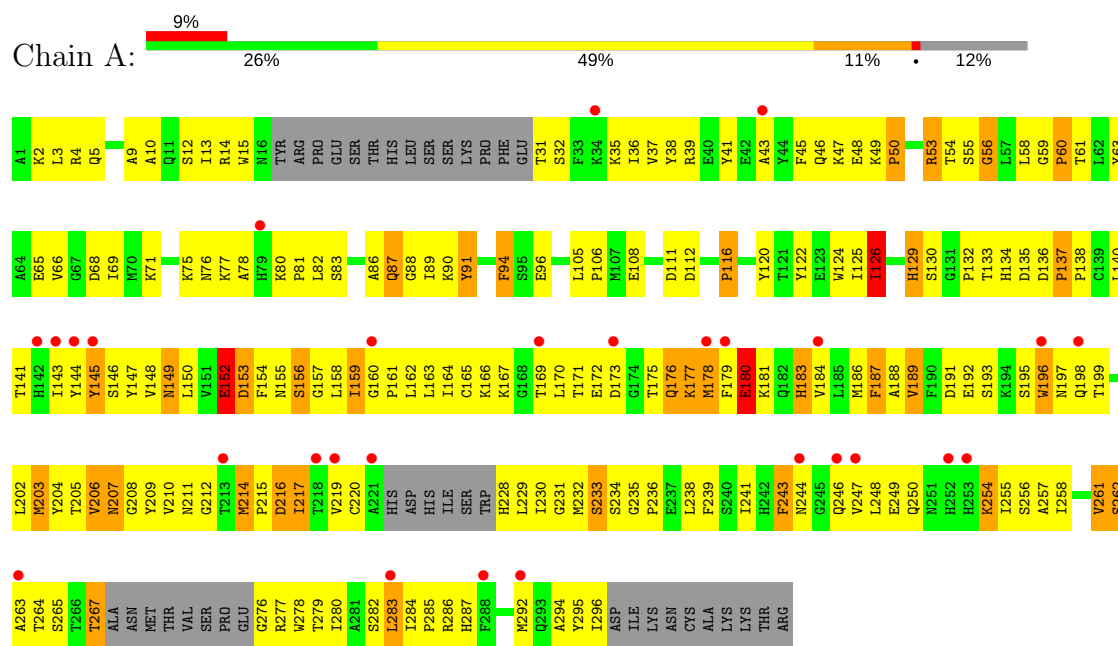
- Molecule 7 is water.

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

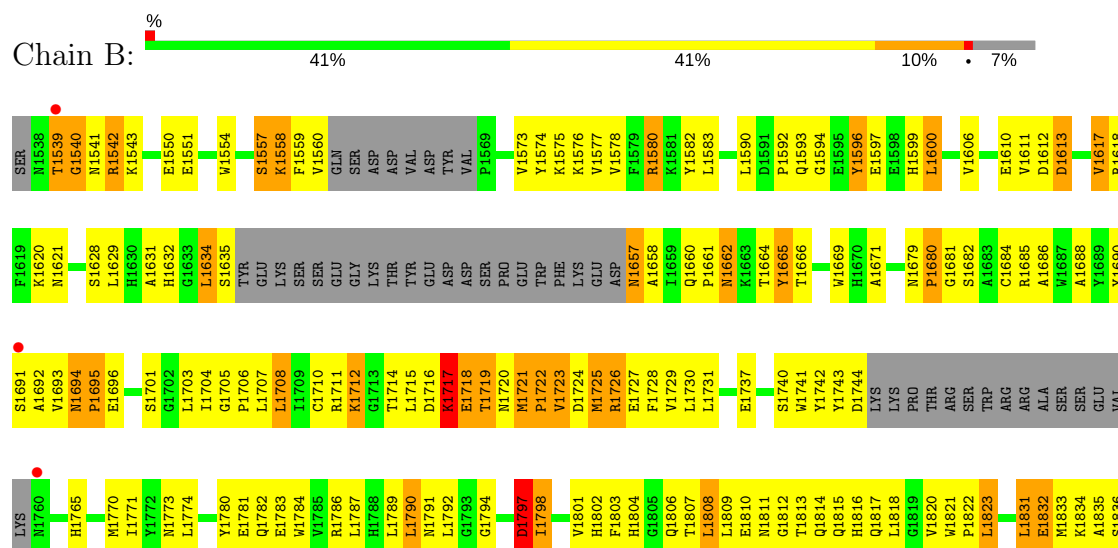
3 Residue-property plots

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



• Molecule 2: Coagulation factor V



L2171	F2178	E2016	K2088	K1837
A2172	G2179	L2017	I2089	
L2173	G2180	Q2018	K2090	L1843
R2174	D2181	G2019	K2091	D1844
L2175	N2182	V2022	I2092	T1845
				E1846
		C2025	V2096	V1847
		S2026	T2097	G1848
		T2027	Q2098	E1849
			G2099	I1850
		G2030	C2100	Q1851
			K2101	R1852
		G2034	E2106	A1853
		K2035	F2107	G1854
		I2036	Y2108	M1855
		E2037	K2109	Q1856
		N2038	V2110	
		K2039	S2111	I1861
		Q2040	Y2112	
			T2113	R1864
		S2044		
		S2045	D2118	K1867
		F2046		M1868
		K2047	T2121	P1869
		K2048	D2122	M1870
		S2049	W2123	G1871
		W2050	K2124	L1872
		W2051	F2125	
		G2052	Y2126	L1876
		N2053	R2127	I1877
		Y2054		
		W2055	M2132	E1886
				F1887
		F2058	N2140	W1888
			N2141	G1889
		L2062	K2142	Y1890
		N2063	V2143	F1891
			R2144	E1892
		K2067	G2145	P1893
		V2068	H2146	K1894
		N2069	V2147	L1895
		A2070	K2148	A1896
		W2071		R1897
		Q2072		L1898
		A2073	F2151	M1899
		K2074	N2152	M1900
		A2075	P2153	
		N2076	F2154	Y1904
		N2077	I2155	M1905
		N2078		A1906
		N2079	I2160	
		Q2080	R2161	K1911
		W2081	T2162	L1912
		L2082		S1913
		Q2083	K2165	T1914
		F2084	T2166	T1915
		D2085	W2167	F1916
		L2086	N2168	M1917
		L2087	Q2169	P1918
			S2170	E1919

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 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
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.80Å)	Xtriage
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%)	DCC
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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 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	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

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 39.

The worst 5 of 548 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 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	593/647 (92%)	479 (81%)	73 (12%)	41 (7%)	1	3
All	All	853/953 (90%)	657 (77%)	119 (14%)	77 (9%)	1	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 ⓘ

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%)	8	22
2	B	526/570 (92%)	467 (89%)	59 (11%)	7	21
All	All	759/839 (90%)	675 (89%)	84 (11%)	7	21

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

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Mol	Chain	Res	Type
2	B	2083	GLN
2	B	1814	GLN
2	B	1851	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 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	14,14,15	0.64	0	15,19,21	0.72	0
3	NAG	A	2186	1	14,14,15	0.51	0	15,19,21	0.71	0
4	NDG	B	2187	2	14,14,15	0.58	0	15,19,21	0.86	1 (6%)
3	NAG	B	2188	2	14,14,15	0.55	0	15,19,21	0.80	1 (6%)
4	NDG	B	2189	2	14,14,15	0.63	0	15,19,21	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	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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2187	NDG	O-C1-C2	-2.07	108.59	111.47
3	B	2188	NAG	C2-N2-C7	-2.06	119.94	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

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

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, 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%)	0.56	28 (10%) 7 4	48, 89, 127, 136	0
2	B	601/647 (92%)	-0.20	6 (0%) 82 77	26, 54, 91, 112	0
All	All	869/953 (91%)	0.03	34 (3%) 40 29	26, 64, 116, 136	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	THR	4.4
1	A	34	LYS	3.7
1	A	247	VAL	3.7
1	A	178	MET	3.6
2	B	1760	ASN	3.6

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NDG	B	2189	14/15	0.90	0.19	-0.19	70,72,74,76	0
5	CU	B	2190	1/1	0.97	0.20	-0.46	65,65,65,65	0
3	NAG	B	2188	14/15	0.89	0.13	-1.25	73,74,76,78	0
3	NAG	A	2186	14/15	0.90	0.16	-1.61	86,88,90,91	0
6	CA	A	2184	1/1	0.95	0.08	-1.93	68,68,68,68	0
4	NDG	B	2187	14/15	0.83	0.34	-	94,98,101,101	0
3	NAG	A	2185	14/15	0.75	0.40	-	127,128,129,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.