



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:56 am GMT

PDB ID : 2R7E
Title : Crystal Structure Analysis of Coagulation Factor VIII
Authors : Stoddard, B.L.; Shen, B.W.
Deposited on : 2007-09-07
Resolution : 3.70 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

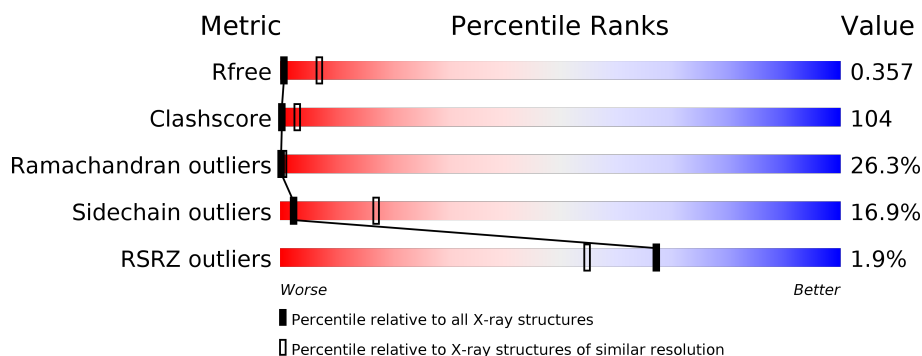
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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	742	<div> <div>2%</div> <div>11% 49% 28% 5% 7%</div> </div>
2	B	770	<div> <div>%</div> <div>11% 47% 23% 16%</div> </div>

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
6	CA	A	2400	-	-	-	X
6	CA	A	2401	-	-	-	X
7	CU	A	2403	-	-	-	X
7	CU	B	2404	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10985 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 VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5590	3592	937	1035	26			

- Molecule 2 is a protein called Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	644	Total	C	N	O	S	0	0	0
			5229	3346	907	944	32			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1838	SER	PHE	ENGINEERED	UNP P00451

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (N-ACETYL-D-GLUCOSAMINE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	7	Total	C	N	O	0	0
			83	46	2	35		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	Ca 3	0	0

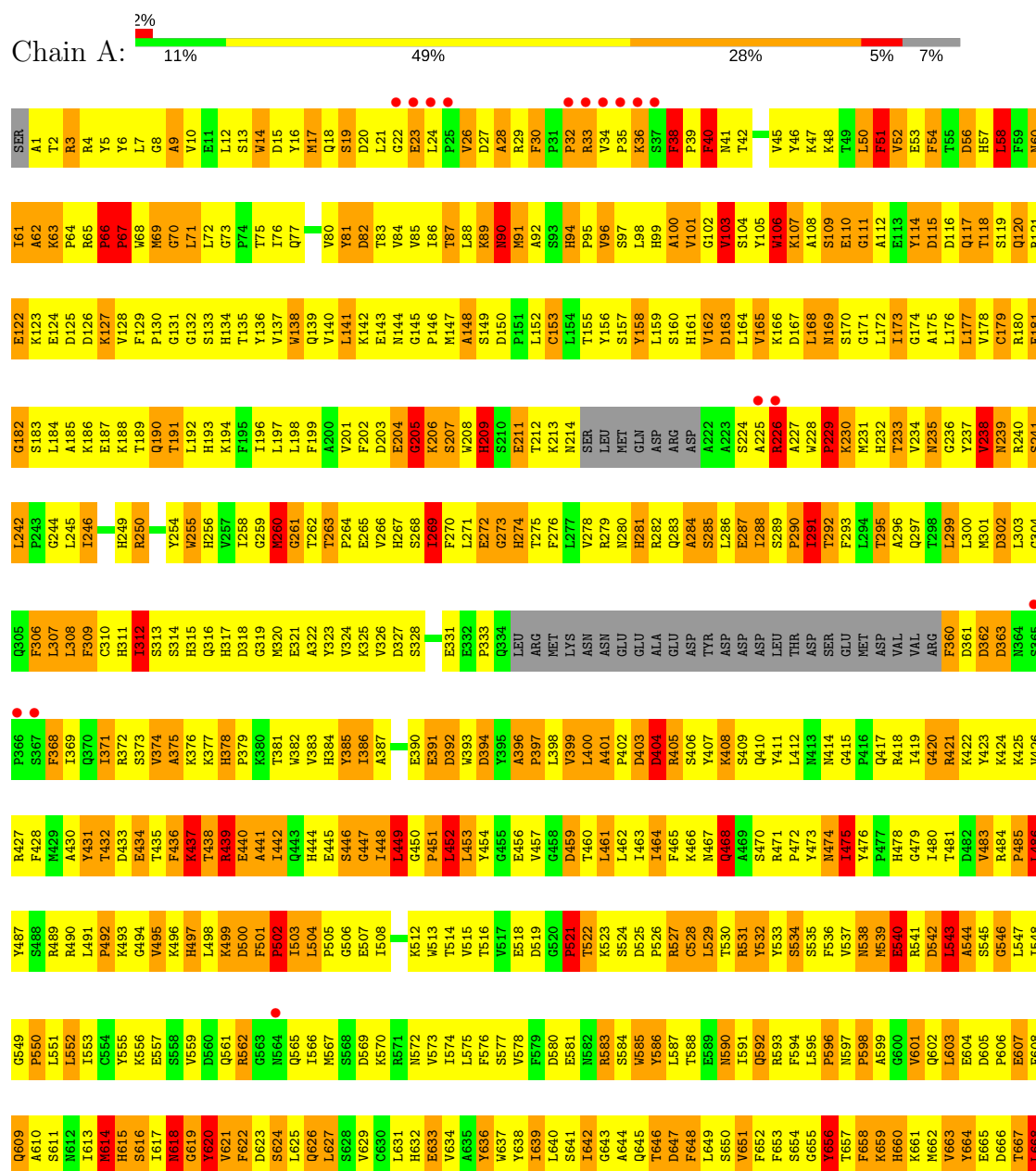
- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Cu 1	0	0
7	A	1	Total 1	Cu 1	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 VIII



LEU	T669
SER	L670
LYS	F671
ASN	P672
ASP	S673
ASN	G675
ALA	E676
ILE	T677
GLU	V678
PRO	F679
ARG	G680
SER	M681
	M682
	E683
	N684
	P685
	G686
	L687
	M688
	L689
	L690
	G691
	C692
	H693
	N694
	R695
	F697
	R698
	N699
	R700
	G701
	M702
	T703
	A704
	L705
	L706
	K707
	V708
	S709
	S710
	C711
	D712
	K713
	N714
	T715
	G716
	D717
	Y718
	D721
	S722
	Y723
	E724
	D725
	ILE
	SER
	ALA
	TYR
	GLU

● Molecule 2: Coagulation factor VIII



ASP	ASP	T1744	K1804	A1866	M1926	P2048	W2112	D2233	L2297
GLU	GLU	Q1745	M1805	H1867	D1927	R2048	Q2113	F2234	D2298
VAL	THR	L1746	N1806	G1868	T1928	L2050	T2114	Q2235	D2299
THR	TRP	P1747	V1807	L1869	L1929	A2051	Y2115	K2236	P2300
ALA	LYS	R1748	K1808	Q1870	P1930	R2052	R2116	L2237	L2301
TRP	ASP	R1749	P1809	Y1871	G1931	L2053	G2117	M2238	L2302
ASN	ASN	G1750	M1810	T1872	L1932	H2054	N2118	K2239	T2303
HIS	HIS	E1751	E1811	V1873	L1933	G1994	S2119	G2242	R2304
TYR	TYR	L1752	T1812	L1874	M1934	G2057	T2120	V2243	R2305
GLY	ARG	N1753	K1813	E1875	L1995	N2060	G2121	E2244	L2306
THR	THR	E1754	T1814	F1876	Q1936	N2061	T2122	T2245	L2307
GLN	ARG	H1755	Y1815	A1877	D1937	A2061	L2123	K2246	L2308
ILE	LEU	L1756	F1816	L1878	Q1938	V2062	M2124	Q2247	H2309
PRO	CYS	G1757	M1817	F1879	R1939	S2063	V2125	G2248	P2310
LYS	SER	L1758	K1818	F1880	L1940	L2064	F2126	V2249	Q2311
GLU	GLN	L1759	M1819	T1881	R1941	K2065	F2127	D2248	Q2312
GLY	ASN	G1760	Q1820	L1882	Y1942	E2066	G2128	Q2250	L2313
TRP	PRO	P1761	H1821	F1883	Q1943	P2067	M2129	L2251	V2314
LYS	LYS	A1701	H1822	D1884	L1944	F2068	V2130	L2252	H2315
SER	SER	E1702	M1823	E1885	L1945	L2069	D2131	L2253	Q2316
GLU	GLU	V1703	A1824	T1886	S1946	W2070	A2132	S2254	L2317
LEU	LEU	E1704	P1825	K1887	G1947	K2071	G2134	Y2255	L2318
GLY	ARG	L1706	E1766	S1888	M1947	L2072	S2135	V2256	L2319
HIS	HIS	Y1707	V1767	Y1889	S1949	D2074	I2135	V2257	R2320
SER	SER	D1708	E1768	Y1890	M1950	L2075	K2136	K2258	M2321
PRO	PRO	Y1709	D1769	F1891	E1951	L2076	H2137	E2259	E2322
GLU	GLU	G1710	D1830	T1892	L2013	L2077	N2138	T2260	V2323
LYS	LYS	M1711	C1832	E1893	F2014	A2077	L2139	L2261	L2324
THR	THR	A1712	M1772	N1894	H1954	P2078	F2140	S2263	G2325
ALA	ALA	S1713	A1834	M1895	V2016	M2079	N2141	S2264	C2326
PHE	ARG	S1713	A1834	E1896	L1956	T2017	P2142	T2265	E2327
LYS	LYS	S1714	M1835	R1897	S2018	L2081	P2143	Q2266	A2328
LYS	LYS	P1715	A1836	R1898	H1957	H2082	P2144	T2267	Q2329
LYS	LEU	H1716	Y1837	C1899	P1959	G2082	L2144	D2268	D2330
GLN	GLN	V1717	S1838	R1900	G1960	L2084	T2145	L2271	L2331
ASP	THR	L1718	S1839	A1901	H1962	K2085	R2147	T2272	L2332
ILE	ASP	R1719	D1840	P1902	T2023	T2086	Y2148	A2208	
LEU	LEU	S1780	D1841	C1903	P2024	F1963	L2149	P2209	
SER	SER	R1721	R1781	N1904	P2025	G2088	L2150	L2210	
LEU	LEU	A1722	P1782	I1905	V1965	A2089	H2152	L2212	
ILE	ILE	Q1723	Y1783	Q1906	P1966	L2026	P2153	L2213	
ALA	ASP	S1724	D1846	Q1907	K1967	F2093	T2154	G2214	
CYS	CYS	G1725	V1847	M1908	E1908	S2094	H2155	N2217	
GLU	GLU	S1726	H1848	D1909	K1968	L2095	Y2156	A2218	
ASP	ASP	V1727	S1787	P1910	E1970	L2096	S2157	V2219	
SER	SER	P1728	G1850	T1911	D1971	Y2097	L2158	Q2284	
THR	THR	Q1729	L1789	F1912	K1972	S2099	R2159	Q2285	
ILE	HIS	F1730	I1851	F1913	P2034	Q2100	S2160	P2221	
ALA	ALA	K1731	G1853	E1914	D2034	Q2036	T2161	Q2222	
VAL	VAL	K1732	P1854	N1915	L1975	F2101	L2162	V2223	
ALA	ALA	V1733	L1855	Y1916	M1977	I2102	R2163	R2224	
ILE	LYS	Y1734	L1856	R1917	L1978	L2103	M2164	N2225	
ASN	ASN	F1735	V1857	F1918	Y1979	M2104	E2165	P2226	
GLU	GLU	Q1736	C1858	H1919	P1980	Y2105	L2166	T2227	
GLY	ASP	E1737	H1859	A1920	G1981	S2106	L2167	E2228	
ASN	GLN	F1738	T1860	I1921	Y2043	L2107	M2168	Q2229	
ASP	ASP	T1739	G1799	N1861	F1982	D2108	G2169	V2230	
LYS	LYS	D1740	A1800	T1862	N1922	Q2044	C2170	L2231	
PRO	PRO	G1741	E1801	L1863	G1923	Q2045	L2170	V2232	
ALA	ALA	S1742	P1802	N1864	Y1924	W2046	Q2210	N2295	
GLU	GLU	F1743	R1803	P1865	I1925	A2047	L2171	S2296	

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.57Å 134.57Å 359.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.37 – 3.70 57.36 – 3.60	Depositor EDS
% Data completeness (in resolution range)	85.0 (57.37-3.70) 81.8 (57.36-3.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.279 , 0.347 0.293 , 0.357	Depositor DCC
R_{free} test set	1536 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	125.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 131.9	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	0.89	EDS
Total number of atoms	10985	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: CA, BMA, NAG, CU, MAN

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	0.56	7/5749 (0.1%)	0.83	9/7806 (0.1%)
2	B	0.44	0/5377	0.75	1/7280 (0.0%)
All	All	0.50	7/11126 (0.1%)	0.79	10/15086 (0.1%)

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
1	A	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ARG	CZ-NH1	8.44	1.44	1.33
1	A	437	LYS	CD-CE	7.11	1.69	1.51
1	A	226	ARG	CZ-NH2	6.99	1.42	1.33
1	A	226	ARG	NE-CZ	5.36	1.40	1.33
1	A	437	LYS	CE-NZ	5.29	1.62	1.49

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	226	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	229	PRO	N-CA-C	6.01	127.74	112.10
1	A	205	GLY	N-CA-C	-6.00	98.11	113.10
1	A	691	GLY	N-CA-C	-5.65	98.99	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TYR	Sidechain
1	A	656	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	5590	0	5429	1198	0
2	B	5229	0	5098	1107	0
3	A	50	0	43	3	0
4	B	28	0	25	0	0
5	B	83	0	70	7	0
6	A	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	10985	0	10665	2260	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 104.

The worst 5 of 2260 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)
1:A:114:TYR:HE1	2:B:1997:ARG:HB2	1.11	1.13
2:B:2284:GLN:HA	2:B:2284:GLN:HE21	1.14	1.13
2:B:1901:ALA:HB1	2:B:1902:PRO:HD2	1.30	1.12
1:A:499:LYS:HG3	1:A:500:ASP:H	1.15	1.12
1:A:651:VAL:HG12	1:A:652:PHE:H	1.15	1.11

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	687/742 (93%)	312 (45%)	180 (26%)	195 (28%)	0	0
2	B	642/770 (83%)	316 (49%)	172 (27%)	154 (24%)	0	1
All	All	1329/1512 (88%)	628 (47%)	352 (26%)	349 (26%)	0	0

5 of 349 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	9	ALA
1	A	17	MET
1	A	19	SER
1	A	23	GLU

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	616/662 (93%)	505 (82%)	111 (18%)	2	14
2	B	572/688 (83%)	482 (84%)	90 (16%)	3	21
All	All	1188/1350 (88%)	987 (83%)	201 (17%)	2	17

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	639	ILE

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Mol	Chain	Res	Type
2	B	1693	LYS
2	B	2232	VAL
1	A	659	LYS
1	A	696	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1736	GLN
2	B	1848	HIS
2	B	2295	ASN
2	B	1778	GLN
2	B	1859	HIS

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 ⓘ

13 carbohydrates 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	$\# Z > 2$
3	NAG	A	2410	1,3	14,14,15	0.84	1 (7%)	15,19,21	0.92	0
3	NAG	A	2411	3	14,14,15	0.70	0	15,19,21	0.79	1 (6%)
3	BMA	A	2412	3	11,11,12	0.79	0	13,15,17	0.72	0
3	MAN	A	2413	3	11,11,12	0.54	0	13,15,17	0.97	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	2420	2,4	14,14,15	0.68	0	15,19,21	0.55	0
4	NAG	B	2421	4	14,14,15	0.72	0	15,19,21	0.56	0
5	NAG	B	2430	2,5	14,14,15	0.71	0	15,19,21	1.34	3 (20%)
5	NAG	B	2431	5	14,14,15	0.53	0	15,19,21	0.92	1 (6%)
5	BMA	B	2432	5	11,11,12	1.55	4 (36%)	13,15,17	1.06	2 (15%)
5	MAN	B	2433	5	11,11,12	1.37	3 (27%)	13,15,17	0.81	0
5	MAN	B	2434	5	11,11,12	1.87	1 (9%)	13,15,17	0.93	1 (7%)
5	BMA	B	2435	5	11,11,12	1.03	1 (9%)	13,15,17	1.45	2 (15%)
5	MAN	B	2436	5	11,11,12	0.69	0	13,15,17	0.93	1 (7%)

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	2410	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2411	3	-	1/6/23/26	0/1/1/1
3	BMA	A	2412	3	-	0/2/19/22	0/1/1/1
3	MAN	A	2413	3	-	0/2/19/22	0/1/1/1
4	NAG	B	2420	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2421	4	-	1/6/23/26	0/1/1/1
5	NAG	B	2430	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2431	5	-	0/6/23/26	0/1/1/1
5	BMA	B	2432	5	-	0/2/19/22	0/1/1/1
5	MAN	B	2433	5	-	0/2/19/22	0/1/1/1
5	MAN	B	2434	5	-	0/2/19/22	0/1/1/1
5	BMA	B	2435	5	-	0/2/19/22	0/1/1/1
5	MAN	B	2436	5	-	0/2/19/22	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2432	BMA	C1-C2	2.02	1.57	1.52
5	B	2433	MAN	C4-C3	2.02	1.57	1.52
5	B	2432	BMA	C4-C5	2.03	1.57	1.53
5	B	2432	BMA	C4-C3	2.08	1.57	1.52
5	B	2433	MAN	C4-C5	2.33	1.58	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2430	NAG	C2-N2-C7	-2.59	119.17	122.94
5	B	2431	NAG	C2-N2-C7	-2.26	119.64	122.94
3	A	2411	NAG	C2-N2-C7	-2.04	119.97	122.94
5	B	2432	BMA	C1-C2-C3	-2.02	107.08	109.65
3	A	2413	MAN	C1-C2-C3	2.05	112.25	109.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2421	NAG	O7-C7-N2-C2
3	A	2411	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2410	NAG	3	0
3	A	2411	NAG	2	0
5	B	2430	NAG	2	0
5	B	2431	NAG	1	0
5	B	2432	BMA	3	0
5	B	2435	BMA	3	0
5	B	2436	MAN	3	0

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	693/742 (93%)	-0.26	17 (2%) 58 45	75, 170, 206, 206	0
2	B	644/770 (83%)	-0.37	9 (1%) 75 64	89, 169, 206, 206	0
All	All	1337/1512 (88%)	-0.32	26 (1%) 67 55	75, 170, 206, 206	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	725	ASP	5.1
1	A	23	GLU	4.7
1	A	225	ALA	4.3
1	A	24	LEU	3.7
1	A	37	SER	3.7

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](#)

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(Å ²)	Q<0.9
5	NAG	B	2430	14/15	0.95	0.15	-0.88	150,153,155,156	0
5	MAN	B	2434	11/12	0.92	0.14	-	190,190,190,190	0
3	MAN	A	2413	11/12	0.69	0.34	-	115,115,115,115	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	2431	14/15	0.88	0.25	-	202,205,205,205	0
5	MAN	B	2436	11/12	0.90	0.18	-	104,104,104,104	11
5	MAN	B	2433	11/12	0.89	0.18	-	187,187,187,187	0
3	NAG	A	2411	14/15	0.79	0.24	-	122,122,122,122	14
3	BMA	A	2412	11/12	0.45	0.32	-	148,148,148,148	11
5	BMA	B	2435	11/12	0.84	0.20	-	145,145,145,145	11
5	BMA	B	2432	11/12	0.82	0.12	-	203,203,203,203	0
3	NAG	A	2410	14/15	0.86	0.18	-	205,205,205,205	0
4	NAG	B	2420	14/15	0.87	0.19	-	205,205,205,205	0
4	NAG	B	2421	14/15	0.84	0.23	-	180,180,180,180	0

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
6	CA	A	2400	1/1	0.56	0.39	6.32	341,341,341,341	0
6	CA	A	2401	1/1	0.98	0.31	4.44	275,275,275,275	0
7	CU	B	2404	1/1	0.98	0.31	2.88	349,349,349,349	0
7	CU	A	2403	1/1	0.96	0.29	2.10	359,359,359,359	0
6	CA	A	2402	1/1	0.96	0.17	-0.07	352,352,352,352	0

6.5 Other polymers [i](#)

There are no such residues in this entry.