



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:40 PM UTC

PDB ID : 2QGX / pdb_00002qgx
Title : Ubiquitin-conjugating enzyme E2Q
Authors : Neculai, D.; Avvakumov, G.V.; Xue, S.; Walker, J.R.; Mackenzie, F.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Sicheri, F.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2007-06-29
Resolution : 2.56 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

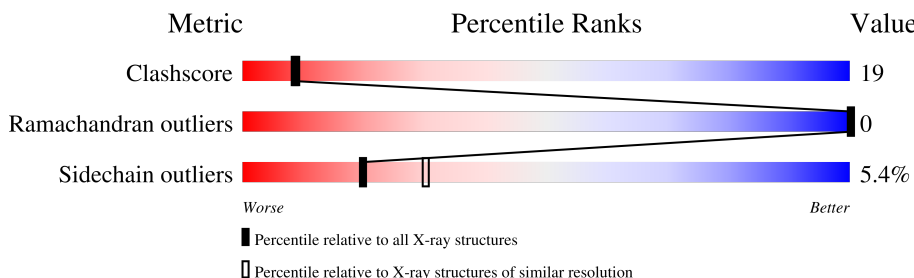
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	169	58% 33% • 8%
1	B	169	55% 37% • 5%
1	C	169	55% 38% •• 5%
1	D	169	55% 36% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5132 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 Ubiquitin-conjugating enzyme E2 Q1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	1	0
			1238	793	210	231	4			
1	B	161	Total	C	N	O	S	0	0	0
			1265	809	213	239	4			
1	C	161	Total	C	N	O	S	0	1	0
			1282	819	219	240	4			
1	D	160	Total	C	N	O	S	0	0	0
			1257	803	212	238	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q7Z7E8
B	-1	GLY	-	expression tag	UNP Q7Z7E8
C	-1	GLY	-	expression tag	UNP Q7Z7E8
D	-1	GLY	-	expression tag	UNP Q7Z7E8

- Molecule 2 is water.

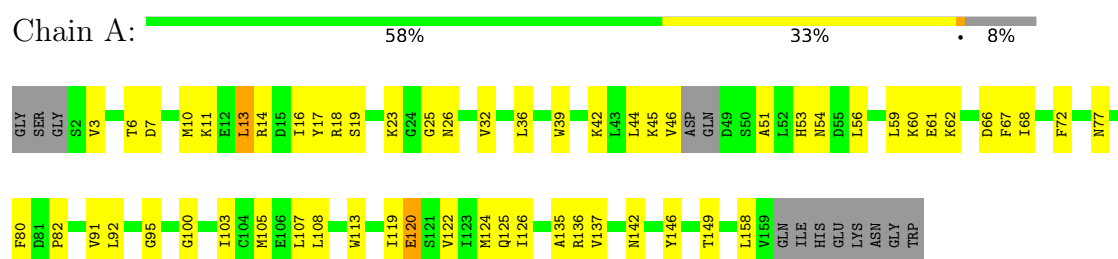
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	20	Total	O	0	0
			20	20		
2	C	13	Total	O	0	0
			13	13		
2	D	37	Total	O	0	0
			37	37		

3 Residue-property plots [i](#)

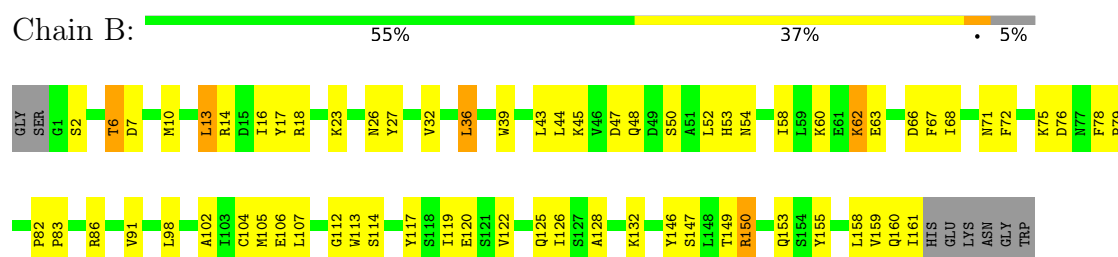
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

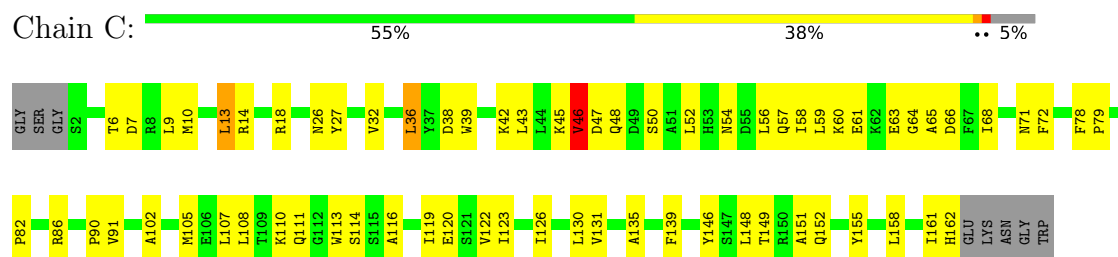
• Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



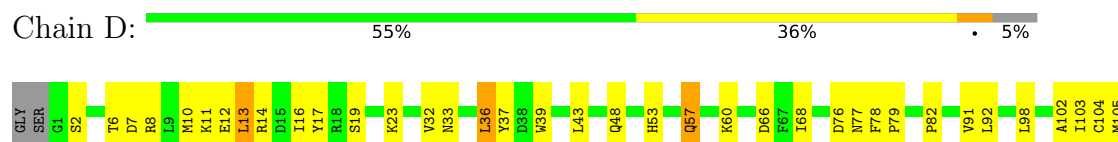
• Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



• Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



• Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



E106	L107		K110	Q111	G112	W113	S114		Y117	S118	I119	E120	S121	V122	I123	M124	Q125	I126		T129		A135	R136		A141	N142	K143	S144	Q145	Y146	S147	L148	T149		Q153		V159	Q160	I161	H162	G163	L164	A165	S166	E167	D168	N169	K170	S171	Q172	L173	I174	V175	A176	S177	E178	D179	N180	K181	S182	Q183	L184	I185	V186	A187	S188	E189	D190	N191	K192	S193	Q194	L195	I196	V197	A198	S199	E200	D201	N202	K203	S204	Q205	L206	I207	V208	A209	S210	E211	D212	N213	K214	S215	Q216	L217	I218	V219	A220	S221	E222	D223	N224	K225	S226	Q227	L228	I229	V230	A231	S232	E233	D234	N235	K236	S237	Q238	L239	I240	V241	A242	S243	E244	D245	N246	K247	S248	Q249	L250	I251	V252	A253	S254	E255	D256	N257	K258	S259	Q260	L261	I262	V263	A264	S265	E266	D267	N268	K269	S270	Q271	L272	I273	V274	A275	S276	E277	D278	N279	K280	S281	Q282	L283	I284	V285	A286	S287	E288	D289	N290	K291	S292	Q293	L294	I295	V296	A297	S298	E299	D300	N301	K302	S303	Q304	L305	I306	V307	A308	S309	E310	D311	N312	K313	S314	Q315	L316	I317	V318	A319	S320	E321	D322	N323	K324	S325	Q326	L327	I328	V329	A330	S331	E332	D333	N334	K335	S336	Q337	L338	I339	V340	A341	S342	E343	D344	N345	K346	S347	Q348	L349	I350	V351	A352	S353	E354	D355	N356	K357	S358	Q359	L360	I361	V362	A363	S364	E365	D366	N367	K368	S369	Q370	L371	I372	V373	A374	S375	E376	D377	N378	K379	S380	Q381	L382	I383	V384	A385	S386	E387	D388	N389	K390	S391	Q392	L393	I394	V395	A396	S397	E398	D399	N400	K401	S402	Q403	L404	I405	V406	A407	S408	E409	D410	N411	K412	S413	Q414	L415	I416	V417	A418	S419	E420	D421	N422	K423	S424	Q425	L426	I427	V428	A429	S430	E431	D432	N433	K434	S435	Q436	L437	I438	V439	A440	S441	E442	D443	N444	K445	S446	Q447	L448	I449	V450	A451	S452	E453	D454	N455	K456	S457	Q458	L459	I460	V461	A462	S463	E464	D465	N466	K467	S468	Q469	L470	I471	V472	A473	S474	E475	D476	N477	K478	S479	Q480	L481	I482	V483	A484	S485	E486	D487	N488	K489	S490	Q491	L492	I493	V494	A495	S496	E497	D498	N499	K500	S501	Q502	L503	I504	V505	A506	S507	E508	D509	N510	K511	S512	Q513	L514	I515	V516	A517	S518	E519	D520	N521	K522	S523	Q524	L525	I526	V527	A528	S529	E530	D531	N532	K533	S534	Q535	L536	I537	V538	A539	S540	E541	D542	N543	K544	S545	Q546	L547	I548	V549	A550	S551	E552	D553	N554	K555	S556	Q557	L558	I559	V560	A561	S562	E563	D564	N565	K566	S567	Q568	L569	I570	V571	A572	S573	E574	D575	N576	K577	S578	Q579	L580	I581	V582	A583	S584	E585	D586	N587	K588	S589	Q590	L591	I592	V593	A594	S595	E596	D597	N598	K599	S600	Q601	L602	I603	V604	A605	S606	E607	D608	N609	K610	S611	Q612	L613	I614	V615	A616	S617	E618	D619	N620	K621	S622	Q623	L624	I625	V626	A627	S628	E629	D630	N631	K632	S633	Q634	L635	I636	V637	A638	S639	E640	D641	N642	K643	S644	Q645	L646	I647	V648	A649	S650	E651	D652	N653	K654	S655	Q656	L657	I658	V659	A660	S661	E662	D663	N664	K665	S666	Q667	L668	I669	V670	A671	S672	E673	D674	N675	K676	S677	Q678	L679	I680	V681	A682	S683	E684	D685	N686	K687	S688	Q689	L690	I691	V692	A693	S694	E695	D696	N697	K698	S699	Q700	L701	I702	V703	A704	S705	E706	D707	N708	K709	S710	Q711	L712	I713	V714	A715	S716	E717	D718	N719	K720	S721	Q722	L723	I724	V725	A726	S727	E728	D729	N730	K731	S732	Q733	L734	I735	V736	A737	S738	E739	D740	N741	K742	S743	Q744	L745	I746	V747	A748	S749	E750	D751	N752	K753	S754	Q755	L756	I757	V758	A759	S760	E761	D762	N763	K764	S765	Q766	L767	I768	V769	A770	S771	E772	D773	N774	K775	S776	Q777	L778	I779	V780	A781	S782	E783	D784	N785	K786	S787	Q788	L789	I790	V791	A792	S793	E794	D795	N796	K797	S798	Q799	L800	I801	V802	A803	S804	E805	D806	N807	K808	S809	Q810	L811	I812	V813	A814	S815	E816	D817	N818	K819	S820	Q821	L822	I823	V824	A825	S826	E827	D828	N829	K830	S831	Q832	L833	I834	V835	A836	S837	E838	D839	N840	K841	S842	Q843	L844	I845	V846	A847	S848	E849	D850	N851	K852	S853	Q854	L855	I856	V857	A858	S859	E860	D861	N862	K863	S864	Q865	L866	I867	V868	A869	S870	E871	D872	N873	K874	S875	Q876	L877	I878	V879	A880	S881	E882	D883	N884	K885	S886	Q887	L888	I889	V890	A891	S892	E893	D894	N895	K896	S897	Q898	L899	I900	V901	A902	S903	E904	D905	N906	K907	S908	Q909	L910	I911	V912	A913	S914	E915	D916	N917	K918	S919	Q920	L921	I922	V923	A924	S925	E926	D927	N928	K929	S930	Q931	L932	I933	V934	A935	S936	E937	D938	N939	K940	S941	Q942	L943	I944	V945	A946	S947	E948	D949	N950	K951	S952	Q953	L954	I955	V956	A957	S958	E959	D960	N961	K962	S963	Q964	L965	I966	V967	A968	S969	E970	D971	N972	K973	S974	Q975	L976	I977	V978	A979	S980	E981	D982	N983	K984	S985	Q986	L987	I988	V989	A990	S991	E992	D993	N994	K995	S996	Q997	L998	I999	V1000	A1001	S1002	E1003	D1004	N1005	K1006	S1007	Q1008	L1009	I1010	V1011	A1012	S1013	E1014	D1015	N1016	K1017	S1018	Q1019	L1020	I1021	V1022	A1023	S1024	E1025	D1026	N1027	K1028	S1029	Q1030	L1031	I1032	V1033	A1034	S1035	E1036	D1037	N1038	K1039	S1040	Q1041	L1042	I1043	V1044	A1045	S1046	E1047	D1048	N1049	K1050	S1051	Q1052	L1053	I1054	V1055	A1056	S1057	E1058	D1059	N1060	K1061	S1062	Q1063	L1064	I1065	V1066	A1067	S1068	E1069	D1070	N1071	K1072	S1073	Q1074	L1075	I1076	V1077	A1078	S1079	E1080	D1081	N1082	K1083	S1084	Q1085	L1086	I1087	V1088	A1089	S1090	E1091	D1092	N1093	K1094	S1095	Q1096	L1097	I1098	V1099	A1100	S1101	E1102	D1103	N1104	K1105	S1106	Q1107	L1108	I1109	V1110	A1111	S1112	E1113	D1114	N1115	K1116	S1117	Q1118	L1119	I1120	V1121	A1122	S1123	E1124	D1125	N1126	K1127	S1128	Q1129	L1130	I1131	V1132	A1133	S1134	E1135	D1136	N1137	K1138	S1139	Q1140	L1141	I1142	V1143	A1144	S1145	E1146	D1147	N1148	K1149	S1150	Q1151	L1152	I1153	V1154	A1155	S1156	E1157	D1158	N1159	K1160	S1161	Q1162	L1163	I1164	V1165	A1166	S1167	E1168	D1169	N1170	K1171	S1172	Q1173	L1174	I1175	V1176	A1177	S1178	E1179	D1180	N1181	K1182	S1183	Q1184	L1185	I1186	V1187	A1188	S1189	E1190	D1191	N1192	K1193	S1194	Q1195	L1196	I1197	V1198	A1199	S1200	E1201	D1202	N1203	K1204	S1205	Q1206	L1207	I1208	V1209	A1210	S1211	E1212	D1213	N1214	K1215	S1216	Q1217	L1218	I1219	V1220	A1221	S1222	E1223	D1224	N1225	K1226	S1227	Q1228	L1229	I1230	V1231	A1232	S1233	E1234	D1235	N1236	K1237	S1238	Q1239	L1240	I1241	V1242	A1243	S1244	E1245	D1246	N1247	K1248	S1249	Q1250	L1251	I1252	V1253	A1254	S1255	E1256	D1257	N1258	K1259	S1260	Q1261	L1262	I1263	V1264	A1265	S1266	E1267	D1268	N1269	K1270	S1271	Q1272	L1273	I1274	V1275	A1276	S1277	E1278	D1279	N1280	K1281	S1282	Q1283	L1284	I1285	V1286	A1287	S1288	E1289	D1290	N1291	K1292	S1293	Q1294	L1295	I1296	V1297	A1298	S1299	E1300	D1301	N1302	K1303	S1304	Q1305	L1306	I1307	V1308	A1309	S1310	E1311	D1312	N1313	K1314	S1315	Q1316	L1317	I1318	V1319	A1320	S1321	E1322	D1323	N1324	K1325	S1326	Q1327	L1328	I1329	V1330	A1331	S1332	E1333	D1334	N1335	K1336	S1337	Q1338	L1339	I1340	V1341	A1342	S1343	E1344	D1345	N1346	K1347	S1348	Q1349	L1350	I1351	V1352	A1353	S1354	E1355	D1356	N1357	K1358	S1359	Q1360	L1361	I1362	V1363	A1364	S1365	E1366	D1367	N1368	K1369	S1370	Q1371	L1372	I1373	V1374	A1375	S1376	E1377	D1378	N1379	K1380	S1381	Q1382	L1383	I1384	V1385	A1386	S1387	E1388	D1389	N1390	K1391	S1392	Q1393	L1394	I1395	V1396	A1397	S1398	E1399	D1400	N1401	K1402	S1403	Q1404	L1405	I1406	V1407	A1408	S1409	E1410	D1411	N1412	K1413	S1414	Q1415	L1416	I1417	V1418	A1419	S1420	E1421	D1422	N1423	K1424	S1425	Q1426	L1427	I1428	V1429	A1430	S1431	E1432	D1433	N1434	K1435	S1436	Q1437	L1438	I1439	V1440	A1441	S1442	E1443	D1444	N1445	K1446	S1447	Q1448	L1449	I1450	V1451	A1452	S1453	E1454	D1455	N1456	K1457	S1458	Q1459	L1460	I1461	V1462	A1463	S1464	E1465	D1466	N1467	K1468	S1469	Q1470	L1471	I1472	V1473	A1474	S1475	E1476	D1477	N1478	K1479	S1480	Q1481	L1482	I1483	V1484	A1485	S1486	E1487	D1488	N1489	K1490	S1491	Q1492	L1493	I1494	V1495	A1496	S1497	E1498	D1499	N1500	K1501	S1502	Q1503	L1504	I1505	V1506	A1507	S1508	E1509	D1510	N1511	K1512	S1513	Q1514	L1515	I1516	V1517	A1518	S1519	E1520	D1521	N1522	K1523	S1524	Q1525	L1526	I1527	V1528	A1529	S1530	E1531	D1532	N1533	K1534	S1535	Q1536	L1537	I1538	V1539	A1540	S1541	E1542	D1543	N1544	K1545	S1546	Q1547	L1548	I1549	V1550	A1551	S1552	E1553	D1554	N1555	K1556	S1557	Q1558	L1559	I1560	V1561	A1562	S1563	E1564	D1565	N1566	K1567	S1568	Q1569	L1570	I1571	V1572	A1573
------	------	--	------	------	------	------	------	--	------	------	------	------	------	------	------	------	------	------	--	------	--	------	------	--	------	------	------	------	------	------	------	------	------	--	------	--	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	60.39Å 60.39Å 172.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.72 – 2.56	Depositor
% Data completeness (in resolution range)	99.1 (38.72-2.56)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.168 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5132	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/1260	0.64	0/1697
1	B	0.26	0/1288	0.66	0/1737
1	C	0.32	1/1306 (0.1%)	0.67	0/1761
1	D	0.26	0/1280	0.64	1/1726 (0.1%)
All	All	0.28	1/5134 (0.0%)	0.65	1/6921 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	VAL	CA-CB	5.99	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	GLN	N-CA-C	-5.52	106.38	113.01

There are no chirality outliers.

There are no planarity outliers.

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	1238	0	1249	47	0
1	B	1265	0	1275	52	0
1	C	1282	0	1288	60	0
1	D	1257	0	1264	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	13	0	0	0	0
2	D	37	0	0	0	0
All	All	5132	0	5076	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 191 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:B:18:ARG:HA	1:B:23:LYS:HE3	1.50	0.94
1:B:60:LYS:HD3	1:B:66:ASP:HB3	1.50	0.91
1:A:42:LYS:HD3	1:A:44:LEU:HD21	1.56	0.87
1:C:52:LEU:HD22	1:C:135:ALA:HB3	1.68	0.74
1:B:71:ASN:HD22	1:B:86:ARG:HE	1.36	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/169 (90%)	142 (93%)	11 (7%)	0	100	100
1	B	159/169 (94%)	149 (94%)	10 (6%)	0	100	100
1	C	160/169 (95%)	148 (92%)	12 (8%)	0	100	100
1	D	158/169 (94%)	152 (96%)	6 (4%)	0	100	100
All	All	630/676 (93%)	591 (94%)	39 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	136/145 (94%)	130 (96%)	6 (4%)	25	37
1	B	139/145 (96%)	129 (93%)	10 (7%)	13	18
1	C	141/145 (97%)	133 (94%)	8 (6%)	18	28
1	D	138/145 (95%)	131 (95%)	7 (5%)	21	32
All	All	554/580 (96%)	523 (94%)	31 (6%)	20	28

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	158	LEU
1	D	57	GLN
1	C	18[A]	ARG
1	D	159	VAL
1	D	13	LEU

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

Mol	Chain	Res	Type
1	C	57	GLN
1	D	138	GLN
1	C	125	GLN
1	D	153	GLN
1	D	57	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.