



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 1, 2017 – 07:22 PM EDT

PDB ID : 1QXP  
Title : Crystal Structure of a mu-like calpain  
Authors : Pal, G.P.; Veyra, T.D.; Elce, J.S.; Jia, Z.  
Deposited on : unknown  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

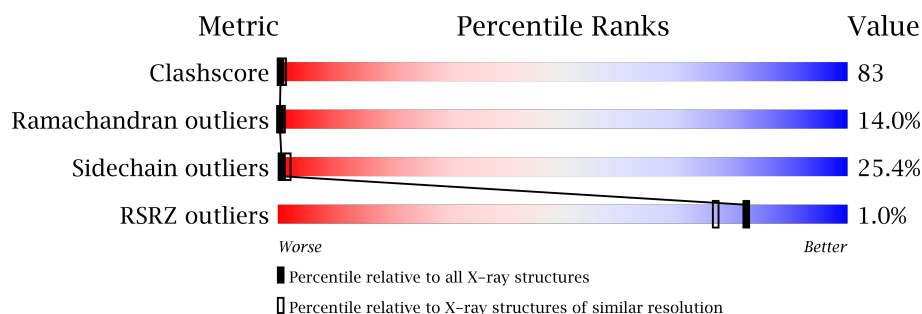
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	900	
1	B	900	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12368 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 mu-like calpain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	783	Total	C	N	O	S	0	0	0
			6053	3846	1037	1143	27			
1	B	788	Total	C	N	O	S	0	0	0
			6003	3830	1015	1129	29			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	ENGINEERED	UNP P97571
B	105	SER	CYS	ENGINEERED	UNP P97571
A	702A	GLY	-	CLONING ARTIFACT	UNP Q07009
A	702B	LYS	-	CLONING ARTIFACT	UNP Q07009
A	702C	LEU	-	CLONING ARTIFACT	UNP Q07009
A	702D	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702E	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702F	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702G	ILE	-	CLONING ARTIFACT	UNP Q07009
A	702H	GLU	-	CLONING ARTIFACT	UNP Q07009
A	702I	HIS	-	EXPRESSION TAG	UNP Q07009
A	702J	HIS	-	EXPRESSION TAG	UNP Q07009
A	702K	HIS	-	EXPRESSION TAG	UNP Q07009
A	702L	HIS	-	EXPRESSION TAG	UNP Q07009
A	702M	HIS	-	EXPRESSION TAG	UNP Q07009
A	702N	HIS	-	EXPRESSION TAG	UNP Q07009
B	702A	GLY	-	CLONING ARTIFACT	UNP Q07009
B	702B	LYS	-	CLONING ARTIFACT	UNP Q07009
B	702C	LEU	-	CLONING ARTIFACT	UNP Q07009
B	702D	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702E	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702F	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702G	ILE	-	CLONING ARTIFACT	UNP Q07009
B	702H	GLU	-	CLONING ARTIFACT	UNP Q07009
B	702I	HIS	-	EXPRESSION TAG	UNP Q07009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	702J	HIS	-	EXPRESSION TAG	UNP Q07009
B	702K	HIS	-	EXPRESSION TAG	UNP Q07009
B	702L	HIS	-	EXPRESSION TAG	UNP Q07009
B	702M	HIS	-	EXPRESSION TAG	UNP Q07009
B	702N	HIS	-	EXPRESSION TAG	UNP Q07009

- Molecule 2 is water.

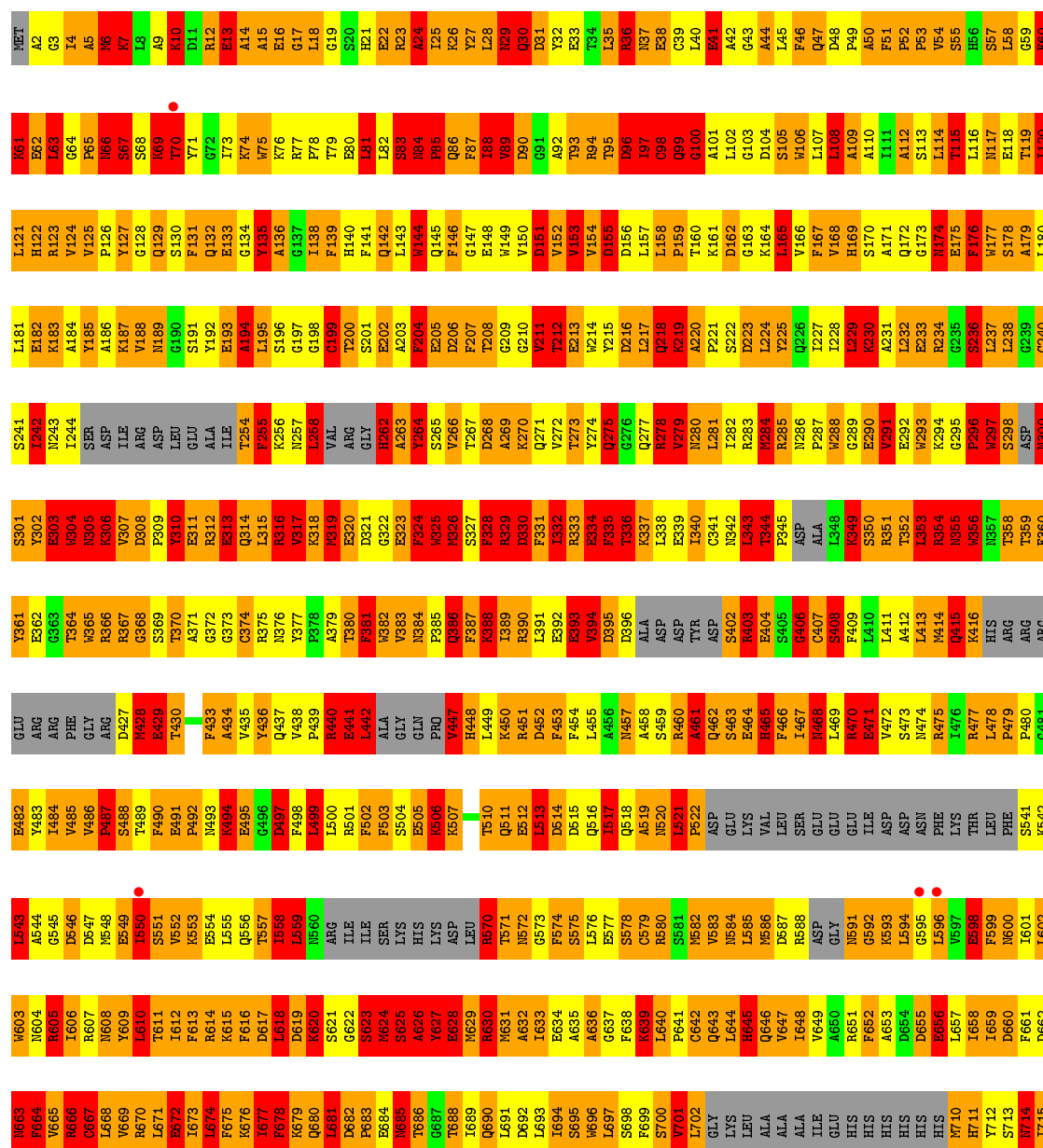
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	172	Total O 172 172	0	0
2	B	140	Total O 140 140	0	0

### 3 Residue-property plots

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

Chain A: 



[illegible]

- Molecule 1: mu-like calpain



F661	D662	N663	F664	V665	R666	C667	V668	F669	B670	L671	E672	L673	L674	F675	K676	L677	F678	K679	G680	L691	D692	L693	L694	G695	G696	L697	F698	G699	F700	G701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	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	L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N714	ILE	N715	GLU	ALA	N718	E719	S720	EO	GLU	E723	R724	Q725	E726	R727	K728	L729	F730	V731	Q732	L733	ALA	GLY	ASP	ASP	N738	E739	V740	S741	A742	T743	E744	L745	N746	ASN	ILE	LEU	ASN	LYS	VAL	VAL	THR	ARG	HIS	PRO	ASP	LEU	LYS	THR	ASP	GLY	F764	G765	I766	D767	T768	C769	R770	S771	M772	V773
A774	V775	M776	D777	S778	D779	T780	T781		L784	G785	F786	E787	E788	F789	K790	Y791	L792	W793	N794	N795	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	N831	Q832	H833	I834		
Y835	S836	M837	I838	I839	R840	ARG	TYR	S843	G847	N848	M849	D850	F851	D852	N853	F854	I855	S856	C857	L858	V859	R860	L861	D862	A863	M864	F865	R866	A867	F868	R869	S870	L871	D872	K873	N874	G875	T876	G877	Q878	I879	Q880	V881	N882	I883	Q884	E885	W886	L887	Q888	L889	T890	M891	Y892	S893					

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.74Å 184.60Å 86.37Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	91.29 – 2.80 49.81 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.6 (91.29-2.80) 87.3 (49.81-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.229 , 0.311 0.232 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 98.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	3.70	964/6177 (15.6%)	2.67	470/8354 (5.6%)
1	B	3.71	932/6128 (15.2%)	2.67	489/8288 (5.9%)
All	All	3.70	1896/12305 (15.4%)	2.67	959/16642 (5.8%)

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	45
1	B	0	39
All	All	0	84

The worst 5 of 1896 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	SER	CA-CB	28.73	1.96	1.52
1	A	339	GLU	CD-OE1	23.66	1.51	1.25
1	A	320	GLU	CD-OE2	20.06	1.47	1.25
1	B	429	GLU	CD-OE1	19.54	1.47	1.25
1	A	811	SER	CA-CB	-18.37	1.25	1.52

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH1	-29.77	105.41	120.30
1	A	329	ARG	NE-CZ-NH1	26.14	133.37	120.30
1	A	329	ARG	NE-CZ-NH2	-24.17	108.22	120.30
1	B	514	ASP	CB-CG-OD2	-18.56	101.59	118.30
1	A	285	ARG	NE-CZ-NH2	-15.96	112.32	120.30

There are no chirality outliers.

5 of 84 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ILE	Mainchain
1	A	152	VAL	Mainchain
1	A	24	ALA	Mainchain
1	A	29	ASN	Mainchain
1	A	99	GLN	Mainchain,Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6053	0	5615	959	3
1	B	6003	0	5477	969	1
2	A	172	0	0	53	1
2	B	140	0	0	45	1
All	All	12368	0	11092	1928	3

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 83.

The worst 5 of 1928 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:583:VAL:CB	1:A:583:VAL:CA	1.74	1.65
1:B:0:GLU:CA	1:B:0:GLU:CB	1.75	1.64
1:B:786:PHE:CA	1:B:786:PHE:CB	1.74	1.64
1:A:550:ILE:CB	1:A:550:ILE:CA	1.75	1.64
1:B:8:LEU:CD2	1:B:8:LEU:CG	1.76	1.63

All (3) 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:457:ASN:OD1	2:B:1033:HOH:O[1_454]	1.56	0.64
1:A:442:LEU:CD2	2:A:922:HOH:O[1_455]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:OD1	1:B:303:GLU:N[2_656]	2.08	0.12

## 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	747/900 (83%)	500 (67%)	143 (19%)	104 (14%)	0	1
1	B	748/900 (83%)	497 (66%)	146 (20%)	105 (14%)	0	1
All	All	1495/1800 (83%)	997 (67%)	289 (19%)	209 (14%)	0	1

5 of 209 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	60	PHE
1	A	63	LEU
1	A	67	SER
1	A	83	SER

### 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	606/782 (78%)	459 (76%)	147 (24%)	1	2
1	B	584/782 (75%)	429 (74%)	155 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1190/1564 (76%)	888 (75%)	302 (25%)	<b>0</b> <b>2</b>

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	853	ASN
1	B	111	ILE
1	B	701	VAL
1	A	874	ASN
1	B	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	853	ASN
1	B	47	GLN
1	B	646	GLN
1	A	878	GLN
1	A	888	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 [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	783/900 (87%)	-0.36	4 (0%) 90 88	16, 49, 81, 98	0
1	B	788/900 (87%)	-0.32	11 (1%) 75 69	17, 51, 84, 102	0
All	All	1571/1800 (87%)	-0.34	15 (0%) 82 77	16, 50, 83, 102	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	596	LEU	3.7
1	B	587	ASP	3.7
1	A	596	LEU	3.3
1	B	712	TYR	3.3
1	B	402	SER	3.2

### 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.