



Full wwPDB X-ray Structure Validation Report ⓘ

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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 Full wwPDB X-ray Structure Validation 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

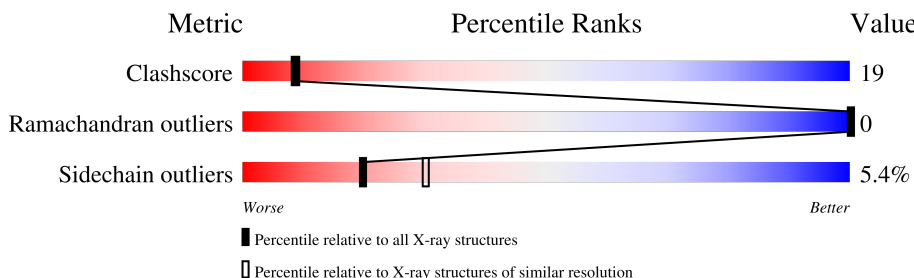
1 Overall quality at a glance

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.

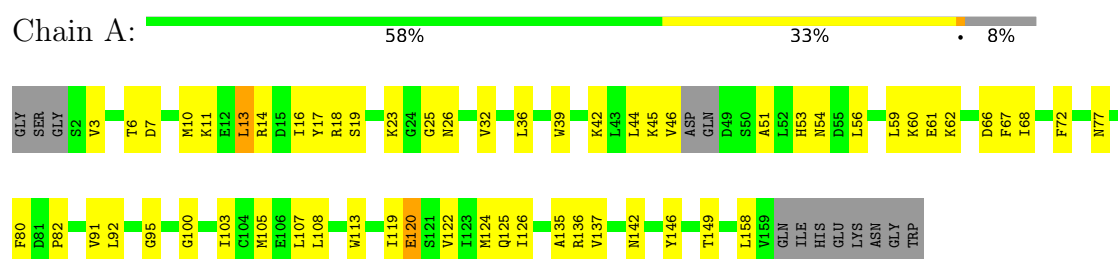
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	20	Total	O	0	0
			20	20		
2	C	13	Total	O	0	0
			13	13		
2	D	37	Total	O	0	0
			37	37		

3 Residue-property plots [i](#)

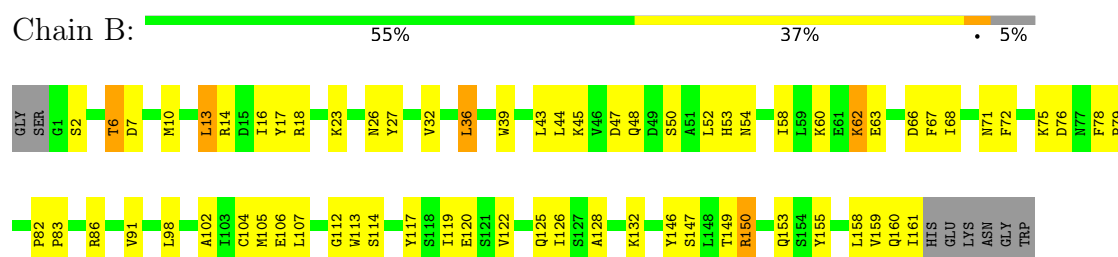
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

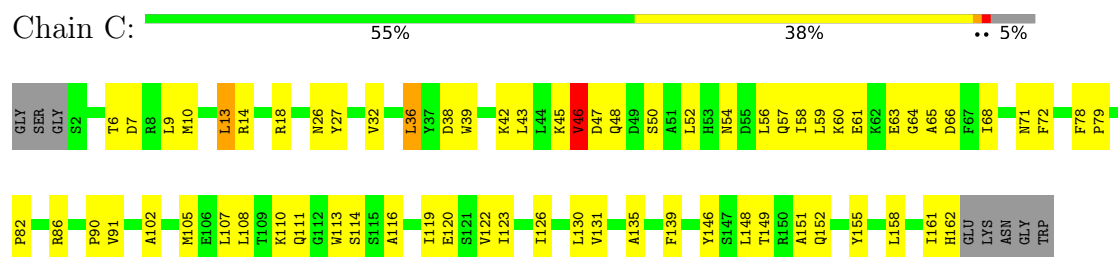
• Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



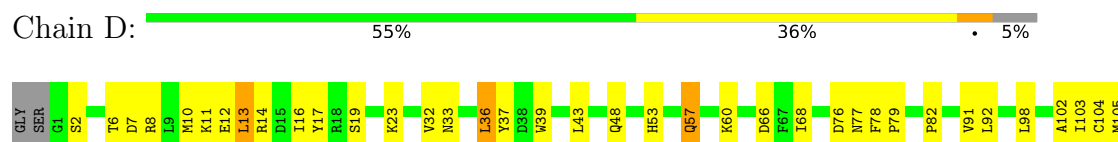
• Molecule 1: Ubiquitin-conjugating enzyme E2 Q1



• 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	Y173	S174	L175	I176	V177	I178	E179	S180	D181	N182	K183	S184	Q185	Y186	S187	L188	I189	V190	I191	E192	S193	D194	N195	K196	S197	Q198	Y199	S200	L201	I202	V203	I204	E205	S206	D207	N208	K209	S210	Q211	Y212	S213	L214	I215	V216	I217	E218	S219	D220	N221	K222	S223	Q224	Y225	S226	L227	I228	V229	I230	E231	S232	D233	N234	K235	S236	Q237	Y238	S239	L240	I241	V242	I243	E244	S245	D246	N247	K248	S249	Q250	Y251	S252	L253	I254	V255	I256	E257	S258	D259	N260	K261	S262	Q263	Y264	S265	L266	I267	V268	I269	E270	S271	D272	N273	K274	S275	Q276	Y277	S278	L279	I280	V281	I282	E283	S284	D285	N286	K287	S288	Q289	Y290	S291	L292	I293	V294	I295	E296	S297	D298	N299	K300	S301	Q302	Y303	S304	L305	I306	V307	I308	E309	S310	D311	N312	K313	S314	Q315	Y316	S317	L318	I319	V320	I321	E322	S323	D324	N325	K326	S327	Q328	Y329	S330	L331	I332	V333	I334	E335	S336	D337	N338	K339	S340	Q341	Y342	S343	L344	I345	V346	I347	E348	S349	D350	N351	K352	S353	Q354	Y355	S356	L357	I358	V359	I360	E361	S362	D363	N364	K365	S366	Q367	Y368	S369	L370	I371	V372	I373	E374	S375	D376	N377	K378	S379	Q380	Y381	S382	L383	I384	V385	I386	E387	S388	D389	N390	K391	S392	Q393	Y394	S395	L396	I397	V398	I399	E400	S401	D402	N403	K404	S405	Q406	Y407	S408	L409	I410	V411	I412	E413	S414	D415	N416	K417	S418	Q419	Y420	S421	L422	I423	V424	I425	E426	S427	D428	N429	K430	S431	Q432	Y433	S434	L435	I436	V437	I438	E439	S440	D441	N442	K443	S444	Q445	Y446	S447	L448	I449	V450	I451	E452	S453	D454	N455	K456	S457	Q458	Y459	S460	L461	I462	V463	I464	E465	S466	D467	N468	K469	S470	Q471	Y472	S473	L474	I475	V476	I477	E478	S479	D480	N481	K482	S483	Q484	Y485	S486	L487	I488	V489	I490	E491	S492	D493	N494	K495	S496	Q497	Y498	S499	L500	I501	V502	I503	E504	S505	D506	N507	K508	S509	Q510	Y511	S512	L513	I514	V515	I516	E517	S518	D519	N520	K521	S522	Q523	Y524	S525	L526	I527	V528	I529	E530	S531	D532	N533	K534	S535	Q536	Y537	S538	L539	I540	V541	I542	E543	S544	D545	N546	K547	S548	Q549	Y550	S551	L552	I553	V554	I555	E556	S557	D558	N559	K560	S561	Q562	Y563	S564	L565	I566	V567	I568	E569	S570	D571	N572	K573	S574	Q575	Y576	S577	L578	I579	V580	I581	E582	S583	D584	N585	K586	S587	Q588	Y589	S590	L591	I592	V593	I594	E595	S596	D597	N598	K599	S600	Q601	Y602	S603	L604	I605	V606	I607	E608	S609	D610	N611	K612	S613	Q614	Y615	S616	L617	I618	V619	I620	E621	S622	D623	N624	K625	S626	Q627	Y628	S629	L630	I631	V632	I633	E634	S635	D636	N637	K638	S639	Q640	Y641	S642	L643	I644	V645	I646	E647	S648	D649	N650	K651	S652	Q653	Y654	S655	L656	I657	V658	I659	E660	S661	D662	N663	K664	S665	Q666	Y667	S668	L669	I670	V671	I672	E673	S674	D675	N676	K677	S678	Q679	Y680	S681	L682	I683	V684	I685	E686	S687	D688	N689	K690	S691	Q692	Y693	S694	L695	I696	V697	I698	E699	S700	D701	N702	K703	S704	Q705	Y706	S707	L708	I709	V710	I711	E712	S713	D714	N715	K716	S717	Q718	Y719	S720	L721	I722	V723	I724	E725	S726	D727	N728	K729	S730	Q731	Y732	S733	L734	I735	V736	I737	E738	S739	D740	N741	K742	S743	Q744	Y745	S746	L747	I748	V749	I750	E751	S752	D753	N754	K755	S756	Q757	Y758	S759	L760	I761	V762	I763	E764	S765	D766	N767	K768	S769	Q770	Y771	S772	L773	I774	V775	I776	E777	S778	D779	N780	K781	S782	Q783	Y784	S785	L786	I787	V788	I789	E790	S791	D792	N793	K794	S795	Q796	Y797	S798	L799	I800	V801	I802	E803	S804	D805	N806	K807	S808	Q809	Y810	S811	L812	I813	V814	I815	E816	S817	D818	N819	K820	S821	Q822	Y823	S824	L825	I826	V827	I828	E829	S830	D831	N832	K833	S834	Q835	Y836	S837	L838	I839	V840	I841	E842	S843	D844	N845	K846	S847	Q848	Y849	S850	L851	I852	V853	I854	E855	S856	D857	N858	K859	S860	Q861	Y862	S863	L864	I865	V866	I867	E868	S869	D870	N871	K872	S873	Q874	Y875	S876	L877	I878	V879	I880	E881	S882	D883	N884	K885	S886	Q887	Y888	S889	L890	I891	V892	I893	E894	S895	D896	N897	K898	S899	Q900	Y901	S902	L903	I904	V905	I906	E907	S908	D909	N910	K911	S912	Q913	Y914	S915	L916	I917	V918	I919	E920	S921	D922	N923	K924	S925	Q926	Y927	S928	L929	I930	V931	I932	E933	S934	D935	N936	K937	S938	Q939	Y940	S941	L942	I943	V944	I945	E946	S947	D948	N949	K950	S951	Q952	Y953	S954	L955	I956	V957	I958	E959	S960	D961	N962	K963	S964	Q965	Y966	S967	L968	I969	V970	I971	E972	S973	D974	N975	K976	S977	Q978	Y979	S980	L981	I982	V983	I984	E985	S986	D987	N988	K989	S990	Q991	Y992	S993	L994	I995	V996	I997	E998	S999	D1000	N1001	K1002	S1003	Q1004	Y1005	S1006	L1007	I1008	V1009	I1010	E1011	S1012	D1013	N1014	K1015	S1016	Q1017	Y1018	S1019	L1020	I1021	V1022	I1023	E1024	S1025	D1026	N1027	K1028	S1029	Q1030	Y1031	S1032	L1033	I1034	V1035	I1036	E1037	S1038	D1039	N1040	K1041	S1042	Q1043	Y1044	S1045	L1046	I1047	V1048	I1049	E1050	S1051	D1052	N1053	K1054	S1055	Q1056	Y1057	S1058	L1059	I1060	V1061	I1062	E1063	S1064	D1065	N1066	K1067	S1068	Q1069	Y1070	S1071	L1072	I1073	V1074	I1075	E1076	S1077	D1078	N1079	K1080	S1081	Q1082	Y1083	S1084	L1085	I1086	V1087	I1088	E1089	S1090	D1091	N1092	K1093	S1094	Q1095	Y1096	S1097	L1098	I1099	V1100	I1101	E1102	S1103	D1104	N1105	K1106	S1107	Q1108	Y1109	S1110	L1111	I1112	V1113	I1114	E1115	S1116	D1117	N1118	K1119	S1120	Q1121	Y1122	S1123	L1124	I1125	V1126	I1127	E1128	S1129	D1130	N1131	K1132	S1133	Q1134	Y1135	S1136	L1137	I1138	V1139	I1140	E1141	S1142	D1143	N1144	K1145	S1146	Q1147	Y1148	S1149	L1150	I1151	V1152	I1153	E1154	S1155	D1156	N1157	K1158	S1159	Q1160	Y1161	S1162	L1163	I1164	V1165	I1166	E1167	S1168	D1169	N1170	K1171	S1172	Q1173	Y1174	S1175	L1176	I1177	V1178	I1179	E1180	S1181	D1182	N1183	K1184	S1185	Q1186	Y1187	S1188	L1189	I1190	V1191	I1192	E1193	S1194	D1195	N1196	K1197	S1198	Q1199	Y1200	S1201	L1202	I1203	V1204	I1205	E1206	S1207	D1208	N1209	K1210	S1211	Q1212	Y1213	S1214	L1215	I1216	V1217	I1218	E1219	S1220	D1221	N1222	K1223	S1224	Q1225	Y1226	S1227	L1228	I1229	V1230	I1231	E1232	S1233	D1234	N1235	K1236	S1237	Q1238	Y1239	S1240	L1241	I1242	V1243	I1244	E1245	S1246	D1247	N1248	K1249	S1250	Q1251	Y1252	S1253	L1254	I1255	V1256	I1257	E1258	S1259	D1260	N1261	K1262	S1263	Q1264	Y1265	S1266	L1267	I1268	V1269	I1270	E1271	S1272	D1273	N1274	K1275	S1276	Q1277	Y1278	S1279	L1280	I1281	V1282	I1283	E1284	S1285	D1286	N1287	K1288	S1289	Q1290	Y1291	S1292	L1293	I1294	V1295	I1296	E1297	S1298	D1299	N1300	K1301	S1302	Q1303	Y1304	S1305	L1306	I1307	V1308	I1309	E1310	S1311	D1312	N1313	K1314	S1315	Q1316	Y1317	S1318	L1319	I1320	V1321	I1322	E1323	S1324	D1325	N1326	K1327	S1328	Q1329	Y1330	S1331	L1332	I1333	V1334	I1335	E1336	S1337	D1338	N1339	K1340	S1341	Q1342	Y1343	S1344	L1345	I1346	V1347	I1348	E1349	S1350	D1351	N1352	K1353	S1354	Q1355	Y1356	S1357	L1358	I1359	V1360	I1361	E1362	S1363	D1364	N1365	K1366	S1367	Q1368	Y1369	S1370	L1371	I1372	V1373	I1374	E1375	S1376	D1377	N1378	K1379	S1380	Q1381	Y1382	S1383	L1384	I1385	V1386	I1387	E1388	S1389	D1390	N1391	K1392	S1393	Q1394	Y1395	S1396	L1397	I1398	V1399	I1400	E1401	S1402	D1403	N1404	K1405	S1406	Q1407	Y1408	S1409	L1410	I1411	V1412	I1413	E1414	S1415	D1416	N1417	K1418	S1419	Q1420	Y1421	S1422	L1423	I1424	V1425	I1426	E1427	S1428	D1429	N1430	K1431	S1432	Q1433	Y1434	S1435	L1436	I1437	V1438	I1439	E1440	S1441	D1442	N1443	K1444	S1445	Q1446	Y1447	S1448	L1449	I1450	V1451	I1452	E1453	S1454	D1455	N1456	K1457	S1458	Q1459	Y1460	S1461	L1462	I1463	V1464	I1465	E1466	S1467	D1468	N1469	K1470	S1471	Q1472	Y1473	S1474	L1475	I1476	V1477	I1478	E1479	S1480	D1481	N1482	K1483	S1484	Q1485	Y1486	S1487	L1488	I1489	V1490	I1491	E1492	S1493	D1494	N1495	K1496	S1497	Q1498	Y1499	S1500	L1501	I1502	V1503	I1504	E1505	S1506	D1507	N1508	K1509	S1510	Q1511	Y1512	S1513	L1514	I1515	V1516	I1517	E1518	S1519	D1520	N1521	K1522	S1523	Q1524	Y1525	S1526	L1527	I1528	V1529	I1530	E1531	S1532	D1533	N1534	K1535	S1536	Q1537	Y1538	S1539	L1540	I1541	V1542	I1543	E1544	S1545	D1546	N1547	K1548	S1549	Q1550	Y1551	S1552	L1553	I1554	V1555	I1556	E1557	S1558	D1559	N1560	K1561	S1562	Q1563	Y1
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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

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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.

All (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
1:C:50:SER:HB3	1:C:131:VAL:HG13	1.71	0.72
1:D:60:LYS:HD3	1:D:66:ASP:HB3	1.71	0.72
1:A:119:ILE:HA	1:A:122:VAL:HG12	1.73	0.71
1:C:91:VAL:HA	1:C:146:TYR:CE2	2.27	0.69
1:D:16:ILE:HG12	1:D:120:GLU:HB3	1.75	0.68
1:A:26:ASN:HA	1:A:45:LYS:HB2	1.75	0.68
1:A:149:THR:HG23	1:C:152:GLN:HE22	1.60	0.66
1:B:54:ASN:O	1:B:58:ILE:HG12	1.96	0.65
1:D:39:TRP:CZ3	1:D:119:ILE:HG21	2.32	0.64
1:D:60:LYS:HB2	1:D:66:ASP:HB3	1.79	0.64
1:A:124:MET:HE2	1:A:124:MET:HA	1.79	0.64
1:B:2:SER:O	1:B:6:THR:HG22	1.97	0.64
1:C:60:LYS:HA	1:C:64:GLY:O	1.98	0.64
1:D:6:THR:HG22	1:D:37:TYR:OH	1.96	0.64
1:C:14:ARG:HG2	1:D:7:ASP:OD2	1.96	0.63
1:A:95:GLY:HA3	1:A:135:ALA:HB2	1.80	0.63
1:D:160:GLN:HE21	1:D:160:GLN:N	1.97	0.62
1:C:59:LEU:HD11	1:C:90:PRO:HG3	1.81	0.62
1:D:105:MET:HE2	1:D:107:LEU:HD21	1.82	0.62
1:C:105:MET:HE1	1:C:126:ILE:HG12	1.82	0.62
1:D:39:TRP:HZ3	1:D:119:ILE:HG21	1.65	0.61
1:C:54:ASN:HA	1:C:57:GLN:HE22	1.66	0.61
1:A:60:LYS:HB2	1:A:66:ASP:HB3	1.82	0.61
1:B:44:LEU:HD23	1:B:67:PHE:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG11	1:A:53:HIS:HA	1.83	0.60
1:D:2:SER:O	1:D:6:THR:HG23	2.02	0.60
1:A:91:VAL:HA	1:A:146:TYR:CE2	2.38	0.59
1:B:16:ILE:HG12	1:B:120:GLU:HB2	1.85	0.59
1:C:14:ARG:HG3	1:D:10:MET:HE3	1.84	0.58
1:B:91:VAL:HA	1:B:146:TYR:CE2	2.38	0.58
1:A:107:LEU:HD22	1:A:125:GLN:NE2	2.19	0.58
1:D:105:MET:HE2	1:D:107:LEU:CD2	2.34	0.58
1:C:105:MET:HE1	1:C:126:ILE:HA	1.85	0.58
1:C:7:ASP:OD1	1:D:14:ARG:HD2	2.04	0.57
1:B:48:GLN:HG3	1:B:53:HIS:CE1	2.39	0.57
1:C:59:LEU:HD11	1:C:90:PRO:CG	2.34	0.57
1:A:105:MET:HE2	1:A:108:LEU:HG	1.86	0.57
1:C:71:ASN:HD22	1:C:86:ARG:HE	1.51	0.56
1:D:114:SER:HB3	1:D:117:TYR:CD1	2.41	0.56
1:A:14:ARG:CZ	1:A:18[A]:ARG:HH22	2.18	0.55
1:B:10:MET:O	1:B:14:ARG:HG3	2.06	0.55
1:B:107:LEU:HD22	1:B:125:GLN:CD	2.31	0.55
1:D:57:GLN:HE21	1:D:57:GLN:HA	1.72	0.55
1:D:110:LYS:HG3	1:D:159:VAL:HA	1.88	0.55
1:C:86:ARG:HD3	1:C:148:LEU:HD13	1.89	0.54
1:D:19:SER:O	1:D:23:LYS:HG3	2.08	0.54
1:C:105:MET:HB3	1:C:108:LEU:HD23	1.89	0.54
1:D:98:LEU:HD21	1:D:104:CYS:HB2	1.88	0.54
1:A:10:MET:HE3	1:B:14:ARG:HG2	1.89	0.54
1:D:149:THR:O	1:D:153:GLN:HG3	2.06	0.54
1:D:98:LEU:HD12	1:D:102:ALA:HB3	1.90	0.54
1:A:135:ALA:O	1:A:136:ARG:HD2	2.08	0.54
1:C:9:LEU:HB3	1:C:36:LEU:HD12	1.90	0.54
1:A:6:THR:HG22	1:A:10:MET:HE2	1.91	0.53
1:B:147:SER:HB2	1:C:61:GLU:HA	1.89	0.53
1:D:60:LYS:HD3	1:D:66:ASP:CB	2.37	0.53
1:C:6:THR:HG22	1:C:10:MET:HE2	1.91	0.53
1:C:14:ARG:NH1	1:D:11:LYS:HB2	2.24	0.53
1:B:47:ASP:O	1:B:50:SER:HB3	2.09	0.53
1:A:61:GLU:HG3	1:A:62:LYS:H	1.73	0.53
1:D:107:LEU:HA	1:D:112:GLY:O	2.09	0.53
1:A:107:LEU:H	1:A:107:LEU:HD23	1.74	0.52
1:A:16:ILE:HG13	1:A:120:GLU:HG2	1.90	0.52
1:C:39:TRP:HB2	1:C:72:PHE:HB2	1.91	0.52
1:C:60:LYS:HE3	1:C:66:ASP:CG	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:O	1:A:113:TRP:HB2	2.10	0.52
1:B:60:LYS:HB2	1:B:66:ASP:HB3	1.91	0.51
1:C:161:ILE:HG23	1:C:162:HIS:CD2	2.45	0.51
1:D:125:GLN:O	1:D:129:THR:HG23	2.10	0.51
1:B:149:THR:O	1:B:153:GLN:HG3	2.11	0.51
1:D:118:SER:O	1:D:122:VAL:HG23	2.10	0.51
1:A:39:TRP:HB2	1:A:72:PHE:HB2	1.91	0.51
1:B:27:TYR:OH	1:B:120:GLU:HG3	2.11	0.50
1:C:161:ILE:HG23	1:C:162:HIS:HD2	1.76	0.50
1:C:110:LYS:HE3	1:C:111:GLN:HE22	1.76	0.50
1:D:68:ILE:HD13	1:D:92:LEU:HD11	1.92	0.50
1:A:122:VAL:O	1:A:126:ILE:HG13	2.12	0.50
1:C:155:TYR:O	1:C:158:LEU:HB3	2.12	0.50
1:C:110:LYS:HG3	1:C:111:GLN:NE2	2.27	0.49
1:C:114:SER:C	1:C:116:ALA:H	2.19	0.49
1:A:105:MET:CE	1:A:108:LEU:HG	2.42	0.49
1:A:7:ASP:OD2	1:B:14:ARG:HD2	2.12	0.49
1:B:43:LEU:HB2	1:B:68:ILE:HB	1.94	0.49
1:D:82:PRO:HG3	1:D:113:TRP:CB	2.43	0.49
1:C:57:GLN:NE2	1:C:57:GLN:H	2.10	0.49
1:D:106:GLU:O	1:D:112:GLY:HA3	2.12	0.49
1:A:103:ILE:HG22	1:A:105:MET:HB2	1.94	0.48
1:D:142:ASN:O	1:D:144:SER:HA	2.13	0.48
1:A:105:MET:HE3	1:A:107:LEU:HD21	1.93	0.48
1:C:50:SER:HB3	1:C:131:VAL:CG1	2.41	0.48
1:D:135:ALA:O	1:D:136:ARG:HD2	2.13	0.48
1:A:14:ARG:HD2	1:B:7:ASP:OD1	2.13	0.48
1:A:51:ALA:O	1:A:54:ASN:HB3	2.14	0.48
1:C:60:LYS:HB3	1:C:65:ALA:HA	1.96	0.48
1:B:114:SER:HB3	1:B:117:TYR:CE2	2.49	0.47
1:C:82:PRO:HG3	1:C:113:TRP:CB	2.43	0.47
1:C:102:ALA:HB2	1:C:151:ALA:O	2.14	0.47
1:B:98:LEU:HD21	1:B:104:CYS:SG	2.55	0.47
1:C:78:PHE:CD1	1:C:79:PRO:HA	2.50	0.47
1:D:91:VAL:HA	1:D:146:TYR:CE2	2.49	0.47
1:B:78:PHE:CD1	1:B:79:PRO:HA	2.50	0.47
1:B:147:SER:CB	1:C:61:GLU:HG3	2.45	0.47
1:A:119:ILE:HA	1:A:122:VAL:CG1	2.41	0.47
1:B:39:TRP:CZ3	1:B:119:ILE:HG21	2.50	0.47
1:B:159:VAL:O	1:B:161:ILE:HG23	2.15	0.47
1:A:3:VAL:HG13	1:B:17:TYR:CE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:NH1	1:B:150:ARG:HB2	2.30	0.46
1:A:42:LYS:HE3	1:A:67:PHE:CD1	2.50	0.46
1:B:83:PRO:HD3	1:B:113:TRP:CH2	2.49	0.46
1:B:147:SER:HB3	1:C:61:GLU:HG3	1.97	0.46
1:C:52:LEU:HB2	1:C:135:ALA:O	2.16	0.46
1:A:19:SER:O	1:A:23:LYS:HG3	2.15	0.46
1:C:43:LEU:HB2	1:C:68:ILE:HB	1.98	0.46
1:D:48:GLN:HG3	1:D:53:HIS:NE2	2.30	0.46
1:D:13:LEU:HD22	1:D:17:TYR:CE2	2.51	0.46
1:D:120:GLU:O	1:D:124:MET:HG3	2.16	0.46
1:A:25:GLY:O	1:A:44:LEU:HB2	2.16	0.46
1:C:32:VAL:HG12	1:C:38:ASP:O	2.16	0.46
1:D:103:ILE:HG22	1:D:105:MET:HG3	1.97	0.46
1:D:110:LYS:HD3	1:D:159:VAL:O	2.16	0.46
1:A:82:PRO:HG3	1:A:113:TRP:CB	2.46	0.45
1:A:92:LEU:HD23	1:A:137:VAL:HA	1.98	0.45
1:B:105:MET:SD	1:B:126:ILE:HD13	2.56	0.45
1:C:47:ASP:HB3	1:C:50:SER:OG	2.16	0.45
1:A:60:LYS:HE2	1:A:66:ASP:OD2	2.15	0.45
1:B:128:ALA:O	1:B:132:LYS:HD3	2.16	0.45
1:C:52:LEU:O	1:C:56:LEU:HG	2.16	0.45
1:C:122:VAL:O	1:C:126:ILE:HG13	2.15	0.45
1:A:13:LEU:HB3	1:B:10:MET:HE1	1.98	0.45
1:C:36:LEU:HD23	1:D:36:LEU:HB2	1.98	0.45
1:C:110:LYS:HG3	1:C:111:GLN:CD	2.41	0.45
1:D:118:SER:HB3	1:D:121:SER:HB2	1.98	0.45
1:C:13:LEU:HG	1:C:39:TRP:CH2	2.52	0.45
1:B:39:TRP:HB2	1:B:72:PHE:HB2	1.99	0.45
1:A:107:LEU:HD11	1:A:122:VAL:HG23	1.98	0.45
1:A:14:ARG:HG2	1:B:10:MET:HE3	1.99	0.45
1:B:52:LEU:HD21	1:B:68:ILE:HD11	1.99	0.44
1:A:61:GLU:HA	1:D:149:THR:HG22	1.99	0.44
1:D:143:LYS:HA	1:D:144:SER:HA	1.49	0.44
1:B:13:LEU:HG	1:B:39:TRP:CZ2	2.52	0.44
1:A:11:LYS:HB2	1:B:14:ARG:NH1	2.33	0.44
1:B:78:PHE:CG	1:B:79:PRO:HA	2.53	0.44
1:A:13:LEU:HD22	1:A:17:TYR:CE2	2.52	0.44
1:A:77:ASN:O	1:A:80:PHE:HB2	2.17	0.44
1:C:107:LEU:O	1:C:113:TRP:HB2	2.18	0.44
1:B:122:VAL:O	1:B:126:ILE:HG12	2.17	0.43
1:C:26:ASN:ND2	1:C:46:VAL:HG13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:LEU:HB2	1:D:68:ILE:HB	2.00	0.43
1:B:48:GLN:C	1:B:50:SER:H	2.27	0.43
1:C:126:ILE:O	1:C:130:LEU:HG	2.19	0.43
1:D:76:ASP:HA	1:D:77:ASN:HA	1.73	0.43
1:C:54:ASN:H	1:C:54:ASN:HD22	1.67	0.43
1:C:57:GLN:H	1:C:57:GLN:CD	2.27	0.43
1:A:56:LEU:HD21	1:A:68:ILE:HD11	2.01	0.42
1:B:62:LYS:HE3	1:B:62:LYS:HA	2.01	0.42
1:B:82:PRO:HG3	1:B:113:TRP:CB	2.48	0.42
1:B:155:TYR:CE1	1:B:161:ILE:HD11	2.54	0.42
1:D:60:LYS:CD	1:D:66:ASP:HB3	2.47	0.42
1:D:78:PHE:CD1	1:D:79:PRO:HA	2.53	0.42
1:C:119:ILE:O	1:C:123:ILE:HG13	2.19	0.42
1:B:98:LEU:HD12	1:B:102:ALA:HB3	2.02	0.42
1:A:142:ASN:ND2	1:D:33:ASN:H	2.17	0.42
1:D:8:ARG:O	1:D:12:GLU:HG2	2.19	0.42
1:A:14:ARG:NH1	1:A:18[A]:ARG:HH22	2.17	0.41
1:B:36:LEU:O	1:B:36:LEU:HD13	2.20	0.41
1:C:13:LEU:HG	1:C:39:TRP:CZ2	2.55	0.41
1:C:59:LEU:CD1	1:C:90:PRO:HG3	2.48	0.41
1:D:48:GLN:HA	1:D:53:HIS:CG	2.55	0.41
1:D:119:ILE:O	1:D:123:ILE:HG13	2.20	0.41
1:C:63:GLU:O	1:C:63:GLU:HG3	2.20	0.41
1:B:26:ASN:HA	1:B:45:LYS:HB2	2.02	0.41
1:C:58:ILE:HG21	1:C:139:PHE:HZ	1.84	0.41
1:B:106:GLU:O	1:B:112:GLY:HA3	2.20	0.41
1:C:114:SER:C	1:C:116:ALA:N	2.78	0.41
1:D:141:ALA:O	1:D:143:LYS:HD2	2.20	0.41
1:B:155:TYR:HE1	1:B:161:ILE:HD11	1.86	0.41
1:B:75:LYS:HA	1:B:75:LYS:HD2	1.83	0.41
1:B:82:PRO:HG3	1:B:113:TRP:HB2	2.02	0.41
1:A:61:GLU:HB2	1:D:147:SER:CB	2.51	0.41
1:B:159:VAL:HG23	1:B:161:ILE:HG12	2.03	0.41
1:C:27:TYR:OH	1:C:120:GLU:HG3	2.20	0.41
1:C:158:LEU:C	1:C:158:LEU:HD13	2.46	0.41
1:C:27:TYR:HA	1:C:42:LYS:O	2.21	0.40
1:C:71:ASN:ND2	1:C:86:ARG:HE	2.17	0.40
1:A:100:GLY:C	1:A:146:TYR:CD1	3.00	0.40
1:D:122:VAL:O	1:D:126:ILE:HG13	2.21	0.40

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 [i](#)

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

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	32	VAL

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	59	LEU
1	A	120	GLU
1	A	158	LEU
1	B	6	THR
1	B	13	LEU
1	B	32	VAL
1	B	36	LEU
1	B	62	LYS
1	B	63	GLU
1	B	76	ASP
1	B	150	ARG
1	B	158	LEU
1	B	160	GLN
1	C	13	LEU
1	C	18[A]	ARG
1	C	18[B]	ARG
1	C	36	LEU
1	C	45	LYS
1	C	46	VAL
1	C	48	GLN
1	C	149	THR
1	D	13	LEU
1	D	32	VAL
1	D	36	LEU
1	D	57	GLN
1	D	149	THR
1	D	159	VAL
1	D	160	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	77	ASN
1	A	111	GLN
1	A	125	GLN
1	A	145	GLN
1	B	4	GLN
1	B	53	HIS
1	B	71	ASN
1	B	145	GLN

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	153	GLN
1	B	160	GLN
1	C	48	GLN
1	C	54	ASN
1	C	57	GLN
1	C	71	ASN
1	C	111	GLN
1	C	125	GLN
1	C	145	GLN
1	C	152	GLN
1	C	160	GLN
1	C	162	HIS
1	D	48	GLN
1	D	53	HIS
1	D	57	GLN
1	D	77	ASN
1	D	125	GLN
1	D	138	GLN
1	D	145	GLN
1	D	153	GLN
1	D	160	GLN

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 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.