



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:50 AM UTC

PDB ID : 1N6E / pdb_00001n6e
Title : tricorn protease in complex with a tridecapeptide chloromethyl ketone derivative
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

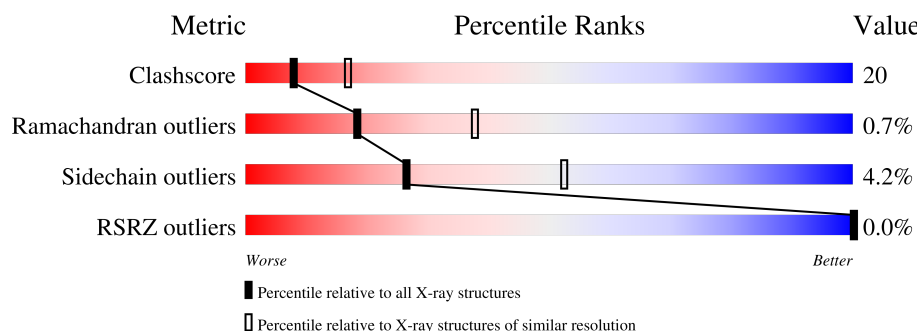
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1071	
1	C	1071	
1	E	1071	
1	G	1071	
1	I	1071	
1	K	1071	

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Mol	Chain	Length	Quality of chain
2	B	14	50% 29% 7% 14%
2	D	14	50% 29% 7% 14%
2	F	14	36% 36% 14% 14%
2	H	14	50% 29% 7% 14%
2	J	14	50% 29% 7% 14%
2	L	14	7% 43% 29% 14% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 50544 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 Tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	C	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	E	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	G	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	I	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	K	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			

- Molecule 2 is a protein called DQTQKAAAELTFF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	D	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	F	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	H	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	J	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	L	12	Total	C	N	O	0	0	1
			87	58	13	16			

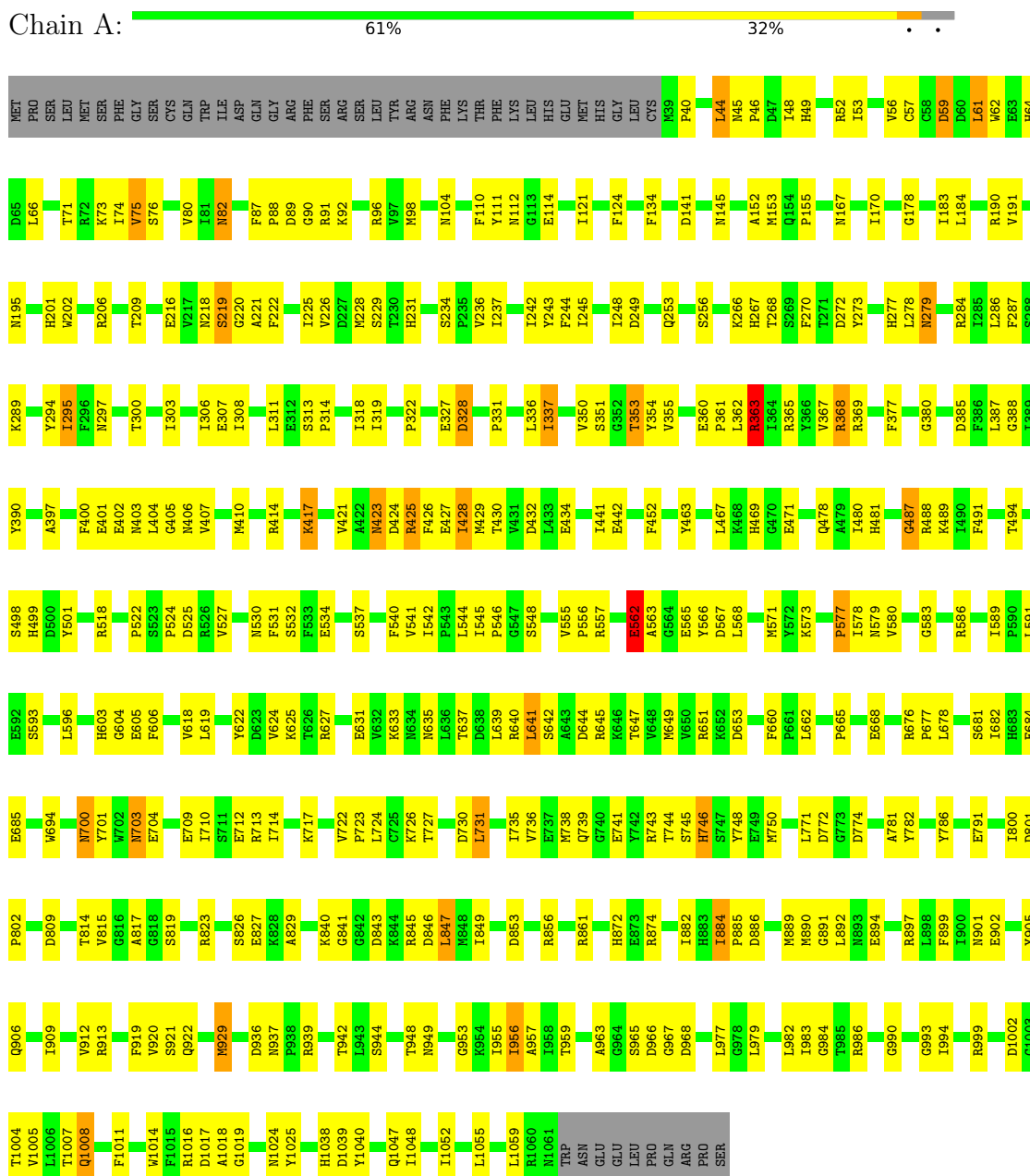
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total 178	O 178	0	0
3	B	2	Total 2	O 2	0	0
3	C	172	Total 172	O 172	0	0
3	D	2	Total 2	O 2	0	0
3	E	138	Total 138	O 138	0	0
3	F	5	Total 5	O 5	0	0
3	G	154	Total 154	O 154	0	0
3	H	2	Total 2	O 2	0	0
3	I	157	Total 157	O 157	0	0
3	J	2	Total 2	O 2	0	0
3	K	146	Total 146	O 146	0	0
3	L	2	Total 2	O 2	0	0

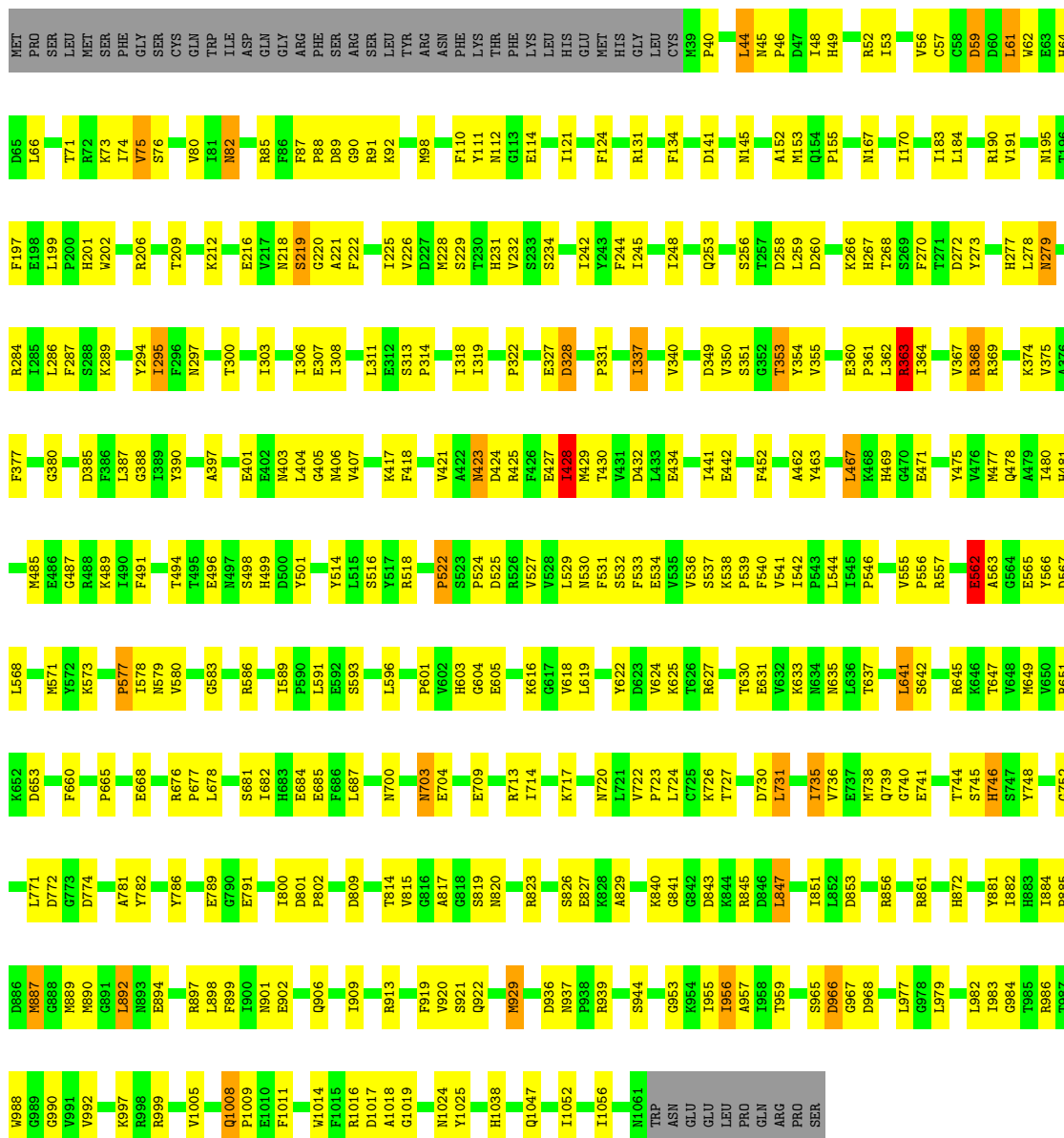
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

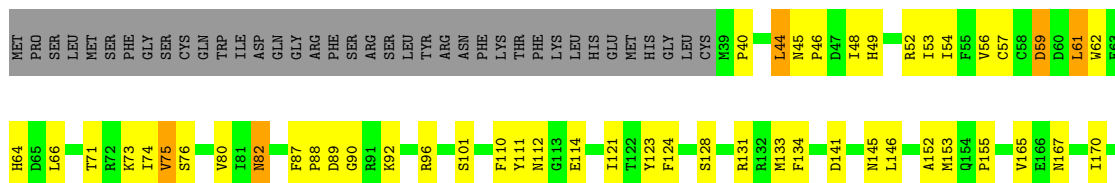
- Molecule 1: Tricorn protease



Chain C:

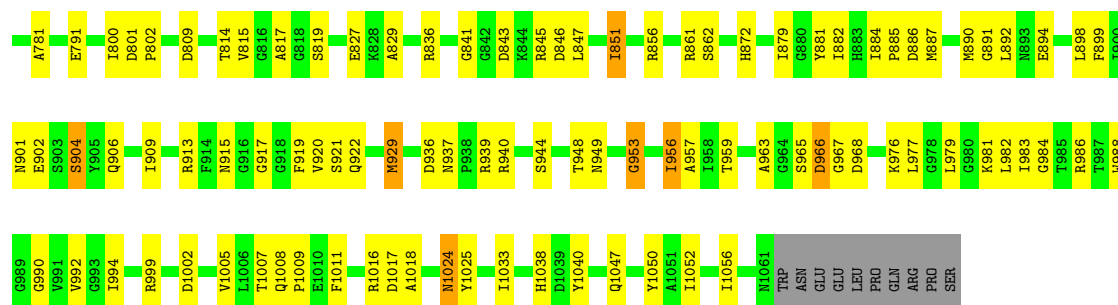


Chain E:



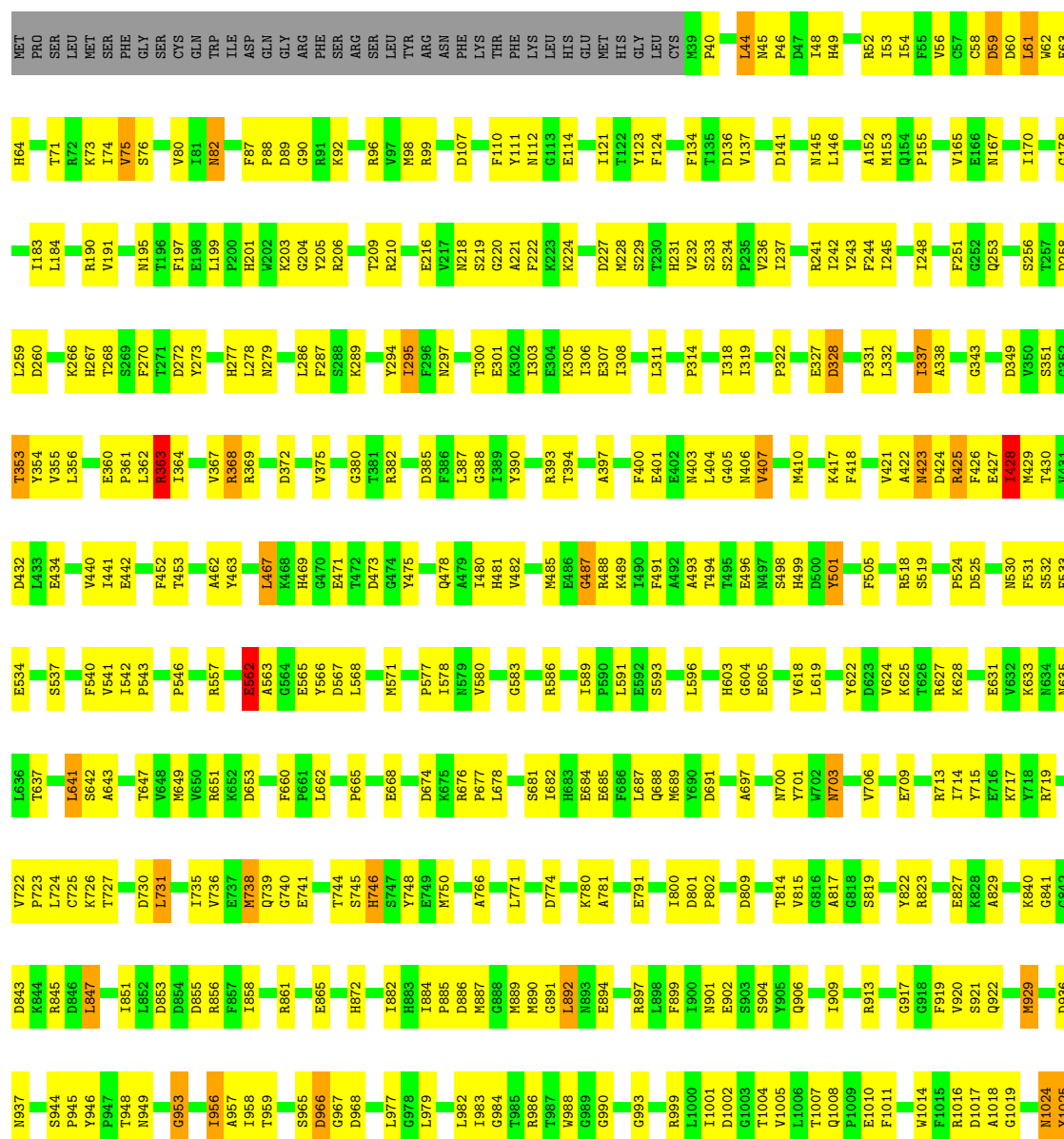
G178	E179	A180	I183	I184	R190	V191	I192	N195	T196	F197	E198	P200	H201	H202	K203	G204	R206	T209	E216	V217	N218	S219	E220	E221	F222	K223	K224	I225	V226	D227	M228	S229	T230	H231	V232	S233	S234	P235	V236	I237	I242	Y243	F244	I245	I248	Q253	S256	T257																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
D258	L259	D260	H267	T268	S269	F270	I271	Y272	H277	L278	N279	L199	D281	L286	F287	K289	Y294	I295	F296	I303	I306	E307	G220	E401	I308	L311	P314	I318	I319	P322	E327	D328	F329	P331	I337	D349	V350	S351	G352	T353	Y354	V355	V358	P359																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
E360	P361	R363	I364	V367	R368	D372	V375	A376	F377	I378	H379	G380	D385	F386	L387	G388	I389	Y390	R393	A397	F400	E401	E402	M403	L404	G405	N406	V407	M410	G411	V412	K417	F418	V421	A422	M423	D424	R425	F426	E427	I428	M429	T430	F431	D432	L433	E434																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
I441	E442	D451	F452	A462	Y463	L467	K468	H469	D473	G474	Y475	Q478	A479	I480	H481	M485	E486	G487	R488	K489	F491	T494	T495	E496	N497	S498	H499	E500	Y501	D506	L515	S516	Y517	R518	P524	D525	V528	L529	N530	F531	S532	F533	E534	V535	V536	S537	K538																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
P539	F540	V541	I542	P546	L554	R557	E562	A563	G564	E565	Y566	D567	L568	N571	P577	I578	N579	V580	G583	R586	F589	L591	S593	L596	H603	G604	E605	F606	Y609	V618	L619	V624	K625	E631	V632	K633	N634	R635	L636	T637	D638	L639																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
E640	L641	S642	T647	V648	M649	P650	R651	D653	F660	P661	L662	P665	E668	E672	T673	D674	P677	L678	S681	I682	H683	E684	E685	A697	N700	Y701	W702	W703	V706	E709	R713	I714	Y715	E716	K717	V722	P723	L724	C725	K726	L731	I735	V736																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
E737	N738	Q739	G740	E741	Y742	R743	T744	S745	H746	S747	Y748	E749	M750	S762	C767	L771	D772	G773	D774	H775	Y776	K780	A781	Y782	E791	I800	D801	P802	D809	G812	E813	T814	V815	G816	A817	G818	S819	N820	E821	Y822	R823	S826	E827	K828	A829	K840	G841	G842	D843																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
K844	R845	D846	L847	I851	L852	D853	R856	R859	E863	R861	S862	H863	H872	Y881	I882	H883	L884	P885	D886	K887	G888	M889	A781	Y782	E791	I800	D801	P802	D809	G812	E813	T814	V815	G816	A817	G818	S819	N820	E821	Y822	R823	S826	E827	K828	A829	K840	G841	G842	D843																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
E826	M829	D836	N837	F838	P838	S844	Y846	P847	T848	N849	G853	I856	A857	T858	T859	Y862	S865	D866	G867	D868	I869	F870	L877	G878	L879	K881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L18





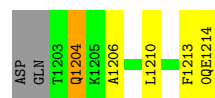
• Molecule 1: Tricorn protease

Chain K: 57% 35%

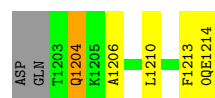




• Molecule 2: DQTQKAAAELTFF



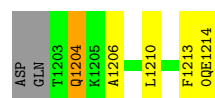
• Molecule 2: DQTQKAAAELTFF



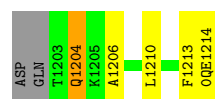
• Molecule 2: DQTQKAAAELTFF



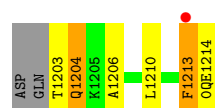
• Molecule 2: DQTQKAAAELTFF



• Molecule 2: DQTQKAAAELTFF



• Molecule 2: DQTQKAAAELTFF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.47Å 245.10Å 157.89Å 90.00° 105.19° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60 6.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.6 (6.00-2.60) 85.4 (6.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.288 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50544	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 0QE

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	0.84	1/8367 (0.0%)	1.04	23/11311 (0.2%)
1	C	0.85	1/8367 (0.0%)	1.04	24/11311 (0.2%)
1	E	0.79	2/8367 (0.0%)	1.04	24/11311 (0.2%)
1	G	0.80	0/8367	1.04	20/11311 (0.2%)
1	I	0.81	1/8367 (0.0%)	1.04	22/11311 (0.2%)
1	K	0.79	0/8367	1.03	21/11311 (0.2%)
2	B	1.21	1/87 (1.1%)	0.87	0/116
2	D	1.24	1/87 (1.1%)	0.84	0/116
2	F	1.13	1/87 (1.1%)	0.84	0/116
2	H	1.25	1/87 (1.1%)	0.85	0/116
2	J	1.16	1/87 (1.1%)	0.83	0/116
2	L	1.02	1/87 (1.1%)	0.86	0/116
All	All	0.82	11/50724 (0.0%)	1.04	134/68562 (0.2%)

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	E	0	2
1	K	0	2
All	All	0	4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1213	PHE	C-O	10.58	1.44	1.23
2	D	1213	PHE	C-O	10.34	1.44	1.23
2	B	1213	PHE	C-O	9.81	1.43	1.23
2	J	1213	PHE	C-O	9.73	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1213	PHE	C-O	9.05	1.41	1.23

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	487	GLY	N-CA-C	-7.57	106.08	115.08
1	G	362	LEU	N-CA-C	7.53	120.03	110.24
1	I	425	ARG	N-CA-C	-7.33	104.07	113.16
1	K	425	ARG	N-CA-C	-7.32	104.09	113.16
1	A	746	HIS	N-CA-C	7.31	121.48	111.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	776	TYR	Sidechain
1	E	822	TYR	Sidechain
1	K	1025	TYR	Sidechain
1	K	822	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	8177	0	8002	319	1
1	C	8177	0	8002	307	1
1	E	8177	0	8002	367	0
1	G	8177	0	8002	324	1
1	I	8177	0	8002	320	1
1	K	8177	0	8002	349	0
2	B	87	0	84	5	0
2	D	87	0	84	5	0
2	F	87	0	84	9	0
2	H	87	0	84	4	0
2	J	87	0	84	5	0
2	L	87	0	84	8	0
3	A	178	0	0	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	172	0	0	25	0
3	D	2	0	0	0	0
3	E	138	0	0	55	0
3	F	5	0	0	2	0
3	G	154	0	0	32	0
3	H	2	0	0	1	0
3	I	157	0	0	19	0
3	J	2	0	0	0	0
3	K	146	0	0	56	0
3	L	2	0	0	1	0
All	All	50544	0	48516	1902	2

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 20.

The worst 5 of 1902 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:I:351:SER:OG	1:I:353:THR:HG22	1.41	1.17
1:C:351:SER:OG	1:C:353:THR:HG22	1.46	1.16
1:G:351:SER:OG	1:G:353:THR:HG22	1.47	1.15
1:A:351:SER:OG	1:A:353:THR:HG22	1.45	1.14
1:E:351:SER:OG	1:E:353:THR:HG22	1.46	1.13

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:N	1:I:143:ASP:OD2[2_545]	2.06	0.14
1:C:167:ASN:N	1:G:143:ASP:OD2[2_455]	2.12	0.08

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	1021/1071 (95%)	948 (93%)	67 (7%)	6 (1%)	21	42
1	C	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	16	34
1	E	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	16	34
1	G	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	16	34
1	I	1021/1071 (95%)	949 (93%)	64 (6%)	8 (1%)	16	34
1	K	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	16	34
2	B	9/14 (64%)	4 (44%)	5 (56%)	0	100	100
2	D	9/14 (64%)	4 (44%)	5 (56%)	0	100	100
2	F	9/14 (64%)	6 (67%)	3 (33%)	0	100	100
2	H	9/14 (64%)	5 (56%)	4 (44%)	0	100	100
2	J	9/14 (64%)	6 (67%)	3 (33%)	0	100	100
2	L	9/14 (64%)	5 (56%)	4 (44%)	0	100	100
All	All	6180/6510 (95%)	5721 (93%)	413 (7%)	46 (1%)	18	38

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	C	219	SER
1	E	219	SER
1	E	1018	ALA
1	G	219	SER

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	883/928 (95%)	848 (96%)	35 (4%)	28	55
1	C	883/928 (95%)	848 (96%)	35 (4%)	28	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	883/928 (95%)	848 (96%)	35 (4%)	28	55
1	G	883/928 (95%)	846 (96%)	37 (4%)	26	52
1	I	883/928 (95%)	847 (96%)	36 (4%)	27	54
1	K	883/928 (95%)	850 (96%)	33 (4%)	30	57
2	B	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	D	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	F	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	H	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	J	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	L	8/10 (80%)	6 (75%)	2 (25%)	0	1
All	All	5346/5628 (95%)	5123 (96%)	223 (4%)	26	52

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	82	ASN
2	L	1204	GLN
1	G	937	ASN
1	K	956	ILE
1	K	353	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	579	ASN
1	I	499	HIS
1	G	703	ASN
1	G	1038	HIS
1	I	703	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 oligosaccharides 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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	1023/1071 (95%)	-1.35	0	100	100	8, 35, 56, 78	20 (1%)
1	C	1023/1071 (95%)	-1.33	0	100	100	8, 36, 56, 78	20 (1%)
1	E	1023/1071 (95%)	-1.21	0	100	100	8, 39, 58, 80	20 (1%)
1	G	1023/1071 (95%)	-1.31	0	100	100	8, 36, 57, 78	20 (1%)
1	I	1023/1071 (95%)	-1.30	0	100	100	8, 37, 56, 78	20 (1%)
1	K	1023/1071 (95%)	-1.23	0	100	100	8, 39, 58, 79	20 (1%)
2	B	11/14 (78%)	-0.72	0	100	100	52, 84, 96, 99	0
2	D	11/14 (78%)	-0.74	0	100	100	52, 84, 96, 99	0
2	F	11/14 (78%)	-0.52	0	100	100	53, 85, 97, 98	0
2	H	11/14 (78%)	-0.78	0	100	100	52, 84, 96, 99	0
2	J	11/14 (78%)	-0.74	0	100	100	52, 84, 96, 99	0
2	L	11/14 (78%)	-0.26	1 (9%)	15	11	54, 84, 96, 99	0
All	All	6204/6510 (95%)	-1.28	1 (0%)	100	100	8, 37, 59, 99	120 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	1213	PHE	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.