



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:42 AM GMT

PDB ID : 3FOA  
Title : Crystal structure of the bacteriophage T4 tail sheath protein, deletion mutant gp18M  
Authors : Aksyuk, A.A.; Leiman, P.G.; Kurochkina, L.P.; Shneider, M.M.; Kostyuchenko, V.A.; Mesyanzhinov, V.V.; Rossmann, M.G.  
Deposited on : 2008-12-29  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
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A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

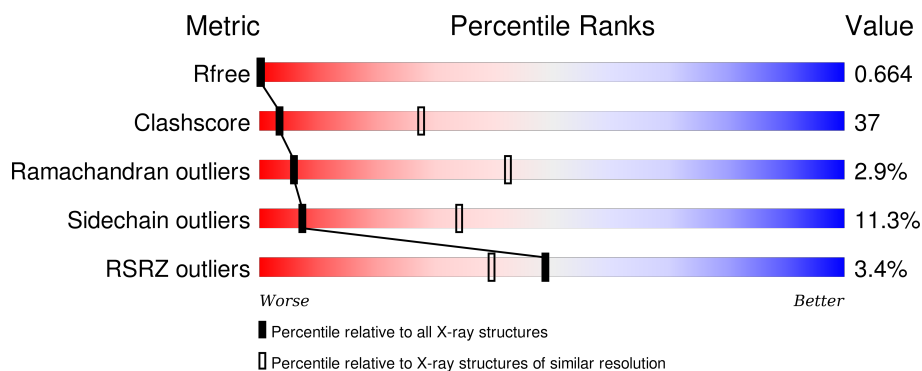
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div>8%</div> <div>39% 44% 10% • 6%</div> </div>
1	B	510	<div> <div>2%</div> <div>38% 43% 11% • 6%</div> </div>
1	C	510	<div> <div>2%</div> <div>42% 41% 10% • 6%</div> </div>
1	D	510	<div> <div>8%</div> <div>42% 41% 9% • 7%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14406 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 Tail sheath protein Gp18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3613	2279	600	726	8			
1	B	478	Total	C	N	O	S	0	0	0
			3605	2275	598	724	8			
1	C	477	Total	C	N	O	S	0	0	0
			3597	2271	596	722	8			
1	D	476	Total	C	N	O	S	0	0	0
			3591	2268	595	720	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLU	ASP	VARIANT	UNP P13332
A	148	ALA	GLY	VARIANT	UNP P13332
A	150	ILE	ASN	VARIANT	UNP P13332
A	151	ILE	TYR	VARIANT	UNP P13332
A	301	GLY	GLU	VARIANT	UNP P13332
A	399	VAL	ALA	VARIANT	UNP P13332
A	454	TYR	HIS	VARIANT	UNP P13332
A	510	PRO	ARG	ENGINEERED	UNP P13332
B	100	GLU	ASP	VARIANT	UNP P13332
B	148	ALA	GLY	VARIANT	UNP P13332
B	150	ILE	ASN	VARIANT	UNP P13332
B	151	ILE	TYR	VARIANT	UNP P13332
B	301	GLY	GLU	VARIANT	UNP P13332
B	399	VAL	ALA	VARIANT	UNP P13332
B	454	TYR	HIS	VARIANT	UNP P13332
B	510	PRO	ARG	ENGINEERED	UNP P13332
C	100	GLU	ASP	VARIANT	UNP P13332
C	148	ALA	GLY	VARIANT	UNP P13332
C	150	ILE	ASN	VARIANT	UNP P13332
C	151	ILE	TYR	VARIANT	UNP P13332
C	301	GLY	GLU	VARIANT	UNP P13332

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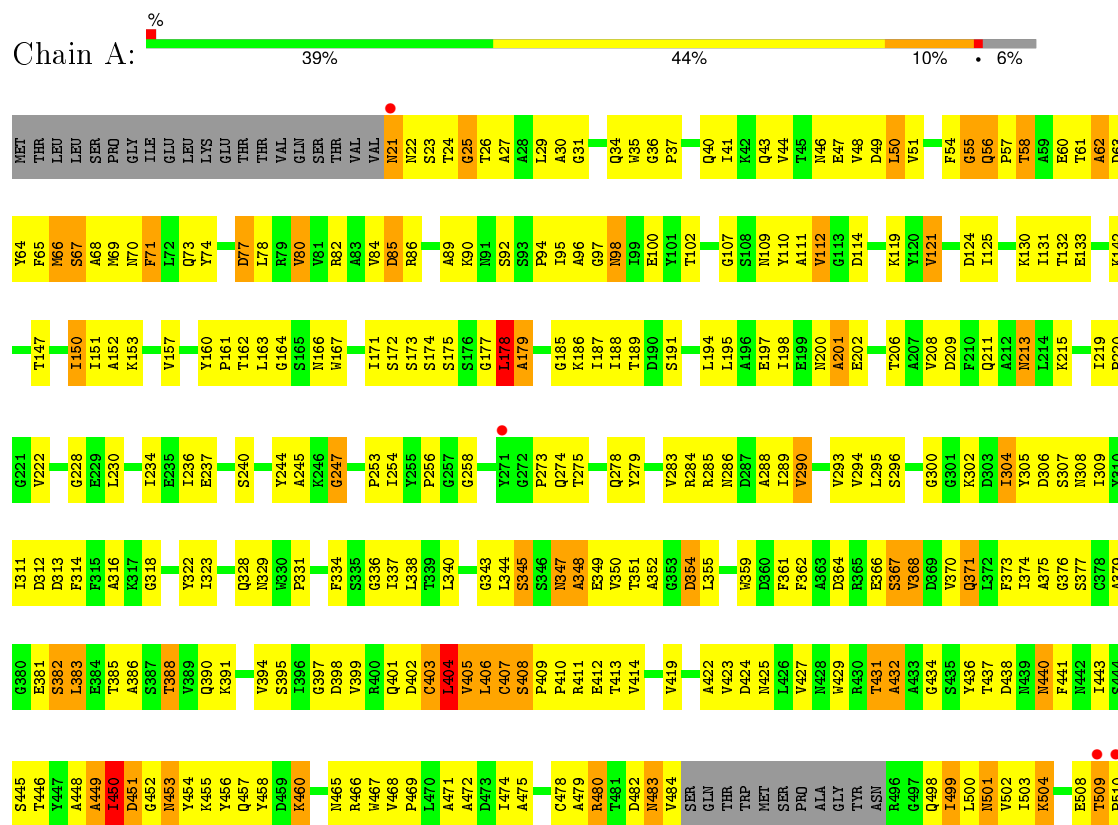
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Chain	Residue	Modelled	Actual	Comment	Reference
C	399	VAL	ALA	VARIANT	UNP P13332
C	454	TYR	HIS	VARIANT	UNP P13332
C	510	PRO	ARG	ENGINEERED	UNP P13332
D	100	GLU	ASP	VARIANT	UNP P13332
D	148	ALA	GLY	VARIANT	UNP P13332
D	150	ILE	ASN	VARIANT	UNP P13332
D	151	ILE	TYR	VARIANT	UNP P13332
D	301	GLY	GLU	VARIANT	UNP P13332
D	399	VAL	ALA	VARIANT	UNP P13332
D	454	TYR	HIS	VARIANT	UNP P13332
D	510	PRO	ARG	ENGINEERED	UNP P13332

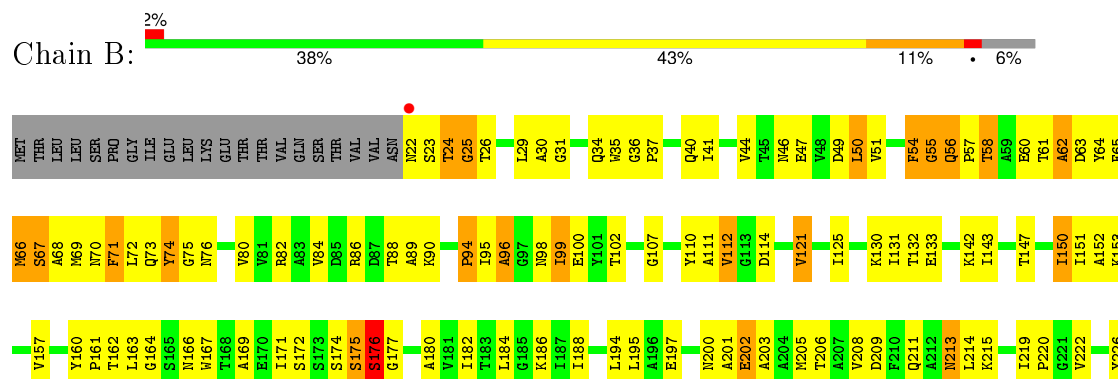
### 3 Residue-property plots

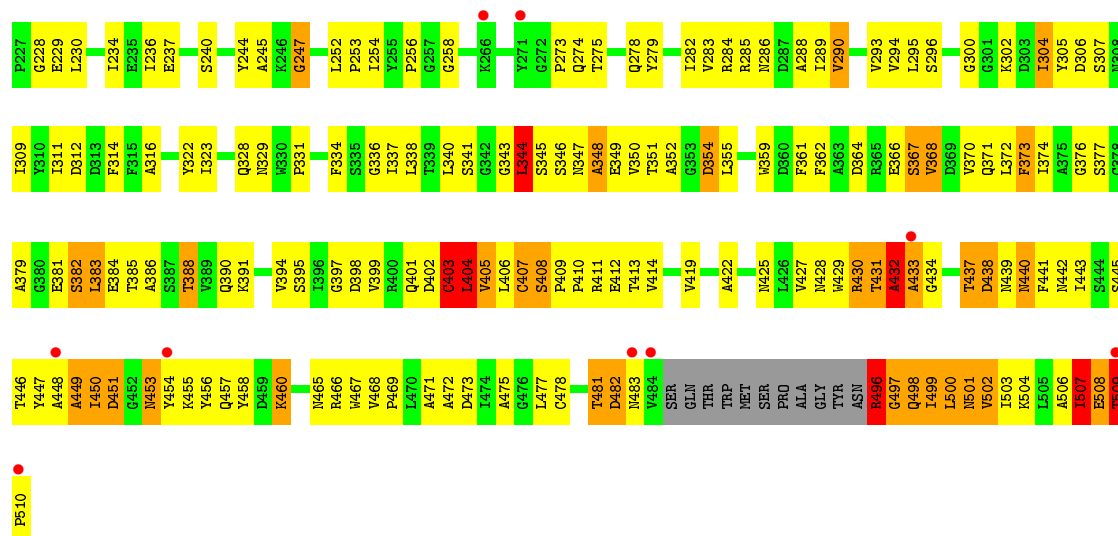
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: Tail sheath protein Gp18

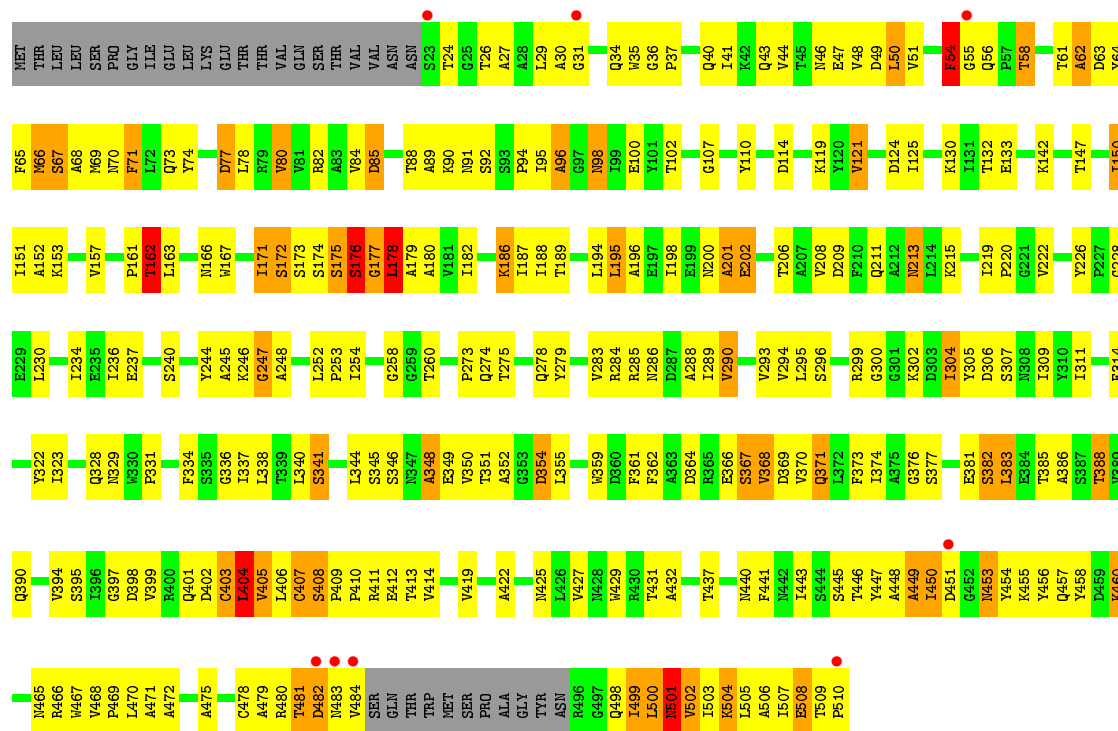
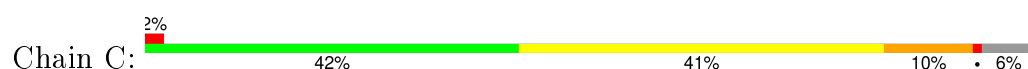


#### • Molecule 1: Tail sheath protein Gp18

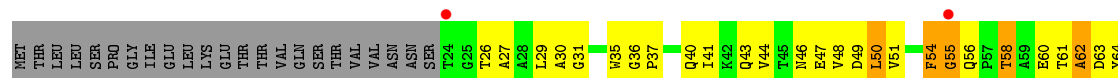
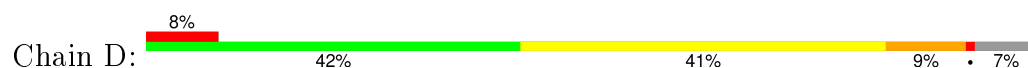




• Molecule 1: Tail sheath protein Gp18



• Molecule 1: Tail sheath protein Gp18



I503	R365	D438	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000	R1001	R1002	R1003	R1004	R1005	R1006	R1007	R1008	R1009	R1010	R1011	R1012	R1013	R1014	R1015	R1016	R1017	R1018	R1019	R1020	R1021	R1022	R1023	R1024	R1025	R1026	R1027	R1028	R1029	R1030	R1031	R1032	R1033	R1034	R1035	R1036	R1037	R1038	R1039	R1040	R1041	R1042	R1043	R1044	R1045	R1046	R1047	R1048	R1049	R1050	R1051	R1052	R1053	R1054	R1055	R1056	R1057	R1058	R1059	R1060	R1061	R1062	R1063	R1064	R1065	R1066	R1067	R1068	R1069	R1070	R1071	R1072	R1073	R1074	R1075	R1076	R1077	R1078	R1079	R1080	R1081	R1082	R1083	R1084	R1085	R1086	R1087	R1088	R1089	R1090	R1091	R1092	R1093	R1094	R1095	R1096	R1097	R1098	R1099	R1100	R1101	R1102	R1103	R1104	R1105	R1106	R1107	R1108	R1109	R1110	R1111	R1112	R1113	R1114	R1115	R1116	R1117	R1118	R1119	R1120	R1121	R1122	R1123	R1124	R1125	R1126	R1127	R1128	R1129	R1130	R1131	R1132	R1133	R1134	R1135	R1136	R1137	R1138	R1139	R1140	R1141	R1142	R1143	R1144	R1145	R1146	R1147	R1148	R1149	R1150	R1151	R1152	R1153	R1154	R1155	R1156	R1157	R1158	R1159	R1160	R1161	R1162	R1163	R1164	R1165	R1166	R1167	R1168	R1169	R1170	R1171	R1172	R1173	R1174	R1175	R1176	R1177	R1178	R1179	R1180	R1181	R1182	R1183	R1184	R1185	R1186	R1187	R1188	R1189	R1190	R1191	R1192	R1193	R1194	R1195	R1196	R1197	R1198	R1199	R1200	R1201	R1202	R1203	R1204	R1205	R1206	R1207	R1208	R1209	R1210	R1211	R1212	R1213	R1214	R1215	R1216	R1217	R1218	R1219	R1220	R1221	R1222	R1223	R1224	R1225	R1226	R1227	R1228	R1229	R1230	R1231	R1232	R1233	R1234	R1235	R1236	R1237	R1238	R1239	R1240	R1241	R1242	R1243	R1244	R1245	R1246	R1247	R1248	R1249	R1250	R1251	R1252	R1253	R1254	R1255	R1256	R1257	R1258	R1259	R1260	R1261	R1262	R1263	R1264	R1265	R1266	R1267	R1268	R1269	R1270	R1271	R1272	R1273	R1274	R1275	R1276	R1277	R1278	R1279	R1280	R1281	R1282	R1283	R1284	R1285	R1286	R1287	R1288	R1289	R1290	R1291	R1292	R1293	R1294	R1295	R1296	R1297	R1298	R1299	R1300	R1301	R1302	R1303	R1304	R1305	R1306	R1307	R1308	R1309	R1310	R1311	R1312	R1313	R1314	R1315	R1316	R1317	R1318	R1319	R1320	R1321	R1322	R1323	R1324	R1325	R1326	R1327	R1328	R1329	R1330	R1331	R1332	R1333	R1334	R1335	R1336	R1337	R1338	R1339	R1340	R1341	R1342	R1343	R1344	R1345	R1346	R1347	R1348	R1349	R1350	R1351	R1352	R1353	R1354	R1355	R1356	R1357	R1358	R1359	R1360	R1361	R1362	R1363	R1364	R1365	R1366	R1367	R1368	R1369	R1370	R1371	R1372	R1373	R1374	R1375	R1376	R1377	R1378	R1379	R1380	R1381	R1382	R1383	R1384	R1385	R1386	R1387	R1388	R1389	R1390	R1391	R1392	R1393	R1394	R1395	R1396	R1397	R1398	R1399	R1400	R1401	R1402	R1403	R1404	R1405	R1406	R1407	R1408	R1409	R1410	R1411	R1412	R1413	R1414	R1415	R1416	R1417	R1418	R1419	R1420	R1421	R1422	R1423	R1424	R1425	R1426	R1427	R1428	R1429	R1430	R1431	R1432	R1433	R1434	R1435	R1436	R1437	R1438	R1439	R1440	R1441	R1442	R1443	R1444	R1445	R1446	R1447	R1448	R1449	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460	R1461	R1462	R1463	R1464	R1465	R1466	R1467	R1468	R1469	R1470	R1471	R1472	R1473	R1474	R1475	R1476	R1477	R1478	R1479	R1480	R1481	R1482	R1483	R1484	R1485	R1486	R1487	R1488	R1489	R1490	R1491	R1492	R1493	R1494	R1495	R1496	R1497	R1498	R1499	R1500	R1501	R1502	R1503	R1504	R1505	R1506	R1507	R1508	R1509	R1510	R1511	R1512	R1513	R1514	R1515	R1516	R1517	R1518	R1519	R1520	R1521	R1522	R1523	R1524	R1525	R1526	R1527	R1528	R1529	R1530	R1531	R1532	R1533	R1534	R1535	R1536	R1537	R1538	R1539	R1540	R1541	R1542	R1543	R1544	R1545	R1546	R1547	R1548	R1549	R1550	R1551	R1552	R1553	R1554	R1555	R1556	R1557	R1558	R1559	R1560	R1561	R1562	R1563	R1564	R1565	R1566	R1567	R1568	R1569	R1570	R1571	R1572	R1573	R1574	R1575	R1576	R1577	R1578	R1579	R1580	R1581	R1582	R1583	R1584	R1585	R1586	R1587	R1588	R1589	R1590	R1591	R1592	R1593	R1594	R1595	R1596	R1597	R1598	R1599	R1600	R1601	R1602	R1603	R1604	R1605	R1606	R1607	R1608	R1609	R1610	R1611	R1612	R1613	R1614	R1615	R1616	R1617	R1618	R1619	R1620	R1621	R1622	R1623	R1624	R1625	R1626	R1627	R1628	R1629	R1630	R1631	R1632	R1633	R1634	R1635	R1636	R1637	R1638	R1639	R1640	R1641	R1642	R1643	R1644	R1645	R1646	R1647	R1648	R1649	R1650	R1651	R1652	R1653	R1654	R1655	R1656	R1657	R1658	R1659	R1660	R1661	R1662	R1663	R1664	R1665	R1666	R1667	R1668	R1669	R1670	R1671	R1672	R1673	R1674	R1675	R1676	R1677	R1678	R1679	R1680	R1681	R1682	R1683	R1684	R1685	R1686	R1687	R1688	R1689	R1690	R1691	R1692	R1693	R1694	R1695	R1696	R1697	R1698	R1699	R1700	R1701	R1702	R1703	R1704	R1705	R1706	R1707	R1708	R1709	R1710	R1711	R1712	R1713	R1714	R1715	R1716	R1717	R1718	R1719	R1720	R1721	R1722	R1723	R1724	R1725	R1726	R1727	R1728	R1729	R1730	R1731	R1732	R1733	R1734	R1735	R1736	R1737	R1738	R1739	R1740	R1741	R1742	R1743	R1744	R1745	R1746	R1747	R1748	R1749	R1750	R1751	R1752	R1753	R1754	R1755	R1756	R1757	R1758	R1759	R1760	R1761	R1762	R1763	R1764	R1765	R1766	R1767	R1768	R1769	R1770	R1771	R1772	R1773	R1774	R1775	R1776	R1777	R1778	R1779	R1780	R1781	R1782	R1783	R1784	R1785	R1786	R1787	R1788	R1789	R1790	R1791	R1792	R1793	R1794</
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.59Å 116.29Å 433.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.50 49.80 – 3.50	Depositor EDS
% Data completeness (in resolution range)	87.8 (49.80-3.50) 87.8 (49.80-3.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.267 , 0.299 0.278 , 0.664	Depositor DCC
$R_{free}$ test set	2266 reflections (7.77%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32322 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	14406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	0.35	0/3677	0.78	21/5001 (0.4%)
1	B	0.29	0/3669	0.91	31/4990 (0.6%)
1	C	0.30	0/3661	0.70	19/4979 (0.4%)
1	D	0.28	0/3655	0.88	27/4971 (0.5%)
All	All	0.30	0/14662	0.82	98/19941 (0.5%)

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	4
1	B	0	13
1	C	0	5
1	D	0	2
All	All	0	24

There are no bond length outliers.

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ALA	N-CA-CB	-22.35	78.81	110.10
1	D	500	LEU	CB-CA-C	-18.07	75.86	110.20
1	A	55	GLY	N-CA-C	18.00	158.11	113.10
1	D	55	GLY	N-CA-C	16.20	153.61	113.10
1	B	55	GLY	N-CA-C	13.58	147.05	113.10

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ASN	Peptide
1	A	450	ILE	Peptide
1	A	451	ASP	Peptide
1	A	452	GLY	Peptide
1	B	22	ASN	Peptide

## 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	3613	0	3554	298	2
1	B	3605	0	3548	280	1
1	C	3597	0	3541	253	1
1	D	3591	0	3536	232	0
All	All	14406	0	14179	1050	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 37.

The worst 5 of 1050 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:PRO:O	1:A:454:TYR:CE1	1.65	1.48
1:A:409:PRO:CD	1:A:451:ASP:O	1.75	1.33
1:B:496:ARG:HG3	1:B:497:GLY:O	1.16	1.29
1:A:379:ALA:CB	1:A:454:TYR:OH	1.84	1.25
1:B:496:ARG:CG	1:B:497:GLY:O	1.89	1.21

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:509:THR:O	1:B:419:VAL:N[4_655]	1.92	0.28
1:A:22:ASN:ND2	1:C:260:THR:OG1[4_555]	2.00	0.20

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	475/510 (93%)	371 (78%)	87 (18%)	17 (4%)	4	37
1	B	474/510 (93%)	365 (77%)	94 (20%)	15 (3%)	5	40
1	C	473/510 (93%)	374 (79%)	84 (18%)	15 (3%)	5	40
1	D	472/510 (92%)	377 (80%)	87 (18%)	8 (2%)	11	54
All	All	1894/2040 (93%)	1487 (78%)	352 (19%)	55 (3%)	6	42

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	201	ALA
1	A	432	ALA
1	B	403	CYS
1	B	502	VAL

### 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	383/411 (93%)	340 (89%)	43 (11%)	7	35
1	B	382/411 (93%)	341 (89%)	41 (11%)	8	37
1	C	381/411 (93%)	337 (88%)	44 (12%)	7	33
1	D	380/411 (92%)	335 (88%)	45 (12%)	6	31
All	All	1526/1644 (93%)	1353 (89%)	173 (11%)	7	34

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	482	ASP
1	C	150	ILE
1	D	404	LEU
1	B	496	ARG
1	C	58	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	390	GLN
1	C	43	GLN
1	D	440	ASN
1	B	440	ASN
1	B	453	ASN

### 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	479/510 (93%)	-0.03	4 (0%) 87 80	24, 65, 121, 227	0
1	B	478/510 (93%)	0.26	10 (2%) 67 58	20, 82, 162, 247	0
1	C	477/510 (93%)	0.15	8 (1%) 73 64	25, 80, 148, 263	0
1	D	476/510 (93%)	0.54	42 (8%) 12 11	26, 116, 254, 407	0
All	All	1910/2040 (93%)	0.23	64 (3%) 49 40	20, 84, 186, 407	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	292	SER	9.9
1	D	325	ALA	6.6
1	B	271	TYR	5.9
1	B	484	VAL	5.2
1	D	484	VAL	5.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.