



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 29, 2017 – 03:16 PM EDT

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-20029824

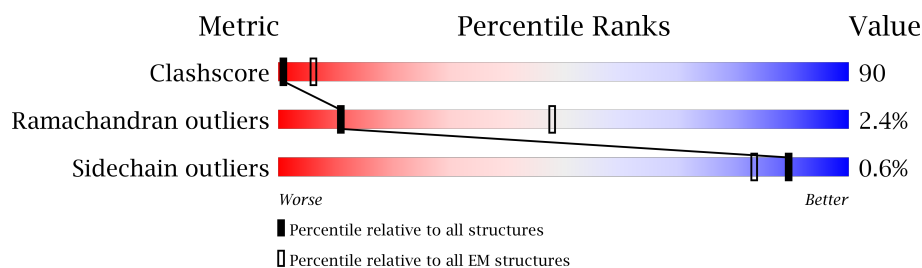
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


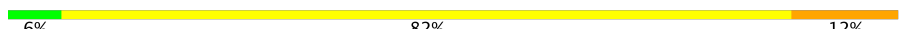
The reported resolution of this entry is 6.60 Å.

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

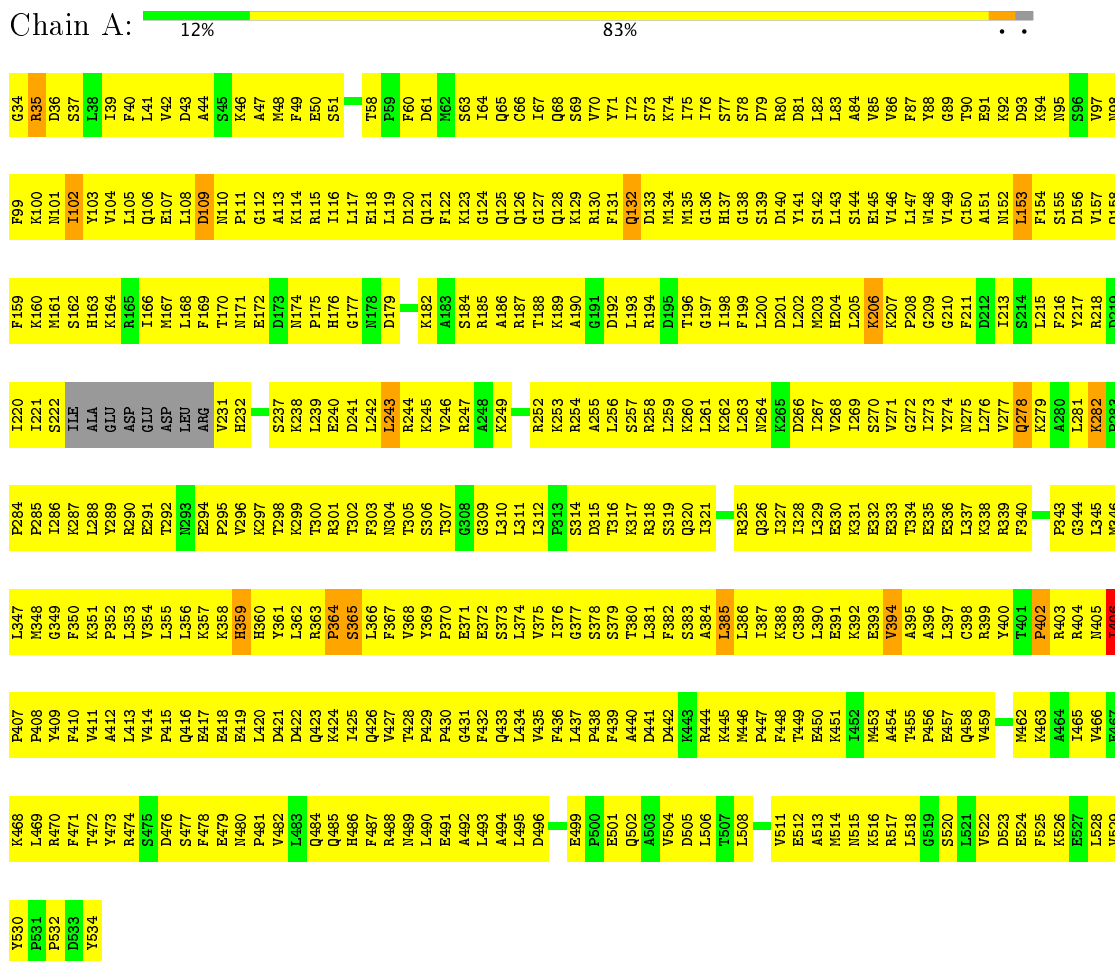
- Molecule 6 is a protein called DNA-dependent protein kinase catalytic subunit.

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

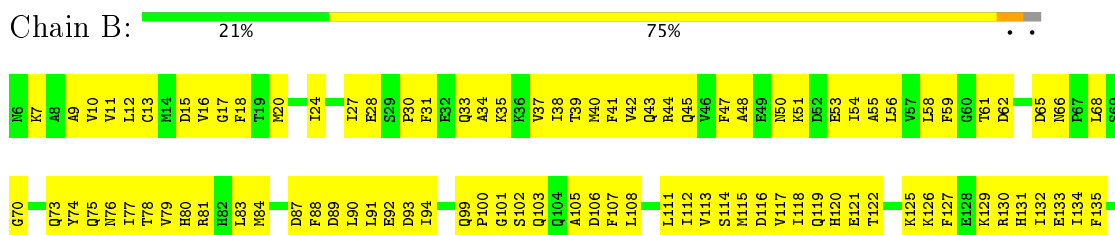
3 Residue-property plots

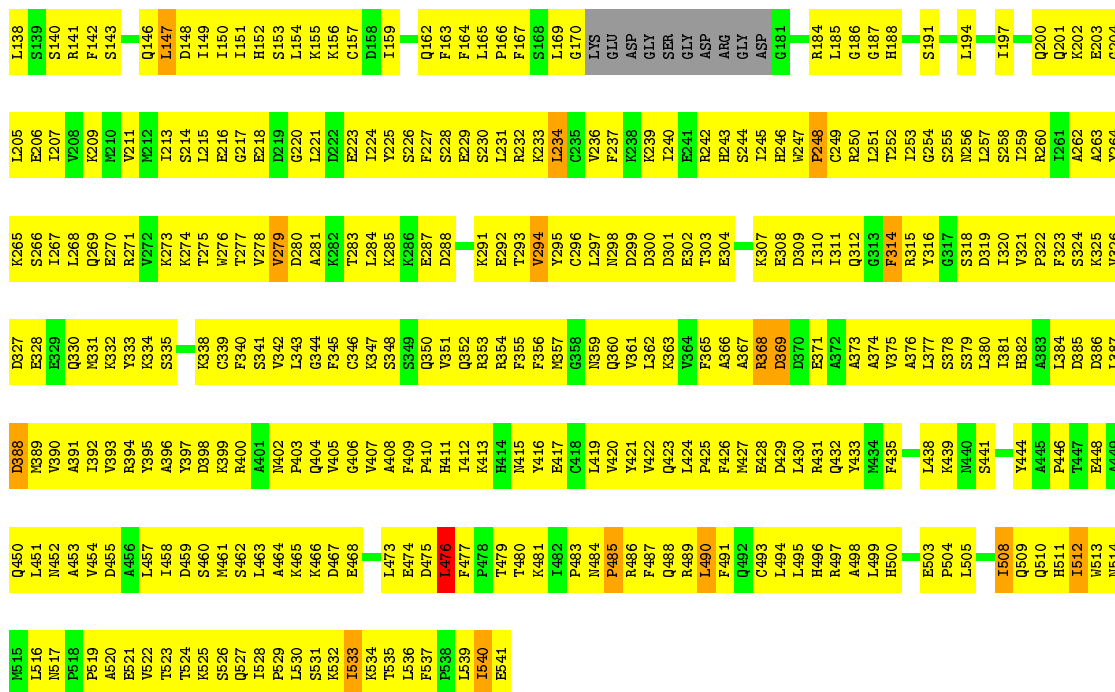
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

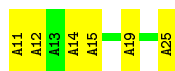


- Molecule 2: X-ray repair cross-complementing protein 5





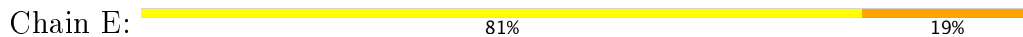
• Molecule 3: PRKDC-Helix



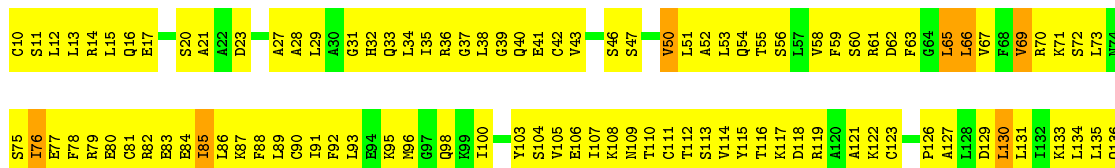
• Molecule 4: DNA (34-MER)



• 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	M754	LYS	R631	V569	ARG	Q448	V386	M326	Y265	G202	R139
D1117	K1057	N997	S875	V875	VAL	K754	HIS	E632	E370	ALA	Y449	E387	Y266	Y265	E203	S140
E1118	S1058	N998	S936	S876	SER	A755	SER	I633	S571	GLY	S450	I388	A328	A266	L204	S141
K1119	L1059	K999	N937	D877	ALA	F756	PRO	L634	V572	GLY	P451	I389	K299	V267	K205	R142
S1120	V1060	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	L1062	E1002	F940	R880	ARG	G759	PRO	R637	L575	ARG	Q454	C392	E332	M268	M208	F147
T1123	L1063	K881	N941	K881	GLU	L760	GLU	Q638	V576	THR	L455	K393	M333	G271	T209	K148
L1124	Q1064	Q1004	L942	S882	ALA	S761	K700	R639	E577	GLY	V456	Q394	H334	L272	L149	L149
Q1125	S1065	D1005	G943	V883	GLN	V762	Y701	E640	K578	LYS	C457	K395	K395	F275	V212	G150
Q1126	L1066	K944	K944	V884	LYS	T763	S702	F641	L579	TRP	C458	F396	K356	A276	R213	E151
C1127	A1067	V1007	A945	A885	GLY	P764	G703	F642	D580	LYS	R459	L397	K337	A277	E214	L152
D1128	L1068	L1008	T946	R886	PHE	L765	F704	E643	E584	VAL	A460	T398	L338	L277	P215	F153
H1129	H1069	A1009	Q947	D887	ASN	L766	A705	P644	E585	PRO	I461	Q399	Q339	H278	K216	S154
A1130	P1070	N948	R888	L1070	LYS	E767	L706	N645	I585	THR	V462	T400	F340	A279	L217	K155
L1131	M1071	E1011	P949	E889	VAL	V768	F707	V646	Q586	TYR	K463	D401	F341	S280	P156	F156
D1132	A1072	A1012	E950	K890	VAL	G769	V708	Y647	T587	K525	V464	D401	M342	Q281	V219	V157
H1133	F1073	I1013	G951	R891	LEU	L770	K709	S648	V588	R526	F465	D405	E343	F282	L220	G158
L1134	K1074	L1014	G952	L892	LYS	M771	F710	F649	G589	H533	R406	D406	Q344	S283	A221	E159
C1135	R1075	D1015	Q953	S893	HIS	G711	G711	S650	E590	V528	A468	F408	F345	T284	C222	L160
R1136	L1076	G1016	G954	F894	LEU	L772	K712	V651	Q591	D529	L468	Y407	Y346	T284	G223	A161
I1137	G1077	I1017	A955	A895	LYS	E713	E713	E652	E592	L530	A470	Q409	G347	L286	L224	L162
A1078	A1078	V1018	V956	V896	LYS	E774	V714	L653	M593	F531	K471	N410	I348	L287	K225	K163
S1079	S1079	D1019	F957	R897	THR	M776	A715	L654	G594	R532	G472	P411	I349	D288	G226	K164
L1080	L1080	P1020	N958	F898	LYS	S777	V716	L655	D595	H533	P473	S412	R390	M289	L227	K165
A1081	V1081	V1021	V959	R899	ASN	L778	K717	Q656	E596	L534	V474	F413	N351	V290	S228	K166
F1082	F1082	D1022	Q960	E900	LEU	M779	M718	S657	P598	V535	L475	L414	V352	V291	S229	A161
H1143	H1083	S1023	L961	M901	SER	Y780	K719	T658	P598	S536	R476	Q415	K353	S292	L230	L169
S1144	H1084	T1024	V962	K902	SER	D781	SER	R659	G599	D537	M477	S416	S354	L293	L231	V170
L1085	L1085	L1025	K963	P903	ASN	R782	K722	L660	V600	E538	C478	V417	M355	F294	C232	L171
M1146	V1086	R1026	R964	V904	GLU	H783	D723	P661	M601	Q539	I479	A418	K396	E295	M233	L171
R1087	R1087	D1027	T965	I905	ALA	M784	E724	L662	M602	M540	S480	S419	K357	V296	K236	L174
F1089	F1089	G1029	F967	L907	R846	Q786	L726	L663	L603	D542	L487	V420	L359	L298	S237	Y175
K1150	K1090	G1030	V968	D908	L848	P787	A727	S664	P604	D542	V482	L421	L360	K299	M238	E176
R1151	R1091	R1031	L968	V909	E849	Y788	S728	G665	T605	S543	H484	L422	S360	K299	E239	L177
L1152	E1092	C1032	L970	F910	E850	Y789	C729	V667	D607	L544	Q465	L424	I361	R300	L178	L178
L1153	E1093	I1033	R971	L911	R851	K790	L730	R668	P608	L546	Q466	D425	I363	A302	D241	G179
S1094	S1094	R1034	L972	P912	R852	D791	T731	L669	A609	D547	L487	T426	R364	A302	P242	L180
R1155	L1095	E1035	A973	R853	R853	I792	F732	L670	A610	E548	I488	V427	G365	T304	Q243	L181
G1156	V1096	F1036	V914	V854	L733	L793	L733	S671	M611	A549	R469	P428	Y366	N305	T244	L182
F1157	E1097	L1037	R977	V855	R854	L794	L734	L672	L612	F550	I490	E429	G367	V306	S245	E183
P1158	Q1098	K1038	Q978	E916	W856	C795	S735	T673	H613	F551	C491	V450	L368	E307	R246	V184
F1159	F1099	M1039	V979	L917	R857	L796	F737	V674	P614	S552	S492	Y431	F369	L308	E247	H185
S1160	S1160	S1040	T980	A918	M858	D797	H738	R675	A615	M554	K493	T432	A370	K309	I248	P186
A1161	F1101	I1041	R981	L919	L859	G798	H738	A677	K616	S555	P494	P433	G371	K310	F249	E187
S1162	E1102	K1042	Q982	T920	G860	Y799	M739	A677	P617	S555	V495	V434	G371	K310	M250	S187
L1163	A1103	Q1043	L983	A921	S861	L800	I740	K678	K618	S556	V496	L435	C373	K313	F251	E188
C1164	L1104	I1044	V984	S922	L862	K801	I741	K678	D619	S557	L497	E436	K374	L313	V252	M189
V1105	V1105	T1045	E985	D923	G863	T802	E742	K681	F620	E558	PRU	H437	V375	A315	V252	L190
L1166	L1106	P1046	F986	R924	G864	S803	L743	Y682	F620	E558	LYS	L438	I376	L316	L253	M191
D1167	Y1107	Q1047	L987	Q925	Q865	A804	D744	PHE	A622	L560	GLY	V439	N377	E317	A255	M192
L1168	M1108	Q1048	V988	T926	R866	L805	V745	GLU	F623	L560	PRO	V439	K378	S318	E256	A193
F1109	F1109	Q1049	V989	K927	M867	R746	R746	GLY	I624	H562	GLU	M441	A378	F319	R257	E194
S1110	S1110	E1050	Q990	V928	K868	A787	VAL	VAL	M625	L563	SER	M441	K379	L320	P258	L196
K1170	K1170	K1051	A929	R869	R869	T809	V748	SER	L626	L564	GLU	T443	D890	K321	Q259	F197
L1172	L1172	S1051	L991	L870	L870	LYS	V749	PRO	V627	Y665	SER	D444	V391	Q322	L260	R198
L1173	L1173	P1053	H993	L871	L871	ASN	P750	LYS	E628	D566	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	F2045	D1983	F1923	F1863	T1681	THR	Y1558	D1495	T1424	L1363	M1303	A1238	C1176	
S2107	L1984	L1984	T1924	D1864	T1682	ILE	F1559	E1496	A1425	C1364	H1304	P1239	G1177	
G2108	K1985	K1985	E1925	T1865	K1683	LEU	R1497	Q1498	Q1426	M1365	L1305	T1240	R1178	
L2109	T2047	L1986	M1926	Q1866	L1684	GLN	S1561	K1498	S1427	T1366	I1306	L1241	P1179	
G2110	V2049	R1987	M1927	L1867	D1685	HIS	L1562	C1499	L1428	H1367	L1307	L1242	Q1180	
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G2113	S2051	R1989	G1929	K1869	H1687	LYS	F1564	P1501	M1369	M1369	ALA	Y1243	GLU	
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E2115	P1991	M1871	M1931	M1871	K1689	CYS	S1566	L1502	L1431	L1431	LYS	S1249	ARG	
D2116	Y2054	L1992	Q1932	G1872	G1690	D1630	I1567	D1504	L1372	CYS	CYS	L1250	HIS	
S2117	S2055	L1993	L1933	Y1873	Q1691	S1630	A1433	L1505	A1433	PHE	PHE	Q1250	LYS	
V2118	S2056	Y1874	L1934	Y1874	A1692	W1632	M1435	S1506	Q1374	GLY	GLY	A1252	SER	
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T2063	K2001	R2001	H1941	Y1881	F1699	P1639	D1576	L1514	V1443	ARG	ARG	L1259	PHE	
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R2065	C1942	S1882	C1942	S1882	T1700	E1640	R1445	L1516	R1445	THR	THR	L1260	VAL	
F2128	R2065	R1883	C1943	R1883	S1701	T1641	R1445	L1516	R1445	G1383	G1383	L1261	VAL	
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K2068	K2068	K1886	M1946	K1886	G1704	A1644	L1582	A1520	L1448	M1386	M1386	L1264	LEU	
R2069	D1947	D1887	C1947	D1887	G1705	V1645	M1583	F1521	S1463	D1388	D1388	L1264	PRO	
L2130	R2070	R2070	A1948	R2070	L1705	V1645	M1583	F1521	S1463	D1388	D1388	E1265	GLY	
R2131	R2071	R2071	R2008	R2071	CYS	L1646	Q1584	G1522	L1468	E1328	E1328	E1265	ASN	
R2132	K2009	K2009	I1949	L1889	L1707	A1647	G1523	G1523	K1456	R1329	R1329	Y1267	ASN	
F2134	E2010	E2010	S1950	H1890	E1708	L1648	S1586	L1524	Q1457	M1268	M1268	M1267	ARG	
N2135	E2011	E2011	V1951	H1890	G1709	L1649	V1587	C1525	Q1458	M1392	M1392	T1269	SER	
D2073	A2011	A2011	V1951	H1890	G1709	L1649	V1587	C1525	Q1458	M1392	M1392	T1269	PRO	
F2074	R2013	R2013	E1952	K1892	L1710	A1650	E1526	E1526	H1459	A1393	A1393	F1270	ASN	
R2075	C1953	C1953	C1953	H1893	R1711	K1394	R1460	L1394	R1460	H1394	H1394	I1271	LEU	
V2076	C1954	C1954	C1954	H1893	R1711	K1394	R1460	L1394	R1460	H1394	H1394	I1271	LEU	
V2077	F1955	F1955	F1955	K1894	L1712	A1652	M1592	VAL	G1462	K1334	K1334	E1272	TRP	
D2078	I1896	I1896	I1896	K1895	L1713	Q1653	V1593	VAL	G1462	K1334	K1334	E1272	TRP	
D2079	N1897	N1897	N1897	N1897	L1714	Q1654	S1594	SER	L1463	T1336	T1336	R1274	LYS	
V2080	Q1898	Q1898	Q1898	Q1898	E1715	L1655	A1595	LEU	L1464	V1337	V1337	T1275	ASP	
L2144	V1899	V1899	F1969	V1899	Q1716	D1656	V1596	LEU	H1465	V1338	V1338	V1276	VAL	
E2082	K1900	K1900	P1900	P1900	L1717	S1657	L1597	LEU	H1466	V1339	V1339	G1277	LEU	
L2145	F1900	F1900	P1900	P1900	L1718	S1658	M1598	LEU	H1467	M1400	M1400	A1278	LEU	
A2146	H1901	H1901	SER	SER	H1721	VAL	G1599	PRO	L1468	I1341	I1341	A1278	LEU	
E2083	G1902	G1902	THR	THR	F1722	ALA	M1600	ALA	L1468	M1402	M1402	L1279	E1214	
M2085	S1903	S1903	ILE	ILE	P1722	PHE	L1601	VAL	Q1471	M1403	M1403	Q1280	E1215	
D2086	Q1904	Q1904	VAL	VAL	P1724	ASN	D1602	LEU	S1472	K1404	K1404	V1281	G1216	
E2087	L1905	L1905	VAL	VAL	M1724	THR	Q1603	SER	Q1472	L1405	L1405	L1282	V1217	
L2088	T1906	T1906	ASP	ASP	M1725	SER	F1604	THR	L1475	K1407	K1407	G1283	S1218	
N2089	E1907	E1907	ALA	ALA	S1726	HIS	F1605	THR	H1476	M1408	M1408	L1284	F1219	
R2090	G1908	G1908	ILE	ILE	R1727	GLY	R1606	SER	H1477	S1409	S1409	E1285	L1220	
C2093	N1909	N1909	ASP	ASP	E1728	SER	E1607	LEU	S1478	L1348	L1348	A1286	I1221	
M2094	E1910	E1910	VAL	VAL	F1729	PHE	R1608	GLY	V1479	M1349	M1349	Q1287	I1221	
A2095	L1911	L1911	LEU	LEU	P1730	PRO	A1609	SER	G1480	M1350	M1350	S1288	F1224	
P2096	L1912	L1912	LYS	LYS	P1731	GLU	ASN	SER	T1481	T1351	T1351	L1291	G1227	
L2097	K1913	K1913	THR	THR	G1732	GLN	GLN	SER	T1481	D1413	D1413	L1291	G1227	
T2098	L1914	L1914	ARG	ARG	T1733	GLN	L1415	GLN	E1482	P1353	P1353	K1292	G1228	
S2099	L1915	L1915	PHE	PHE	R1734	HIS	L1483	HIS	L1415	E1354	E1354	L1292	G1228	
E2099	L1916	L1916	VAL	VAL	P1735	GLM	S1549	GLM	E1416	G1355	G1355	A1295	Q1230	
L2100	K1917	K1917	GLY	GLY	F1736	GLY	L1486	GLY	S1485	H1356	H1356	F1297	Q1231	
V2101	L1918	L1918	LEU	LEU	F1737	THR	L1486	SER	L1486	K1357	K1357	F1297	P1232	
R2102	C1919	C1919	L1798	L1798	M1737	LEU	L1486	SER	L1486	L1368	L1368	L1298	S1233	
H2103	Q2042	Q2042	E1799	E1799	N1738	LYS	L1486	LEU	L1486	L1369	L1369	E1299	G1234	
														I2165

S3083	Q3084	I3019	L2968	L2897	Q2834	S2774	M2534	M2473	L2411	K2350	P2226	S2166
E3085	E3086	D3020	A2959	L2898	A2835	Z2775	T2636	Y2474	Y2442	Q2351	K2227	P2167
L3086	A2961	S3021	E2960	R2899	L2836	R2776	L2536	M2475	F2413	E2352	R2228	L2168
S3087	L2901	F3024	L2837	L2900	L2837	H2777	D2537	I2476	Q2414	Q2353	A2229	L2169
L3088	S2963	P3025	Q2838	L2901	Q2838	G2778	L2415	L2477	L2415	L2354	V2230	Q2170
L3089	D2964	D3026	D2839	L2902	D2839	D2779	L2539	M2478	K2416	T2355	F2231	L2171
Y3090	L2965	L3027	F2840	A2903	F2840	L2780	L2540	M2479	S2417	Q2295	R2232	A2172
L3091	Y2966	N3028	M2841	E2904	M2841	P2781	A2541	L2480	D2418	S2296	H2233	A2173
L3092	S2967	N3029	R2842	L2905	R2842	D2782	L2542	H2481	R2419	S2297	N2234	S2174
L3093	E2968	K3030	F2843	P2906	F2843	L2783	N2543	D2482	F2420	F2360	L2235	E2175
D3094	A2969	M3031	L2844	A2907	Q2784	L2784	S2544	N2483	V2421	I2361	E2236	N2176
D3095	K2970	K3032	M2845	V2910	M2845	L2785	L2545	Y2484	Q2422	V2362	I2237	M2177
V3096	Q2971	E3033	T2847	R2911	T2846	H2786	S2546	R2485	Y2423	C2363	I2238	G2178
D3097	Y2972	F3034	F2850	R2912	T2847	S2788	P2548	P2487	M2424	L2364	K2239	G2179
K3098	K2973	F3035	F2850	G2913	F2850	S2789	K2549	E2488	R2425	N2365	T2240	E2180
A3099	E2974	F3036	F2851	K2914	F2851	L2790	K2549	E2488	R2426	V2364	L2241	G2181
K3100	A2975	Q3037	P2852	R2915	P2852	L2791	L2550	S2489	D2428	N2305	V2242	H2182
Y3101	L2976	E3038	P2853	L2916	P2853	T2792	L2551	S2489	T2368	N2306	E2243	H2183
Y3102	M2977	T3039	F2854	P2917	F2854	P2793	V2552	D2482	D2429	M2307	C2244	Y2184
I3103	K2978	Y3040	V2855	P2918	V2855	L2794	H2553	D2482	E2430	S2370	C2245	M2185
K3104	D2979	L3041	S2856	D2919	S2856	Q2795	F2554	D2494	R2431	F2371	K2246	V2186
N3105	D2980	P3042	C2857	V2920	C2857	A2796	L2556	S2495	Q2432	P2372	D2247	Y2187
G3106	W2981	M3043	Q2858	L2921	Q2858	V2797	L2557	Q2496	K2433	P2373	C2248	E2188
I3107	W2982	M3044	Q2859	L2922	Q2859	A2798	L2558	E2497	V2434	L2374	L2249	I2189
Q3108	D2983	I3045	D2860	K2923	D2860	Q2799	T2559	I2488	C2435	A2375	S2260	V2190
S3109	R3046	I3046	L2861	W2924	L2861	Q2799	T2559	F2489	L2436	E2314	L2251	A2191
F3110	S3047	S3047	E2985	V2925	E2985	R2800	N2560	K2500	D2437	Y2316	P2252	I2192
M3111	K3048	K3048	P2863	L2926	P2863	L2801	F2561	I2438	F2377	E2317	Y2252	I2193
Q3112	T2987	L3049	Q2864	A2927	Q2864	R2802	L2562	A2502	M2379	A2318	R2254	L2194
N3113	E2988	K3050	R2865	K2928	R2865	L2803	L2563	K2503	Y2440	K2319	L2255	S2195
S3114	A2989	L3051	A2866	L2929	A2866	L2804	E2564	D2504	K2441	A2320	L2256	V2196
S3115	E2990	L3052	A2867	V2930	A2867	L2805	M2565	V2505	M2442	E2321	F2257	T2197
I3116	K2991	L3052	L2868	R2931	L2868	L2806	T2567	L2506	M2443	V2322	E2258	G2198
D3118	D2992	F2993	L2869	S2932	L2869	L2807	M2568	Q2508	K2444	R2323	E2258	G2198
V3119	F2993	W2994	S2870	I2933	S2870	F2809	G2569	G2509	F2445	L2324	F2260	A2200
I3120	E2995	E2995	D2872	Q2934	D2872	S2810	P2570	L2510	L2446	L2325	S2261	T2201
L3121	L2996	L2996	P2873	E2935	P2873	S2811	D2571	I2511	P2448	L2326	G2262	P2202
H3122	G2936	G2936	A2874	R2937	A2874	L2812	Y2572	D2512	V2449	K2388	D2264	T2203
Q3123	S2938	T3063	A2875	D2937	A2875	F2813	N2574	I2514	E2450	R2328	D2264	G2205
S3124	L2999	F3064	V2876	V2938	V2876	G2814	M2576	P2515	L2451	F2389	P2265	V2205
R3125	I3000	I3065	S2877	R2940	S2877	G2815	P2576	P2516	R2452	V2392	P2266	P2206
L3126	C3001	D3066	A2878	G2941	A2878	L2817	M2576	L2517	L2454	E2332	D2269	D2208
T3127	Y3002	I3067	A2882	L2942	A2882	K2818	GLU	Q2518	L2455	K2333	N2270	E2209
K3128	N3003	A3068	A2882	F2943	A2882	E2819	HIS	M2456	M2456	E2332	S2271	V2210
L3129	H3004	M3069	S2883	T2944	S2883	M2820	PRO	I2520	P2457	M2335	V2272	L2211
Q3130	L3005	S2945	L2884	S2945	L2884	D2821	LEU	P2521	V2458	I2336	G2273	A2212
S3131	E3007	E3072	Q2885	E2946	Q2885	K2822	SER	R2522	V2459	L2337	I2274	N2213
V3132	E3007	E3072	Q2886	I2947	Q2886	F2823	GLU	M2523	E2460	E2338	Q2275	R2214
Q3133	M3008	L3073	P2887	G2948	P2887	K2824	CYS	F2524	F2461	V2400	L2276	L2215
L3134	K3009	Q3074	V2888	T2948	V2888	T2825	GLN	M2526	V2462	V2401	L2277	L2216
L3135	S3010	K3075	G2889	R2950	G2889	L2826	GLU	M2526	L2462	L2402	G2278	N2217
T3136	L3011	A3076	I2890	S2951	I2890	S2827	ASP	S2526	C2403	C2342	F2218	F2218
E3137	I3012	I3077	R2891	Q2952	R2891	E2828	GLN	H2527	R2404	E2343	V2280	L2219
L3138	Y3013	L3078	L2892	T2953	L2892	K2829	VAL	E2528	V2405	M2281	M2281	M2220
G3139	G3014	E3079	L2893	Q2954	L2893	M2830	THR	T2468	T2468	V2345	K2221	K2221
E3140	L3081	H3080	E2894	S2955	E2894	N2831	ILE	L2531	C2469	A2346	M2282	H2222
F3141	H3081	H3081	E2895	L2832	E2895	L2832	ASP	L2470	E2471	K2347	D2284	V2223
I3142	Y3082	Y3082	A2896	L2957	A2896	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	F3955	S3891	L3829	Q3769	G3707	G3645	P3581	S3458	G3331	D3271	K3147
F4077	M4016	V3956	T3892	S3830	Y3770	R3708	S3649	E3519	N3459	T3332	M3272	Q3148
V4078	E4017	P3957	S3893	D3831	K3771	G3709	S3649	E3460	E3460	T3333	L3273	G3149
A4079	Q4018	L3958	F3894	R3832	N3772	K3710	K3650	A3461	A3461	T3334	V3274	N3150
M4080	K4019	L3959	F3897	R3833	G3773	P3711	L3651	R3522	R3462	R3335	S3275	L3151
A4081	M4020	P3960	F3898	A3834	I3774	E3714	L3652	D3523	L3463	I3336	M3276	S3152
R4082	L4021	F3961	L3898	P3835	L3775	K3715	R3653	N3524	K3464	I3337	V3277	S3153
G4083	K4022	F3962	A3899	P3836	A3776	Y3715	M3654	Y3525	F3465	A3338	Q3278	Q3154
S4084	K4023	L3963	L3900	C3837	Q3777	H3716	K3655	P3526	P3466	N3339	S3279	N3155
K4085	G4024	R3964	A3901	E3838	D3778	V3717	L3656	Q3527	K3467	A3340	Y3280	P3156
D4086	W4027	T3964	S3902	R3839	S3779	R3718	S3657	A3528	L3468	L3341	C3281	R3159
H4087	R4028	R3965	H3903	K3840	A3780	I3719	D3658	R3529	L3469	S3342	R3282	L3160
M4088	Q4029	Q3966	F3904	D3841	C3781	G3720	F3659	V3530	Q3470	V3345	L3283	L3161
I4089	M4030	F3967	A3905	S3842	S3782	A3721	N3660	Y3531	F3471	V3409	S3284	L3162
R4090	E4031	L3968	S3906	L3843	Q3783	F3722	D3661	F3532	I3472	G3348	H3285	T3163
A4091	I4031	N3969	S3907	T3844	A3784	D3723	L3662	R3533	E3473	L3349	C3286	W3164
Q4092	M4032	L3970	H3908	T3844	L3785	K3724	T3663	I3534	R3474	A3349	R3287	M3164
E4093	V4033	M3971	A3909	S3847	L3786	R3725	M3664	L3535	Y3475	E3350	S3288	T3165
P4094	A4034	L3972	L3910	G3848	Q3787	V3726	M3665	S3536	Y3476	I3351	R3289	N3166
E4095	E4035	P3973	I3911	K3849	L3788	R3727	L3666	S3537	E3477	E3352	S3290	R3167
S4096	K4036	K3974	C3912	H3850	R3789	V3728	L3667	E3538	E3478	E3353	Q3291	Y3168
G4097	H4037	K3975	I3913	H3850	T3790	M3729	L3668	S3539	T3479	D3354	G3292	P3169
L4098	W4038	G3976	S3914	G3853	Y3791	A3730	K3669	Y3540	L3480	K3355	C3293	K3172
S4099	Y4039	T3977	H3915	A3854	S3792	S3731	M3670	S3541	R3481	C3294	S3294	M3173
E4100	P4040	L3978	V3916	R3855	F3793	L3732	N3671	F3542	L3482	R3357	E3295	R3174
E4101	R4041	L3979	I3917	M3856	Q3794	R3733	K3672	K3543	M3483	R3358	F3296	D3174
T4102	Q4042	L3980	L3918	L3857	P3795	R3734	D3673	T3544	T3484	Q3297	V3297	P3175
Q4103	K4043	G3981	G3919	M3858	K3796	P3735	D3674	M3603	Q3422	L3359	L3298	M3176
V4104	L4044	S3982	I3920	R3859	T3797	K3736	K3675	E3486	K3485	LEU	L3299	N3177
K4105	C4045	I3983	D3921	K3860	S3798	R3737	P3676	H3549	I3487	GLU	K3299	N3178
Y4106	Y4046	M3984	G3922	G3861	L3800	I3738	G3677	K3550	S3488	LEU	M3240	I3179
L4107	A4047	V3985	R3923	A3862	L3800	I3739	G3678	N3551	S3489	GLY	K3301	M3180
M4108	K4048	H3986	L3919	L3863	G3801	I3740	N3679	K3552	V3490	GLY	M3242	D3181
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	N3185
D4113	G4053	F3991	M3929	R3868	E3807	E3747	S3684	R3557	F3495	GLY	E3309	N3186
P4114	A4054	T3989	V3930	T3869	N3808	H3748	P3685	I3558	I3496	GLY	E3309	N3186
M4115	M4055	S3993	A3931	S3870	N3808	E3749	K3686	K3559	S3497	LYS	Q3249	R3186
I4116	P4056	D3994	M3932	F3871	T3809	F3749	M3687	S3560	M3498	GLY	N3310	I3188
G4117	A4057	R3872	E3933	R3872	V3810	F3750	S3688	E3438	E3438	V3373	M3311	F3189
G4118	V4058	K3873	T3934	K3874	T3811	L3751	D3689	K3561	L3439	I3374	S3312	S3191
R4119	R4109	L3998	G3935	R3874	L3812	V3752	F3690	L3562	Q3440	A3375	F3252	K3192
T4120	T4060	T3999	G3936	E3875	K3813	K3753	K3691	D3563	Q3441	G3376	S3313	K3193
M4121	C4061	M4000	V3937	S3876	D3814	G3754	V3692	Q3564	Y3442	L3377	O3254	E3194
D4122	D4062	T4001	I3938	K3877	L3815	G3755	E3693	G3565	P3443	Y3378	M3257	E3195
G4123	E4063	M4002	G3939	K3877	L3816	E3756	F3694	V3567	A3504	Q3379	S3317	K3196
W4124	L4064	D4003	I3940	P3879	L3817	D3757	L3695	L3505	L3445	R3380	K3318	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	K3260	P3199
W4127	G4067	V4006	G3943	L3882	M3820	Q3760	E3698	F3571	K3449	G3383	L3321	E3261
H4068	H4068	K4007	H3944	L3883	S3821	D3761	L3699	I3572	M3450	H3384	A3322	L3262
E4069	E4069	A4008	G3947	K3884	Q3822	Q3762	L3699	N3574	Q3510	L3386	F3323	H3263
K4070	K4070	P4009	S3947	R3885	R3823	R3763	E3700	A3574	A3911	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.