



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:15 PM GMT

PDB ID : 1JF6
Title : Crystal structure of thermoactinomyces vulgaris r-47 alpha-amylase mutant F286Y
Authors : Ohtaki, A.; Kondo, S.; Shimura, Y.; Tonozuka, T.; Sakano, Y.; Kamitori, S.
Deposited on : 2001-06-20
Resolution : 3.20 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

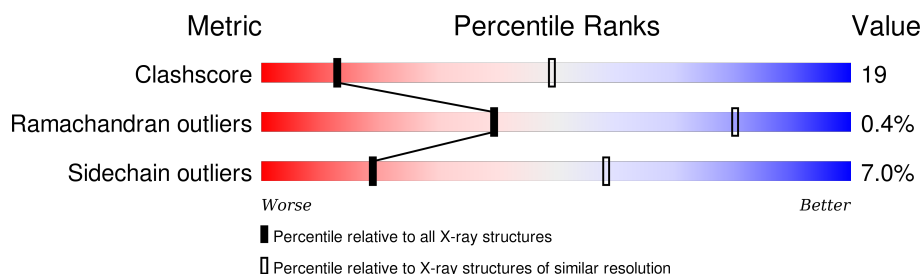
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	585	 58% 39%
1	B	585	 59% 37%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9556 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 ALPHA AMYLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4777	3056	831	875	15			
1	B	585	Total	C	N	O	S	0	0	0
			4777	3056	831	875	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	TYR	PHE	ENGINEERED	UNP Q08751
B	286	TYR	PHE	ENGINEERED	UNP Q08751

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

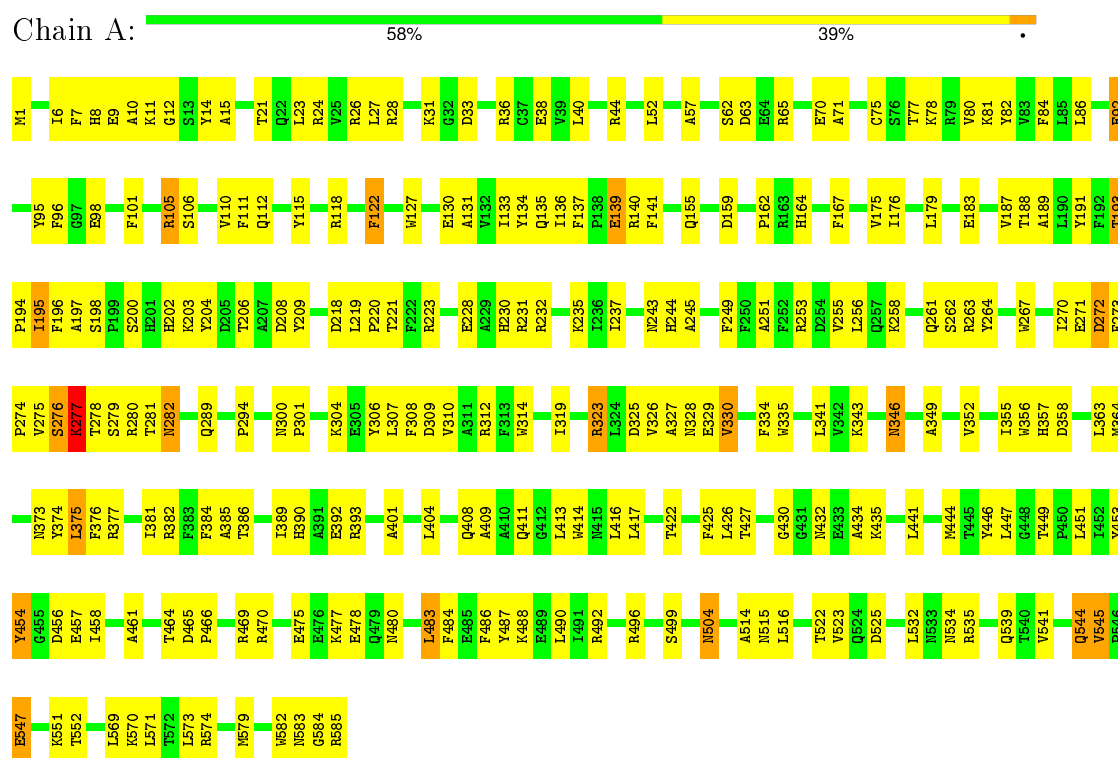
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

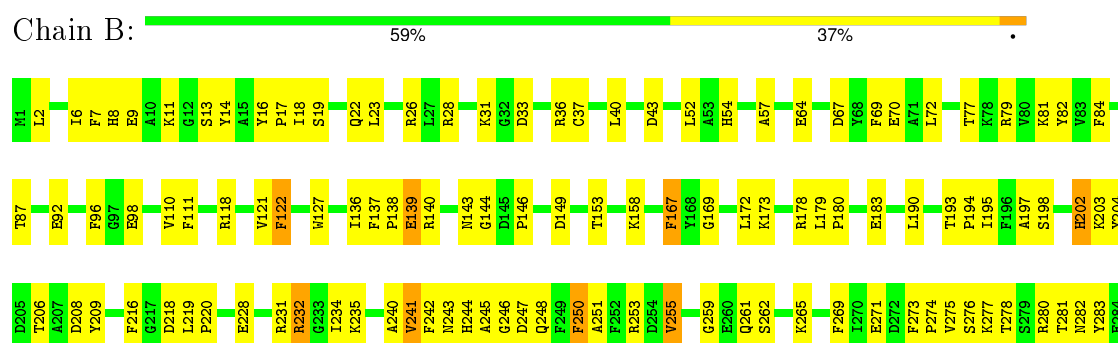
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: ALPHA AMYLASE II



• Molecule 1: ALPHA AMYLASE II



R469	R470	P471	M472	K473	L474	E475	E478	L483	F486	Y487	L491	R492	L493	R494	L497	A498	S499	L500	R504	V505	A514	A518	R521	T522	V523	Q526	H527	V530	L531	L532	N533	N534	R535	Q539	V545	P546	E547	K551	T552	N553	L554	D555	C556	E560
E561	V562	L569	K570	L571	T572	L573	Y576	M579	H580	L581	W582	N583	G584	R585	L597	A598	S599	L600	R604	V605	A614	A618	R621	T622	V623	Q626	H627	V630	L631	L632	N633	N634	R635	Q639	V645	P646	E647	K651	T652	N653	L654	D655	C656	E660
E661	V662	L669	K670	L671	T672	L673	Y676	M679	H680	L681	W682	N683	G684	R685	L697	A698	S699	L700	R704	V705	A714	A718	R721	T722	V723	Q726	H727	V730	L731	L732	N733	N734	R735	Q739	V745	P746	E747	K751	T752	N753	L754	D755	C756	E760
E761	V762	L769	K770	L771	T772	L773	Y776	M779	H780	L781	W782	N783	G784	R785	L797	A798	S799	L800	R804	V805	A814	A818	R821	T822	V823	Q826	H827	V830	L831	L832	N833	N834	R835	Q839	V845	P846	E847	K851	T852	N853	L854	D855	C856	E860
E861	V862	L869	K870	L871	T872	L873	Y876	M879	H880	L881	W882	N883	G884	R885	L897	A898	S899	L900	R904	V905	A914	A918	R921	T922	V923	Q926	H927	V930	L931	L932	N933	N934	R935	Q939	V945	P946	E947	K951	T952	N953	L954	D955	C956	E960
E961	V962	L969	K970	L971	T972	L973	Y976	M979	H980	L981	W982	N983	G984	R985	L997	A998	S999	L1000	R1004	V1005	A1014	A1018	R1021	T1022	V1023	Q1026	H1027	V1030	L1031	L1032	N1033	N1034	R1035	Q1039	V1045	P1046	E1047	K1051	T1052	N1053	L1054	D1055	C1056	E1060
E1061	V1062	L1069	K1070	L1071	T1072	L1073	Y1076	M1079	H1080	L1081	W1082	N1083	G1084	R1085	L1097	A1098	S1099	L1100	R1104	V1105	A1114	A1118	R1121	T1122	V1123	Q1126	H1127	V1130	L1131	L1132	N1133	N1134	R1135	Q1139	V1145	P1146	E1147	K1151	T1152	N1153	L1154	D1155	C1156	E1160
E1161	V1162	L1169	K1170	L1171	T1172	L1173	Y1176	M1179	H1180	L1181	W1182	N1183	G1184	R1185	L1197	A1198	S1199	L1200	R1204	V1205	A1214	A1218	R1221	T1222	V1223	Q1226	H1227	V1230	L1231	L1232	N1233	N1234	R1235	Q1239	V1245	P1246	E1247	K1251	T1252	N1253	L1254	D1255	C1256	E1260
E1261	V1262	L1269	K1270	L1271	T1272	L1273	Y1276	M1279	H1280	L1281	W1282	N1283	G1284	R1285	L1297	A1298	S1299	L1300	R1304	V1305	A1314	A1318	R1321	T1322	V1323	Q1326	H1327	V1330	L1331	L1332	N1333	N1334	R1335	Q1339	V1345	P1346	E1347	K1351	T1352	N1353	L1354	D1355	C1356	E1360
E1361	V1362	L1369	K1370	L1371	T1372	L1373	Y1376	M1379	H1380	L1381	W1382	N1383	G1384	R1385	L1397	A1398	S1399	L1400	R1404	V1405	A1414	A1418	R1421	T1422	V1423	Q1426	H1427	V1430	L1431	L1432	N1433	N1434	R1435	Q1439	V1445	P1446	E1447	K1451	T1452	N1453	L1454	D1455	C1456	E1460
E1461	V1462	L1469	K1470	L1471	T1472	L1473	Y1476	M1479	H1480	L1481	W1482	N1483	G1484	R1485	L1497	A1498	S1499	L1500	R1504	V1505	A1514	A1518	R1521	T1522	V1523	Q1526	H1527	V1530	L1531	L1532	N1533	N1534	R1535	Q1539	V1545	P1546	E1547	K1551	T1552	N1553	L1554	D1555	C1556	E1560
E1561	V1562	L1569	K1570	L1571	T1572	L1573	Y1576	M1579	H1580	L1581	W1582	N1583	G1584	R1585	L1597	A1598	S1599	L1600	R1604	V1605	A1614	A1618	R1621	T1622	V1623	Q1626	H1627	V1630	L1631	L1632	N1633	N1634	R1635	Q1639	V1645	P1646	E1647	K1651	T1652	N1653	L1654	D1655	C1656	E1660
E1661	V1662	L1669	K1670	L1671	T1672	L1673	Y1676	M1679	H1680	L1681	W1682	N1683	G1684	R1685	L1697	A1698	S1699	L1700	R1704	V1705	A1714	A1718	R1721	T1722	V1723	Q1726	H1727	V1730	L1731	L1732	N1733	N1734	R1735	Q1739	V1745	P1746	E1747	K1751	T1752	N1753	L1754	D1755	C1756	E1760
E1761	V1762	L1769	K1770	L1771	T1772	L1773	Y1776	M1779	H1780	L1781	W1782	N1783	G1784	R1785	L1797	A1798	S1799	L1800	R1804	V1805	A1814	A1818	R1821	T1822	V1823	Q1826	H1827	V1830	L1831	L1832	N1833	N1834	R1835	Q1839	V1845	P1846	E1847	K1851	T1852	N1853	L1854	D1855	C1856	E1860
E1861	V1862	L1869	K1870	L1871	T1872	L1873	Y1876	M1879	H1880	L1881	W1882	N1883	G1884	R1885	L1897	A1898	S1899	L1900	R1904	V1905	A1914	A1918	R1921	T1922	V1923	Q1926	H1927	V1930	L1931	L1932	N1933	N1934	R1935	Q1939	V1945	P1946	E1947	K1951	T1952	N1953	L1954	D1955	C1956	E1960
E1961	V1962	L1969	K1970	L1971	T1972	L1973	Y1976	M1979	H1980	L1981	W1982	N1983	G1984	R1985	L1997	A1998	S1999	L2000	R2004	V2005	A2014	A2018	R2021	T2022	V2023	Q2026	H2027	V2030	L2031	L2032	N2033	N2034	R2035	Q2039	V2045	P2046	E2047	K2051	T2052	N2053	L2054	D2055	C2056	E2060
E2061	V2062	L2069	K2070	L2071	T2072	L2073	Y2076	M2079	H2080	L2081	W2082	N2083	G2084	R2085	L2097	A2098	S2099	L2100	R2104	V2105	A2114	A2118	R2121	T2122	V2123	Q2126	H2127	V2130	L2131	L2132	N2133	N2134	R2135	Q2139	V2145	P2146	E2147	K2151	T2152	N2153	L2154	D2155	C2156	E2160
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E2261	V2262	L2269	K2270	L2271	T2272	L2273	Y2276	M2279	H2280	L2281	W2282	N2283	G2284	R2285	L2297	A2298	S2299	L2300	R2304	V2305	A2314	A2318	R2321	T2322	V2323	Q2326	H2327	V2330	L2331	L2332	N2333	N2334	R2335	Q2339	V2345	P2346	E2347	K2351	T2352	N2353	L2354	D2355	C2356	E2360
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E2461	V2462	L2469	K2470	L2471	T2472	L2473	Y2476	M2479	H2480	L2481	W2482	N2483	G2484	R2485	L2497	A2498	S2499	L2500	R2504	V2505	A2514	A2518	R2521	T2522	V2523	Q2526	H2527	V2530	L2531	L2532	N2533	N2534	R2535	Q2539	V2545	P2546	E2547	K2551	T2552	N2553	L2554	D2555	C2556	E2560
E2561	V2562	L2569	K2570	L2571	T2572	L2573	Y2576	M2579	H2580	L2581	W2582	N2583	G2584	R2585	L2597	A2598	S2599	L2600	R2604	V2605	A2614	A2618	R2621	T2622	V2623	Q2626	H2627	V2630	L2631	L2632	N2633	N2634	R2635	Q2639	V2645	P2646	E2647	K2651	T2652	N2653	L2654	D2655	C2656	E2660
E2661	V2662	L2669	K2670	L2671	T2672	L2673	Y2676	M2679	H2680	L2681	W2682	N2683	G2684	R2685	L2697	A2698	S2699	L2700	R2704	V2705	A2714	A2718	R2721	T2722	V2723	Q2726	H2727	V2730	L2731	L2732	N2733	N2734	R2735	Q2739	V2745	P2746	E2747	K2751	T2752	N2753	L2754	D2755	C2756	E2760
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E3161	V3162	L3169	K3170	L3171	T3172	L3173	Y3176	M3179	H3180	L3181	W3182	N3183	G3184	R3185	L3197	A3198	S3199	L3200	R3204	V3205	A3214	A3218	R3221	T3222	V3223	Q3226	H3227	V3230	L3231	L3232	N3233	N3234	R3235	Q3239	V3245	P3246	E3247	K3251	T3252	N3253	L3254	D3255	C3256	E3260
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E3361	V3362	L3369	K3370	L3371	T3372	L3373	Y3376	M3379	H3380	L3381	W3382	N3383	G3384	R3385	L3397	A3398	S3399	L3400	R3404	V3405	A3414	A3418	R3421	T3422	V3423	Q3426	H3427	V3430	L3431	L3432	N3433	N3434	R3435	Q3439	V3445	P3446	E3447	K3451	T3452	N3453	L3454	D3455	C3456	E3460
E3461	V3462	L3469	K3470	L3471	T3472	L3473	Y3476	M3479	H3480	L3481	W3482	N3483	G3484	R3485	L3497	A3498																												

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.25Å 117.94Å 113.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.39 – 3.20	Depositor
% Data completeness (in resolution range)	91.7 (38.39-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9556	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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

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	0.49	0/4907	0.66	0/6643
1	B	0.50	0/4907	0.66	0/6643
All	All	0.50	0/9814	0.66	0/13286

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	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	4777	0	4607	184	0
1	B	4777	0	4607	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	9556	0	9214	361	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 19.

The worst 5 of 361 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:328:ASN:HB3	1:A:355:ILE:HD12	1.40	1.02
1:A:255:VAL:HA	1:A:262:SER:OG	1.67	0.93
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.60	0.83
1:B:26:ARG:HG2	1:B:70:GLU:HG2	1.62	0.81
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.62	0.79

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	583/585 (100%)	551 (94%)	28 (5%)	4 (1%)	26	72
1	B	583/585 (100%)	552 (95%)	30 (5%)	1 (0%)	52	88
All	All	1166/1170 (100%)	1103 (95%)	58 (5%)	5 (0%)	39	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	SER

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Continued from previous page...

Mol	Chain	Res	Type
1	A	547	GLU
1	B	547	GLU
1	A	277	LYS
1	A	195	ILE

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	493/493 (100%)	455 (92%)	38 (8%)	16	54
1	B	493/493 (100%)	462 (94%)	31 (6%)	22	63
All	All	986/986 (100%)	917 (93%)	69 (7%)	19	58

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	MET
1	B	13	SER
1	B	464	THR
1	A	454	TYR
1	A	544	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	GLN
1	B	261	GLN
1	B	539	GLN
1	B	135	GLN
1	B	328	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.