



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 6, 2017 – 06:10 PM EST

PDB ID : 5Y3R
EMDB ID: : EMD-6803
Title : Cryo-EM structure of Human DNA-PK Holoenzyme
Authors : Yin, X.; Liu, M.; Tian, Y.; Wang, J.; Xu, Y.
Deposited on : unknown
Resolution : 6.60 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

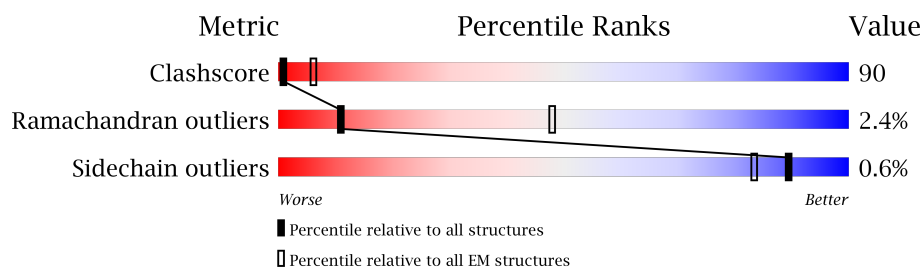
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


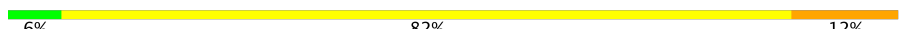
The reported resolution of this entry is 6.60 Å.

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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	501	
2	B	536	
3	K	15	
4	D	34	
5	E	36	
6	C	4119	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 38766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	493	3982	2550	675	739	18	0	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	526	4210	2696	707	784	23	0	0

- Molecule 3 is a protein called PRKDC-Helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	K	15	75	45	15	15	0	0

- Molecule 4 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	34	700	336	123	207	34	0	0

- Molecule 5 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	36	733	354	132	212	35	0	0

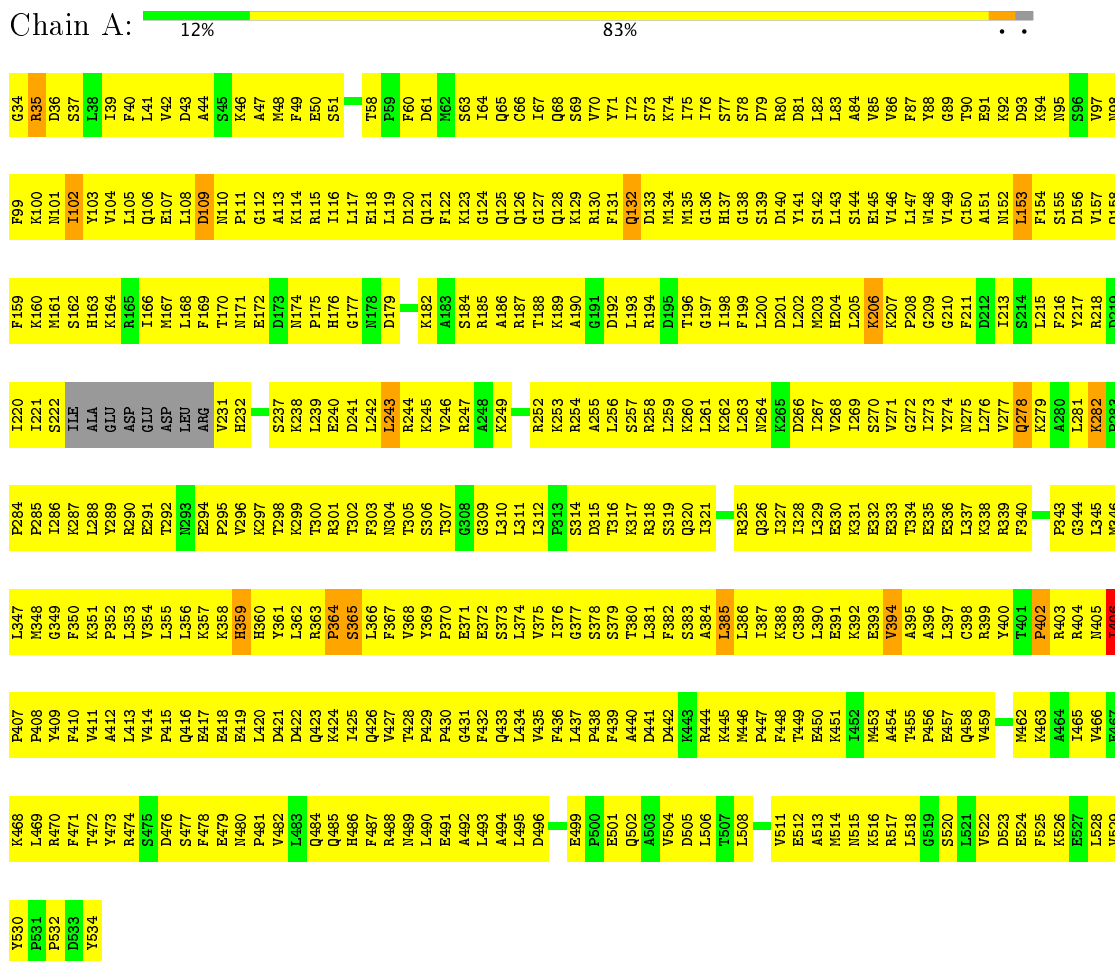
- Molecule 6 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	3636	29066	18608	4912	5356	190	0	0

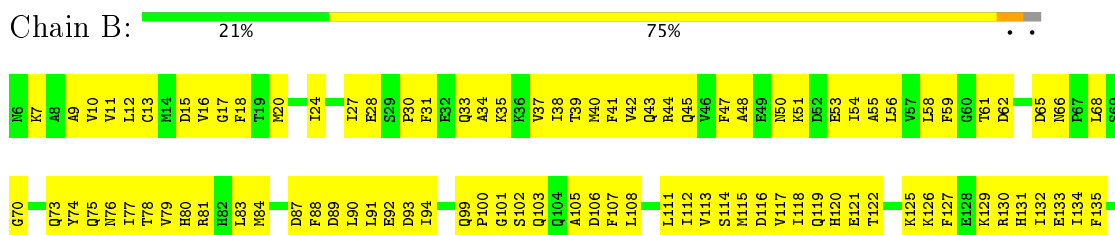
3 Residue-property plots

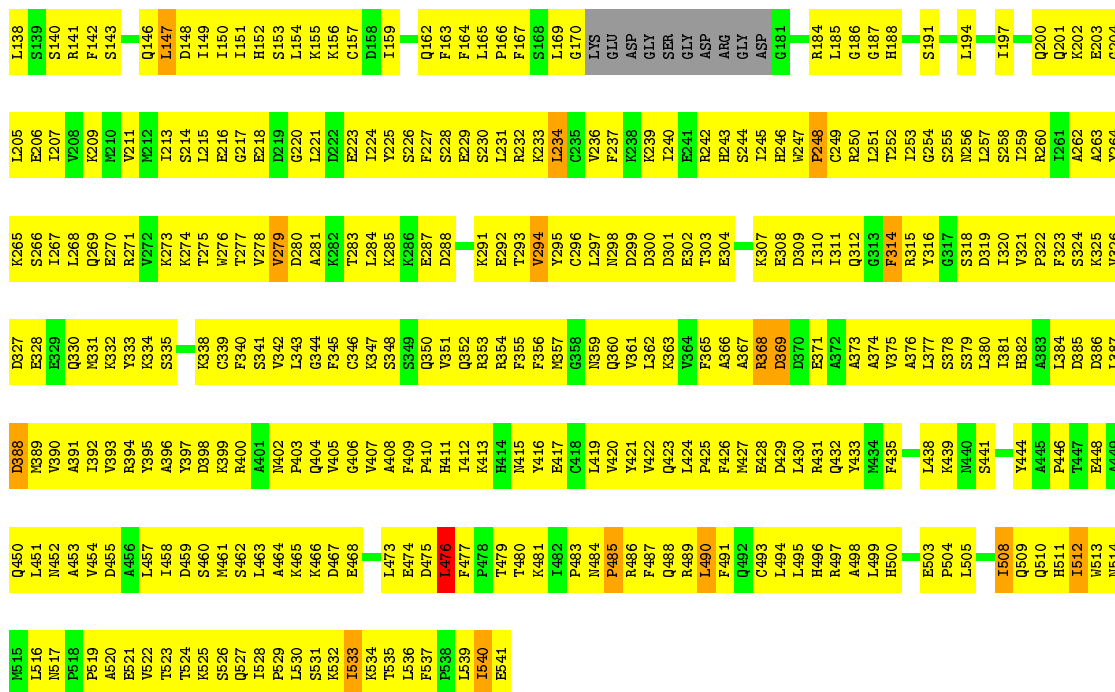
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: X-ray repair cross-complementing protein 6



- Molecule 2: X-ray repair cross-complementing protein 5





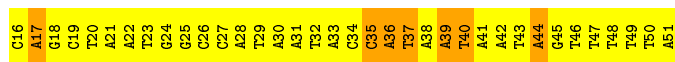
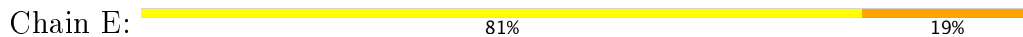
• Molecule 3: PRKDC-Helix



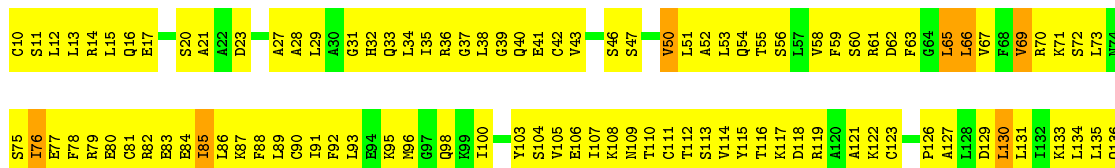
• Molecule 4: DNA (34-MER)



• Molecule 5: DNA (36-MER)



• Molecule 6: DNA-dependent protein kinase catalytic subunit



A1114	V1054	H994	E932	T872	ASN	A751	SER	F629	E567	ASP	F446	V384	S324	L262	F200	T137
H1115	M1055	F995	L933	V873	TRP	L752	LEU	C630	F668	HIS	P447	I385	M325	K263	L201	F138
A1116	T1056	T996	L934	V874	GLU	M753	LYS	R631	V569	ARG	Q448	V386	M326	Y265	G202	R139
D1117	K1057	N997	S875	M754	VAL	K754	HIS	E632	E370	ALA	Y449	E387	Y266	E203	E203	S140
E1118	S1058	K998	S936	S876	SER	A755	SER	I633	S571	GLY	S450	I388	A328	A266	L204	S141
K1119	L1059	N999	N937	D877	ALA	F756	PRO	L634	V572	GLY	P451	I389	K299	V267	K205	R142
S1120	K1060	K1000	V938	E878	LEU	K757	GLU	P835	L573	GLU	K452	Q390	M330	P268	T206	L143
L1121	K1061	F1001	N939	M879	ASP	L758	ASP	E636	K574	VAL	M453	R391	A331	S269	Q207	L147
G1122	E1062	E1002	F940	R880	ARG	G759	PRO	R637	L575	ARG	Q454	C392	E332	M268	M208	F147
T1123	L1063	S1003	K881	L760	GLU	L760	GLU	Q638	V576	THR	L455	K393	M333	G271	T209	K148
I1124	Q1064	Q1004	L942	S761	ALA	S761	K700	R639	E577	GLY	V456	Q394	H334	L272	L149	L149
Q1125	S1065	D1005	G943	V762	GLN	V762	Y701	E640	K578	LYS	C457	K395	K395	F275	V212	G150
L1126	L1066	K944	K644	T763	LYS	T763	S702	F641	L579	TRP	C458	F396	K356	A276	V219	E151
C1127	A1067	V1007	A945	P764	GLY	P764	G703	F642	D580	LYS	R459	L397	K337	E214	E214	L152
D1128	L1068	L1008	T946	L765	PHE	L765	F704	E643	E584	VAL	A460	T398	L338	L277	P215	F153
H1129	H1069	A1009	R947	R766	ASP	R766	A705	P644	E585	PRO	I461	Q399	Q339	H278	K216	S154
L1130	P1070	R948	R888	E767	LYS	E767	L706	M645	I585	THR	V462	T400	F340	A279	L217	K155
I1131	M1071	E1011	E889	V768	VAL	V768	F707	V646	Q586	THR	K463	D401	F341	S280	P156	F156
A1132	A1072	A1012	K890	G769	VAL	G769	V708	Y647	T587	LYS	V464	D401	M342	Q281	V219	V157
H1133	F1073	L1013	R891	L770	LEU	L770	K709	S648	V588	LYS	F465	D405	E343	F282	L220	G158
L1134	K1074	L1014	R892	M771	LYS	M771	F710	F649	G589	VAL	R406	D406	Q344	S283	A221	E159
C1135	R1075	D1015	S893	G711	HIS	G711	V528	S650	E590	PRO	A468	V408	F345	T284	C222	L160
R1136	L1076	G1016	F894	L772	LEU	L772	K712	S651	Q591	THR	V468	Y408	F346	T284	G223	A161
I1137	G1077	I1017	A895	E713	LYS	E713	E743	E652	E592	LYS	A470	Q409	G347	L286	L224	L162
A1138	A1078	V1018	E956	E714	LYS	E714	V714	L653	M593	LYS	K471	M410	I348	L287	K225	K163
E1139	S1079	D1019	F897	M776	THR	M776	A715	L654	G594	THR	G472	P411	I349	D288	K226	K164
K1140	L1080	P1020	M958	S777	LYS	S777	V716	L655	D595	THR	P473	S412	R390	M289	L227	K165
L1141	A1081	V1021	F959	R778	ASN	R778	K717	Q656	E596	LYS	V474	F413	M351	V290	S228	E172
H1142	F1082	D1022	Q960	Y779	LEU	Y779	M718	S657	P598	LYS	L475	L414	V352	V291	S229	K173
V1143	M1083	S1023	L961	T780	SER	T780	K719	T658	P598	LYS	R476	Q415	K353	S292	L230	V174
L1144	L1084	T1024	V962	D781	SER	D781	R781	R659	G599	LYS	M477	S416	S354	L293	L231	T169
L1145	I1085	L1025	K963	R782	ASN	R782	K722	L660	V600	THR	C478	V417	M355	F294	C232	L171
M1146	V1086	R1026	R964	H783	GLU	H783	D723	P661	M601	THR	I479	A418	K396	E295	M233	L171
K1147	R1087	D1027	T965	V784	ALA	V784	E724	L662	M602	LYS	S480	S419	K357	V296	K236	E172
A1148	F1088	F1028	R966	R785	ALA	R785	L725	L663	L603	LYS	L487	V426	L359	L298	P242	L180
K1149	F1089	G1029	F967	Q786	TRP	Q786	L726	S664	P604	LYS	V482	L421	L360	L299	P242	L180
L1150	R1090	G1030	V968	L787	L848	L787	A727	G665	T605	LYS	V483	L422	K299	K299	M238	E176
R1151	E1091	R1031	L968	Y788	E849	Y788	S728	P666	S686	LYS	H484	Y423	I361	E239	E239	L177
L1152	E1092	C1032	L970	Y789	E850	Y789	C729	V667	D607	LYS	Q485	L424	A362	C301	E240	L178
L1153	E1093	I1033	R971	K790	R851	K790	L730	R668	P608	LYS	Q486	D425	I363	A302	D241	L178
S1094	S1094	R1034	L972	D791	R852	D791	T731	L669	A609	LYS	L487	T426	R364	R303	P242	L180
R1155	L1095	E1035	R973	I792	R853	I792	F732	L670	A610	LYS	I488	V427	G365	T304	Q243	L181
G1156	V1096	F1036	V914	L793	R854	L793	L733	S671	M611	LYS	I488	V427	G365	T304	Q243	L181
F1157	E1097	L1037	R977	F794	E855	F794	L734	L672	M612	LYS	I490	E429	G367	V306	T244	E183
P1158	Q1098	K1038	Q978	C795	W856	C795	S735	T673	H613	LYS	C491	V430	L368	E307	R246	V184
F1159	F1099	M1039	V979	L796	R857	L796	F737	V674	P614	LYS	S492	Y431	F369	L308	E247	H185
S1160	S1160	S1040	T980	R918	R858	R918	H738	R675	A615	LYS	K493	T432	A370	K309	I248	P186
A1161	F1101	I1041	R981	G798	L859	G798	H738	A677	K616	LYS	P494	P433	G371	K310	F249	E187
S1162	E1102	K1042	Q982	V799	G860	V799	M739	A677	P617	LYS	V495	V434	G371	K310	M250	E188
L1163	A1103	Q1043	L983	L800	S861	L800	I740	K678	K618	LYS	V496	L435	C373	P251	M189	E188
C1164	L1104	I1044	V984	K801	L862	K801	I741	L678	D619	LYS	L497	E436	K374	F251	M189	E188
V1105	V1105	T1045	E985	T802	G863	T802	E742	K681	F620	LYS	PRU	H437	V375	A315	V252	L190
L1166	L1106	P1046	R986	S803	G864	S803	L743	Y682	E598	LYS	LYS	L438	I376	L316	L253	M191
L1167	Y1107	Q1047	L987	A804	PHE	A804	D744	PHE	A622	LYS	GLY	V439	N377	E317	A255	M192
L1168	M1108	Q1048	V988	L805	GLU	L805	V745	GLU	F623	LYS	PRO	V440	K378	S318	E256	A193
F1109	F1109	Q1049	V989	M867	GLY	M867	R746	GLY	I624	LYS	GLU	M441	K379	F319	R257	E194
S1110	S1110	E1050	Q990	K868	VAL	K868	A746	VAL	M625	LYS	SER	M441	D890	L320	P258	L196
K1170	L1111	K1051	A929	R869	SER	L626	V748	SER	L626	LYS	GLU	T443	V391	K321	Q259	F197
L1172	L1112	S1051	R930	L870	PRO	L870	V749	PRO	V627	LYS	SER	D444	K382	G322	I260	R198
L1173	L1113	P1053	H993	L871	LYS	L871	P750	LYS	E628	LYS	GLU	S445	F383	V323	D261	A199

M2104	F2043	L1981	D1921	S1861	L1679	ALA	G1556	P1493	K1422	K1361	I1301	L1236	A1174
H2105	D2044	I1982	A1922	T1862	A1680	THR	E1557	G1494	I1423	D1362	AL1302	A1237	H1175
R2106	F1923	F1983	F1923	F1863	A1681	THR	F1558	D1495	T1424	L1363	M1303	C1176	C1176
S2107	L1984	L1984	T1924	M1743	T1682	ILE	F1559	E1496	A1425	C1364	H1304	P1239	G1177
G2108	K1985	K1985	K1745	K1745	K1683	LEU	Q1426	R1497	Q1426	M1365	L1240	T1240	R1178
L2109	L1986	L1986	M1926	Q1866	L1684	GLN	S1561	Q1498	S1427	T1366	L1306	L1241	P1179
G2110	V2049	R1987	M1927	L1867	L1688	HIS	L1562	C1499	L1428	H1367	L1307	L1242	Q1180
Q2112	Q2050	L1988	A1928	L1868	L1686	TRP	F1563	L1500	E1429	L1368	A1308	Y1243	THR
G2113	S2051	R1989	G1929	K1869	H1687	LYS	F1564	F1501	M1369	M1369	ALA	Y1243	GLU
E2114	F1990	K1870	E1930	K1870	L1688	LYS	E1565	L1431	R1370	R1370	GLY	F1248	CYS
E2115	P1991	M1871	M1931	M1871	K1689	CYS	L1566	L1502	L1431	L1502	LYS	S1249	ARG
D2116	Y2064	F1992	Q1932	G1872	G1690	ASP	I1567	D1504	L1372	CYS	CYS	L1250	HIS
S2117	S2065	L1993	L1933	L1873	Q1691	S1630	M1568	L1505	A1433	PHE	PHE	Q1250	LYS
V2118	S2066	Y1994	L1934	Y1874	A1692	W1632	T1569	S1506	M1435	GLY	GLY	A1252	SER
R2119	Q2057	R1995	E1935	K1875	E1570	W1633	E1570	K1507	L1436	THR	THR	T1253	ILE
R2120	D2058	L1996	R1936	L1876	L1694	A1634	L1571	K1508	Y1437	GLY	GLY	T1254	GLU
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R2126	A2062	K2000	Y1940	R1880	F1698	L1575	D1576	L1514	V1443	ASN	ASN	D1258	LYS
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K2134	Q2071	R2009	I1949	L1889	S1706	L1646	Q1584	G1522	D1444	E1328	E1328	E1266	ASN
N2135	R2072	E2010	S1950	H1890	L1707	A1647	S1585	G1523	K1456	Q1390	R1329	Y1267	ARG
D2136	D2073	A2011	V1951	H1891	E1708	L1648	S1586	L1524	Q1457	Y1391	Y1390	M1268	SER
F2137	F2074	E2012	I1952	K1892	E1709	L1649	V1587	C1525	L1458	M1392	M1331	T1269	PRO
V2138	R2075	R2013	C1953	L1893	L1710	A1650	K1591	E1526	H1459	A1393	Y1332	F1270	ASN
V2139	V2076	E2014	C1954	H1894	R1711	H1651	R1460	ARG	R1460	H1394	S1333	I1271	LEU
L2140	R2077	G2017	F1955	K1895	H1712	L1652	M1592	VAL	L1468	L1402	K1334	E1272	TRP
N2141	D2078	D2018	L1957	I1897	L1713	Q1654	V1593	VAL	G1462	M1403	K1342	Q1280	LEU
I2142	V2080	S2019	M1957	N1897	E1715	L1655	S1594	SER	L1464	E1343	E1343	V1281	LYS
R2143	V2081	D2020	L1959	Q1898	Q1716	D1656	A1595	LEU	H1465	V1337	T1336	R1275	ASP
L2144	L2081	D2021	L1959	V1899	L1717	S1657	L1597	LEU	H1466	C1399	V1338	V1276	VAL
F2145	E2082	G2021	K1960	F1900	I1718	S1658	M1598	LEU	H1466	M1400	V1339	G1277	LEU
A2146	L2083	P2022	F1961	H1901	H1721	VAL	G1599	PRO	L1468	I1341	R1340	A1278	K1213
E2084	M2085	S2023	Y1962	G1902	F1722	PHE	M1600	ALA	Q1471	M1402	M1341	L1279	E1214
K2148	D2086	Y2024	Q1963	S1903	P1723	ASN	L1601	VAL	S1472	K1404	E1342	Q1280	E1215
L2149	D2086	M2025	G1964	I1904	M1724	THR	D1602	SER	L1472	L1405	F1344	L1282	G1216
V2150	E2087	L2028	L1966	L1905	M1724	THR	Q1603	SER	L1475	L1406	T1345	G1283	S1218
I2151	N2089	S2029	F1967	E1907	Q1725	SER	F1604	THR	H1476	K1407	T1346	G1284	F1219
T2153	R2090	Y2030	S1968	G1908	S1726	HIS	F1605	ALA	H1477	M1408	T1347	E1285	L1220
E2154	C2093	L2081	E1969	M1909	R1727	GLY	R1606	SER	S1478	S1409	L1348	A1286	I1221
E2155	M2094	A2032	K1970	E1910	F1728	PHE	E1607	LEU	V1479	P1410	L1349	Q1287	F1224
F2156	A2095	D2033	P1971	L1911	P1730	PRO	R1608	GLY	G1480	Y1411	M1350	S1288	F1224
R2158	P2096	S2034	E1972	L1912	P1731	GLU	ASN	SER	T1481	K1412	T1351	L1291	G1227
P2159	L2097	T2035	K1973	K1913	T1732	GLN	GLN	SER	T1481	D1413	S1352	L1291	G1227
L2160	T2098	S2037	L1975	L1915	G1733	GLM	LYS	GLN	E1482	I1414	P1353	K1292	C1228
A2161	A2099	E2038	L1976	L1916	P1734	HIS	HIS	GLM	L1483	L1415	E1354	L1292	C1228
K2162	L2100	E2039	I1977	I1917	R1736	VAL	GLN	GLY	L1484	E1416	G1355	A1295	Q1230
R2163	V2101	M2040	F1978	K1917	F1736	GLY	GLY	SER	S1485	T1417	H1356	F1297	Q1231
W2164	K2102	S2041	E1979	L1918	M1737	LEU	L1486	GLY	L1486	H1418	K1357	F1297	P1232
L2165	H2103	Q2042	L1798	L1988	M1738	LYS	L1486	LEU	I1491	L1420	L1359	E1299	G1234
			E1799	E1799	E1799	LEU	L1678	LEU	A1492	E1421	K1360	S1300	I1235

S3083	Q3084	I3019	L2968	L2897	Q2834	S2774	M2534	M2473	L2411	K2350	P2226	S2166
E3085	E2960	D3020	A2959	L2898	A2835	Z2775	T2636	Y2474	Y2442	Q2351	K2227	P2167
L3086	A2961	S3021	E2960	R2899	L2836	R2776	L2636	M2475	F2443	E2352	R2228	L2168
S3087	A2962	L2901	L2837	L2900	L2837	H2777	D2637	I2476	Q2414	Q2353	A2229	L2169
L3088	S2963	P3025	D2839	L2902	Q2838	G2778	L2539	L2477	L2415	L2354	V2230	Q2170
L3089	L2964	D3026	F2840	A2903	F2840	L2780	L2540	M2478	K2416	T2355	F2231	L2171
Y3090	L2965	L3027	M2841	E2904	L2781	P2781	A2541	M2479	S2417	Q2295	R2232	A2172
L3091	S2966	N3028	R2842	L2905	D2782	D2782	L2542	L2480	D2418	S2296	H2233	A2173
L3092	E2967	K3029	F2843	L2906	L2783	L2783	N2543	H2481	F2420	F2360	N2234	S2174
Q3093	A2968	L3030	Q2844	A2907	Q2784	Q2784	S2544	D2482	F2421	I2361	L2235	E2175
D3094	A2969	W3031	M2845	V2910	L2785	L2785	L2545	N2483	V2422	V2362	E2236	N2176
D3095	K2970	K2970	T2846	V2911	K2786	K2786	L2546	Y2484	Q2422	V2362	I2237	M2177
V3096	Q2971	Q2971	T2847	R2911	H2787	H2787	S2547	R2485	Y2423	C2368	I2238	G2178
D3097	Y2972	G2972	F2850	R2912	S2788	S2788	F2548	P2487	M2424	L2364	K2239	G2179
K3098	D2973	K2913	T2850	K2913	S2789	S2789	K2549	E2488	R2425	N2365	T2240	E2180
A3099	E2974	A2914	F2851	R2914	L2790	L2790	L2550	E2488	R2426	V2374	L2241	G2181
K3100	A2975	R2915	P2852	R2915	L2791	L2791	L2551	S2489	D2428	N2305	V2242	H2182
Y3101	L2976	L2916	P2853	P2917	T2792	T2792	V2552	E2497	E2429	N2306	E2243	H2183
Y3102	K2977	P2917	F2854	P2917	P2793	P2793	P2553	V2552	D2430	M2307	C2244	Y2184
Y3103	M2978	P2918	V2855	P2918	L2794	L2794	L2554	D2482	E2431	S2308	C2245	M2185
K3104	Q2979	D2919	S2856	D2919	Q2795	Q2795	L2556	D2494	R2431	R2311	K2246	V2186
N3105	D2980	V2920	C2857	V2920	A2796	A2796	S2557	S2495	Q2432	P2372	D2247	Y2187
G3106	W2981	L2921	I2858	L2921	V2797	V2797	L2557	E2497	L2374	Y2312	C2248	E2188
I3107	W2982	W2982	Q2859	Q2922	A2798	A2798	A2558	I2488	V2434	K2313	L2249	I2189
Q3108	D2983	K2923	D2860	K2923	Q2799	Q2799	T2559	F2489	L2436	E2314	L2251	V2190
S3109	R3046	V2924	L2861	V2924	R2800	R2800	N2560	Q2500	D2437	Y2316	P2252	A2191
F3110	S3047	E2925	S2862	E2925	D2801	D2801	F2561	L2501	F2377	R2311	P2252	L2192
K3111	K3048	L2926	C2863	L2926	P2802	P2802	L2562	A2502	F2378	Y2312	P2252	I2193
Q3112	T2987	A2927	Q2864	A2927	L2803	L2803	L2563	Y2439	M2379	A2318	R2254	L2194
N3113	E2988	K2928	H2865	K2928	L2804	L2804	L2564	K2503	Y2440	K2319	L2255	S2195
S3114	A2989	L2929	A2866	L2929	A2805	A2805	E2564	D2504	K2441	A2320	L2256	V2196
S3115	E2990	Y2930	A2867	Y2930	A2806	A2806	L2565	V2505	M2442	E2321	F2257	T2197
S3116	K2991	R2931	L2868	R2931	Q2807	Q2807	L2567	L2506	M2443	V2382	E2258	G2198
I3117	D2992	S2932	L2869	S2932	L2808	L2808	M2568	Q2507	P2444	R2323	E2258	L2199
D3118	F2993	I2933	S2870	I2933	F2809	F2809	S2569	G2509	K2445	L2385	F2260	A2200
W3119	W2994	Q2934	L2871	Q2934	S2810	S2810	P2570	L2510	L2446	L2386	S2261	T2201
E2995	E2995	E2935	D2872	E2935	S2811	S2811	D2571	I2511	P2448	P2387	G2262	P2202
L2996	L2996	L2996	P2873	L2996	L2812	L2812	Y2572	D2512	V2449	K2388	K2263	T2203
S2997	S2997	D2937	A2874	D2937	F2813	F2813	M2574	I2514	E2450	F2389	D2264	G2205
S2998	S2998	V2938	A2875	V2938	L2814	L2814	N2575	P2515	L2451	H2390	P2265	V2205
L2999	L2999	L2939	V2876	L2939	G2815	G2815	M2576	P2516	R2452	G2391	P2266	P2206
I3000	I3000	R2940	S2877	R2940	L2816	L2816	P2576	L2517	E2453	V2392	G2269	D2208
C3001	C3001	G2941	A2878	G2941	L2817	L2817	M2576	L2518	L2454	K2394	N2270	E2209
Y3002	Y3002	L2942	A2882	L2942	K2818	K2818	GLU	Q2518	L2455	T2395	S2271	V2210
N3003	N3003	F2943	S2883	F2943	E2819	E2819	HIS	I2519	M2456	N2396	V2272	L2211
M3068	H3004	T2944	L2888	T2944	M2820	M2820	PRO	I2520	P2457	I2336	G2273	A2212
L3069	G2945	S2945	G2889	G2945	D2821	D2821	LEU	E2521	V2458	L2337	G2274	N2213
H3070	A3006	E2946	Q2885	E2946	K2822	K2822	SER	R2522	V2459	E2338	Q2275	R2214
E3007	E3007	I2947	Q2886	I2947	F2823	F2823	GLU	N2523	E2460	E2339	L2276	L2215
M3008	M3008	G2948	P2887	G2948	K2824	K2824	CYS	F2524	V2461	V2401	L2277	L2216
K3009	T2949	T2949	V2888	T2949	T2825	T2825	GLN	M2525	V2462	L2402	G2278	N2217
S3010	K2950	G2950	G2889	K2950	L2826	L2826	PHE	S2526	L2403	C2342	G2278	F2218
L3011	Q2951	I2890	I2890	Q2951	S2827	S2827	GLN	H2527	R2404	E2342	I2279	L2219
I3012	I2952	L2891	L2891	I2952	E2828	E2828	GLU	E2528	V2405	M2281	V2280	L2219
Y3013	Y3013	T2953	L2892	T2953	K2829	K2829	THR	T2529	T2467	V2405	M2281	M2220
G3014	Q2954	Q2954	L2893	Q2954	M2830	M2830	THR	E2530	C2468	E2406	M2282	K2221
S2955	E2894	L2831	E2894	S2955	L2831	L2831	ILE	L2531	C2469	G2407	M2282	H2222
A2956	E2895	L2832	E2895	A2956	L2832	L2832	ASP	L2531	R2470	M2408	D2284	V2223
L2957	L2957	T2833	A2896	L2957	T2833	T2833	SER	S2533	Q2472	E2410	P2286	H2225

P4072	F4011	A3949	F3887	K3825	E3765	G3703	D3641	V8514	L3454	N3327	K3267	S3143
A4073	D4012	T3950	V3888	A3826	Q3766	Q3704	K3642	Q3514	K3465	I3328	T3268	F3144
F4074	W4013	Q3951	K3889	A3827	L3767	Y3705	F3643	H3516	L3466	I3329	R3269	I3145
R4075	K4014	F3952	M3890	Y3828	F3768	D3706	H3644	S3517	N3457	A3330	D3270	S3146
D4076	M4015	F3953	S3891	L3829	Q3769	G3707	G3645	P3581	S3458	G3331	D3271	K3147
F4077	F4016	V3955	T3892	S3830	Y3770	R3708	S3649	E3519	N3459	T3332	M3272	Q3148
V4078	E4017	P3956	S3893	D3831	M3771	G3709	S3649	E3460	E3460	T3333	L3273	G3149
A4079	Q4018	E3957	P3894	R3832	N3772	G3709	K3650	I3461	A3396	T3334	V3274	N3150
K4080	L4019	L3958	F3897	R3833	K3773	P3711	L3651	R3522	R3462	R3335	S3275	L3151
A4081	M4020	P3959	F3897	A3834	I3774	E3714	L3652	D3523	I3463	I3336	M3276	S3152
R4082	L4021	Q3960	L3898	P3835	L3775	E3715	R3653	N3524	K3464	I3337	V3277	S3153
G4083	K4022	F3961	A3899	P3836	A3776	Y3715	M3654	Y3525	F3465	A3338	Q3278	Q3154
S4084	K4023	L3900	L3900	C3837	Q3777	H3716	K3655	P3526	P3466	N3339	S3279	N3155
K4085	G4024	R3963	A3901	E3838	D3778	V3717	L3656	Q3527	K3467	A3340	Y3280	P3156
D4086	W4027	T3964	S3902	L3839	S3779	R3718	S3657	A3528	I3468	L3341	C3281	R3159
H4087	R4028	R3965	H3903	K3840	A3780	I3719	D3657	L3529	L3469	S3342	R3282	L3160
M4088	Q4029	Q3966	F3904	D3841	C3781	A3720	F3659	V3530	Q3470	V3345	L3283	L3161
I4089	I4030	F3967	A3905	S3842	S3782	G3721	N3660	Y3531	F3471	F3349	S3284	L3162
R4090	E4031	L3968	S3906	L3843	Q3783	F3722	D3661	F3532	I3472	L3348	H3285	T3163
A4091	I4031	N3969	S3907	T3844	A3784	D3723	L3662	R3533	E3473	A3349	C3286	W3164
Q4092	M4032	L3970	H3908	T3844	L3785	R3724	T3663	I3534	R3474	A3349	R3287	
E4093	V4033	M3971	A3909	S3847	L3786	K3725	M3664	L3535	Y3475	E3350	S3288	R3166
P4094	A4034	L3972	L3910	G3848	Q3787	R3726	M3665	S3536	Y3476	I3351	R3289	T3165
E4095	E4035	P3973	I3911	K3849	L3788	V3727	L3666	S3537	E3477	E3352	S3290	R3167
S4096	K4036	K3974	C3912	H3850	R3789	L3728	L3667	E3538	E3478	E3353	Q3291	Y3168
G4097	H4037	K3975	I3913	H3850	T3790	M3729	L3668	S3539	T3479	D3354	G3292	P3169
L4098	W4038	E3976	S3914	G3853	Y3791	A3730	K3669	Y3540	L3480	K3355	C3293	K3172
S4099	Y4039	T3977	H3915	A3854	S3792	S3731	M3670	S3541	R3481	C3294	S3294	K3173
E4100	P4040	Q3978	V3916	L3855	F3793	L3732	N3671	F3542	L3482	R3357	E3295	D3174
E4101	R4041	L3979	I3917	M3856	Q3794	R3733	K3672	K3543	M3483	R3358	F3296	R3175
T4102	Q4042	L3980	L3918	L3857	P3795	R3734	D3673	T3544	T3484	Q3297	V3297	
Q4103	K4043	M3981	G3919	M3858	M3796	P3735	L3674	K3485	Q3423	L3359	L3298	M3176
L4104	L4044	S3982	I3920	L3859	T3797	R3736	K3675	E3486	Q3424	LEU	L3299	M3177
K4105	C4045	I3983	D3921	K3860	S3798	R3737	P3676	H3549	R3425	GLU	K3299	N3177
Y4106	Y4046	M3984	G3922	G3861	I3738	L3738	G3677	S3487	R3426	LEU	M3240	L3178
L4107	A4047	V3985	R3923	A3862	L3800	I3739	G3678	K3551	S3488	GLY	K3301	W3179
M4108	K4048	H3986	L3919	L3863	G3801	I3740	N3679	K3552	Y3490	GLY	M3242	D3180
D4109	R4049	A3987	L3925	R3864	L3802	R3741	L3680	E3553	P3491	GLY	S3303	D3181
Q4110	K4050	L3988	M3926	T3865	L3803	G3742	K3681	F3554	C3492	GLY	S3305	I3182
A4111	L4051	R3989	N3927	E3866	E3804	H3743	E3682	V3555	M3493	GLU	L3307	I3183
T4112	A4052	A3990	F3928	T3867	L3806	R3746	C3683	A3556	Q3494	ASP	D3308	T3184
D4113	G4053	F3991	M3929	T3869	E3807	E3747	S3684	R3557	F3495	GLY	E3309	N3185
P4114	A4054	V3990	V3930	S3870	N3808	H3748	P3685	I3558	I3496	GLY	E3309	N3185
M4115	M4055	S3993	A3931	F3871	L3809	P3749	M3687	K3559	S3497	LYS	Q3249	R3186
I4116	P4056	D3994	M3932	F3871	T3809	F3750	K3688	S3560	M3498	GLY	N3310	I3188
G4117	A4057	L3997	E3933	R3872	V3810	F3750	S3688	E3438	E3438	V3373	M3311	F3189
G4118	V4058	T3997	T3934	K3873	T3811	L3751	D3689	K3561	L3439	I3374	V3312	L3190
R4119	R4109	L3998	G3935	R3874	L3812	V3752	F3690	L3562	Q3440	A3375	S3313	K3192
T4120	T4060	T3999	G3936	E3875	K3813	K3753	K3691	D3563	Q3441	G3376	S3314	K3193
W4121	C4061	M4000	V3937	S3876	D3814	G3754	V3692	Q3564	Y3442	L3377	Y3315	E3194
D4122	D4062	T4001	I3938	K3877	L3815	G3755	E3693	G3565	P3443	Y3378	S3317	E3195
G4123	E4063	M4002	G3939	K3877	L3816	G3756	F3694	Y3567	A3504	Q3379	K3318	K3196
W4124	L4064	D4003	I3940	P3879	L3817	D3757	L3695	L3505	L3445	R3380	L3318	T3198
E4125	L4065	F4004	D3941	A3880	N3818	L3758	R3696	L3506	V3446	A3381	N3319	T3199
P4126	L4066	F4005	F3942	S3881	T3819	R3759	P3697	Q3569	V3447	F3382	I3320	K3260
W4127	G4067	V4006	G3943	L3882	M3820	Q3760	E3698	F3571	K3449	G3383	L3321	E3261
H4068	H4068	K4007	H3944	L3883	S3821	D3761	L3699	I3572	Q3510	H3384	A3322	L3262
E4069	E4069	A4008	G3947	K3884	Q3822	Q3762	L3699	M3574	A3911	L3386	F3323	H3263
K4070	K4070	P4009	S3947	H3885	R3823	R3763	I3701	A3911	K3451	S3386	R3324	K3264
A4071	S4010	S4010	S3948	A3886	E3824	V3764	P3702	L3575	A3513	A3388	Q3326	S3266

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	53451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.51	0/4060	0.75	3/5468 (0.1%)
2	B	0.45	0/4297	0.69	4/5798 (0.1%)
3	K	0.28	0/74	0.36	0/102
4	D	1.44	1/784 (0.1%)	1.23	5/1209 (0.4%)
5	E	1.38	2/822 (0.2%)	1.23	8/1266 (0.6%)
6	C	0.54	1/29665 (0.0%)	0.77	41/40094 (0.1%)
All	All	0.59	4/39702 (0.0%)	0.78	61/53937 (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	12
2	B	0	8
6	C	0	89
All	All	0	109

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	DG	C3'-O3'	-5.56	1.36	1.44
5	E	36	DA	N9-C4	-5.48	1.34	1.37
6	C	2245	TRP	CB-CG	-5.41	1.40	1.50
5	E	39	DA	C3'-O3'	-5.16	1.37	1.44

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2323	LEU	CA-CB-CG	-9.10	94.38	115.30
6	C	734	LEU	CA-CB-CG	-8.80	95.05	115.30
5	E	44	DA	O4'-C4'-C3'	-8.59	100.85	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1257	LEU	CA-CB-CG	-8.10	96.68	115.30
6	C	2884	LEU	CA-CB-CG	-7.98	96.96	115.30

There are no chirality outliers.

5 of 109 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ILE	Peptide
1	A	109	ASP	Peptide
1	A	206	LYS	Peptide
1	A	268	VAL	Peptide
1	A	35	ARG	Peptide

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	3982	0	4064	899	0
2	B	4210	0	4250	708	0
3	K	75	0	74	5	0
4	D	700	0	388	182	0
5	E	733	0	410	214	0
6	C	29066	0	29396	5262	0
All	All	38766	0	38582	6927	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 90.

The worst 5 of 6927 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)
6:C:3809:THR:HA	6:C:3930:VAL:O	1.25	1.32
6:C:3740:ILE:HB	6:C:3748:HIS:O	1.38	1.22
1:A:378:SER:O	1:A:382:PHE:HB3	1.39	1.21
6:C:700:LYS:N	6:C:703:CYS:HG	1.35	1.21
2:B:264:TYR:HB2	2:B:363:LYS:O	1.43	1.19

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 PDB entries followed by that with respect to all EM entries.

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	489/501 (98%)	411 (84%)	74 (15%)	4 (1%)	22	66
2	B	522/536 (97%)	444 (85%)	71 (14%)	7 (1%)	14	56
3	K	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	C	3608/4119 (88%)	2742 (76%)	764 (21%)	102 (3%)	6	39
All	All	4632/5171 (90%)	3609 (78%)	910 (20%)	113 (2%)	11	42

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	368	ARG
6	C	430	VAL
6	C	473	PRO
6	C	905	ILE
6	C	1977	ILE

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 PDB entries followed by that with respect to all EM entries.

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	448/455 (98%)	447 (100%)	1 (0%)	94	97
2	B	474/481 (98%)	473 (100%)	1 (0%)	94	97
6	C	3238/3667 (88%)	3217 (99%)	21 (1%)	89	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4160/4603 (90%)	4137 (99%)	23 (1%)	89 94

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C	2419	ASP
6	C	2480	ILE
6	C	3719	ILE
6	C	2476	ILE
6	C	2507	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
6	C	1374	GLN
6	C	1866	GLN
6	C	3679	ASN
6	C	1426	GLN
6	C	1552	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.