wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 08:30 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

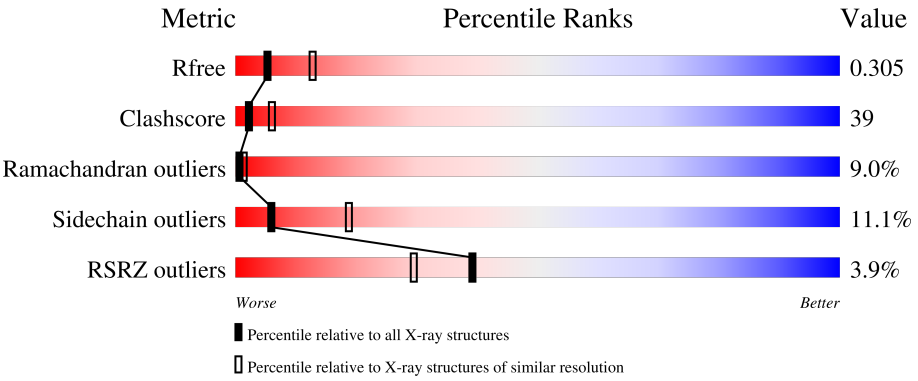
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	306	9% 26% 49% 11% • 12%
2	B	647	% 41% 41% 10% • 7%

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.

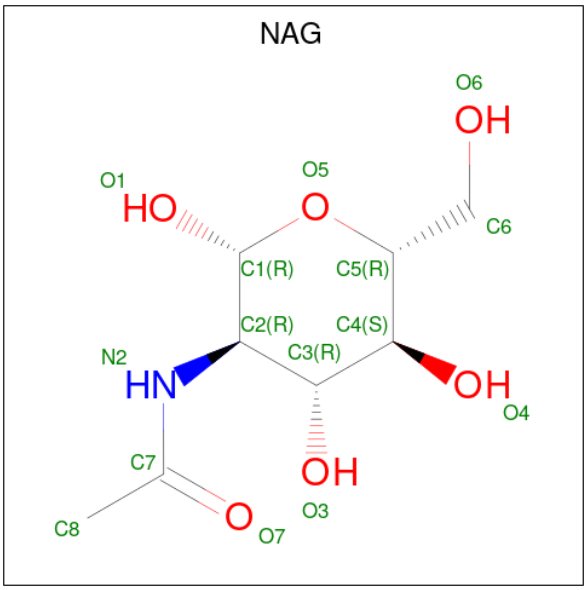
- Molecule 1 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 2-acetamido-2-deoxy-beta-D-glucopyranose (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		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 6 is water.

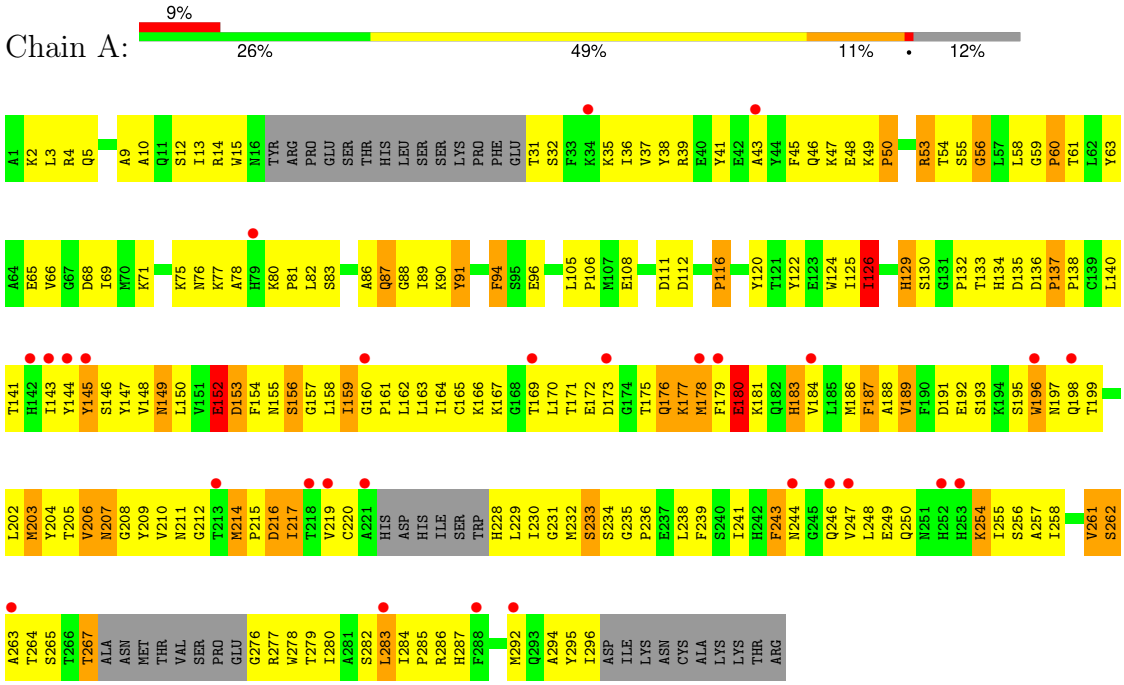
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	47	Total O 47 47	0	0
6	B	142	Total O 142 142	0	0

3 Residue-property plots (i)

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.

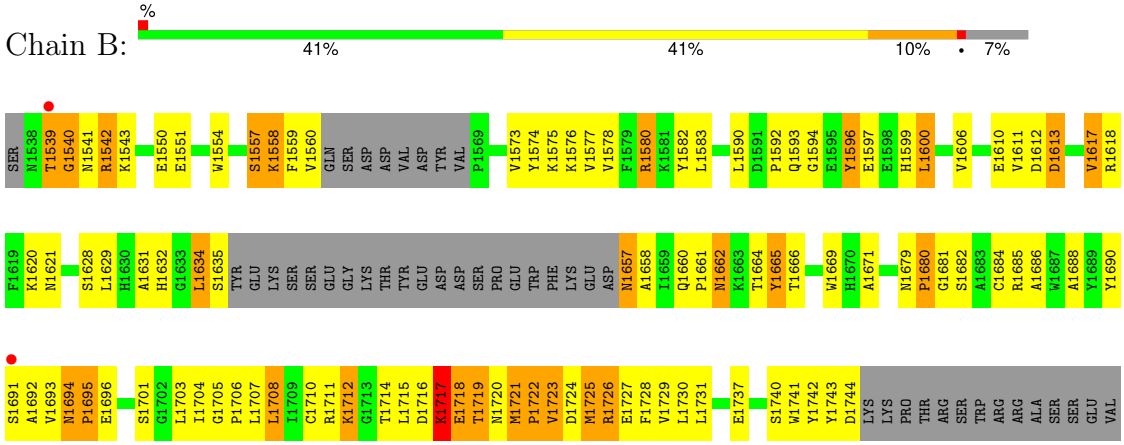
- Molecule 1: Coagulation factor V

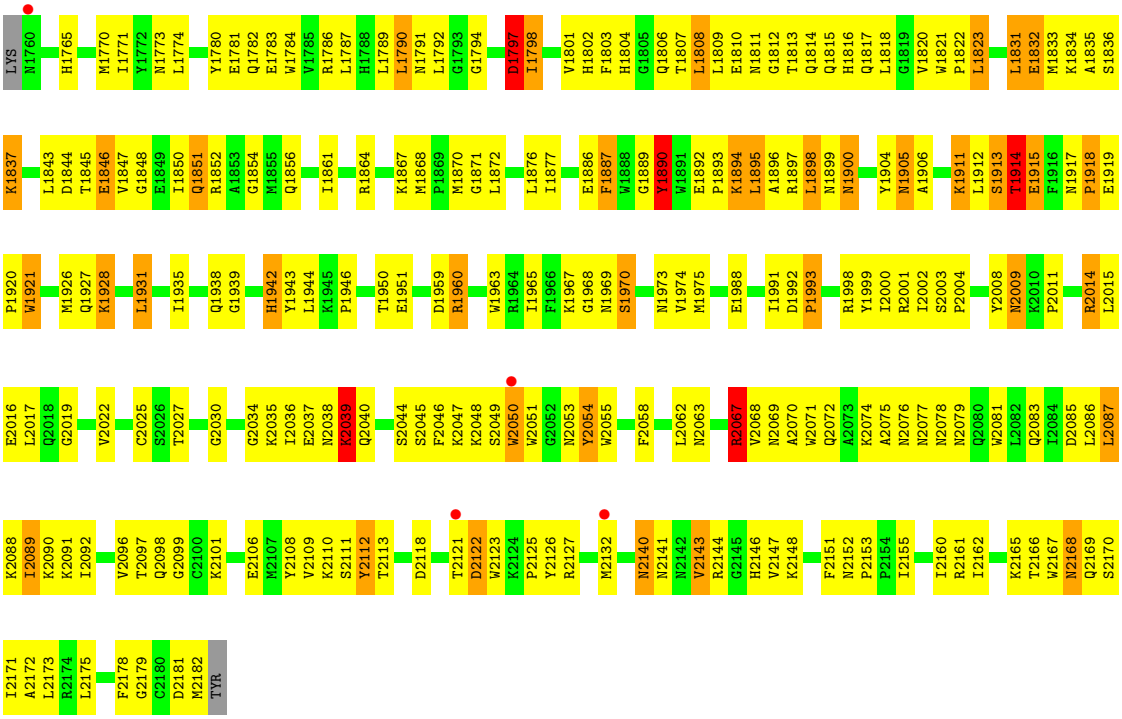
Chain A:



- Molecule 2: Coagulation factor V

Chain B:




LYS N1760 H1765 M1770 I1771 Y1772 N1773 L1774 Y1780 E1781 Q1782 E1783 W1784 V1785 R1786 L1787 H1788 L1789 L1790 N1791 L1792 G1793 G1794 D1797 I1798 V1801 H1802 F1803 H1804 G1805 Q1806 T1807 L1808 L1809 E1810 N1811 G1812 T1813 Q1814 Q1815 H1816 Q1817 L1818 G1819 V1820 W1821 P1822 L1823 L1831 E1832 M1833 K1834 A1835 S1836
K1837 L1843 D1844 T1845 E1846 V1847 G1848 E1849 I1850 Q1851 R1852 A1853 G1854 M1855 Q1856 I1861 R1864 K1867 M1868 P1869 M1870 G1871 L1872 L1876 I1877 E1886 F1887 W1888 G1889 Y1890 W1891 E1892 P1893 K1894 L1895 A1896 R1897 L1898 N1899 N1900 Y1904 N1905 A1906 K1911 L1912 S1913 T1914 E1915 F1916 N1917 P1918 E1919
P1920 W1921 M1926 Q1927 K1928 L1931 I1935 Q1938 G1939 H1942 Y1943 L1944 K1945 P1946 T1950 E1951 D1959 R1960 W1963 R1964 I1965 F1966 K1967 G1968 N1969 S1970 N1973 V1974 M1975 E1988 I1991 D1992 P1993 R1998 Y1999 I2000 R2001 I2002 S2003 P2004 Y2008 N2009 K2010 P2011 R2014 L2015
E2016 L2017 Q2018 G2019 V2022 C2025 S2026 T2027 G2030 G2034 K2035 I2036 E2037 N2038 K2039 Q2040 S2044 S2045 F2046 K2047 K2048 S2049 W2050 W2051 G2052 N2053 Y2054 W2055 F2058 L2062 N2063 R2067 V2068 N2069 A2070 W2071 Q2072 A2073 K2074 A2075 N2076 N2077 N2078 N2079 Q2080 W2081 L2082 Q2083 I2084 D2085 L2086 L2087
K2088 I2089 K2090 K2091 I2092 V2096 T2097 Q2098 G2099 C2100 K2101 E2106 M2107 Y2108 V2109 K2110 S2111 Y2112 T2113 D2118 T2121 D2122 W2123 K2124 P2125 Y2126 R2127 M2132 N2140 N2141 N2142 V2143 R2144 G2145 H2146 V2147 K2148 F2151 N2152 P2153 P2154 I2155 I2160 R2161 I2162 K2165 T2166 W2167 N2168 Q2169 S2170
I2171 A2172 L2173 R2174 L2175 F2178 G2179 C2180 D2181 M2182 TYR

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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%)	wwPDB-VP
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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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

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

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(^{o})	Ideal(^{o})
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	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	549	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 549 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 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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 (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%)	208 (89%)	25 (11%)	6 20
2	B	526/570 (92%)	467 (89%)	59 (11%)	6 18
All	All	759/839 (90%)	675 (89%)	84 (11%)	6 19

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

Mol	Chain	Res	Type
2	B	1895	LEU
2	B	2079	ASN
2	B	1900	ASN
2	B	1921	TRP
2	B	2113	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2168	ASN
2	B	2065	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 monosaccharides 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	A	2186	1	14,14,15	0.53	0	17,19,21	0.70	0
3	NAG	B	2189	2	14,14,15	0.66	0	17,19,21	0.68	0
3	NAG	B	2187	2	14,14,15	0.61	0	17,19,21	0.79	0
3	NAG	B	2188	2	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
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	A	2186	1	-	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	B	2187	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	2188	2	-	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(^{o})	Ideal(^{o})
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	2189	NAG	3	0
3	B	2187	NAG	4	0
3	B	2188	NAG	4	0
3	A	2185	NAG	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

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	268/306 (87%)	0.56	28 (10%) 6 3	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%) 39 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

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

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, 95^{th} 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(Å^2)	Q<0.9
3	NAG	A	2185	14/15	0.75	0.40	127,128,129,130	0
3	NAG	B	2187	14/15	0.83	0.34	94,98,101,101	0
3	NAG	B	2188	14/15	0.89	0.13	73,74,76,78	0
3	NAG	A	2186	14/15	0.90	0.16	86,88,90,91	0
3	NAG	B	2189	14/15	0.90	0.19	70,72,74,76	0
4	CA	A	2184	1/1	0.95	0.08	68,68,68,68	0
5	CU	B	2190	1/1	0.97	0.20	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.