



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:41 PM UTC

PDB ID : 6MIX / pdb_00006mix
EMDB ID : EMD-9132
Title : Human TRPM2 ion channel in apo state
Authors : Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on : 2018-09-20
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

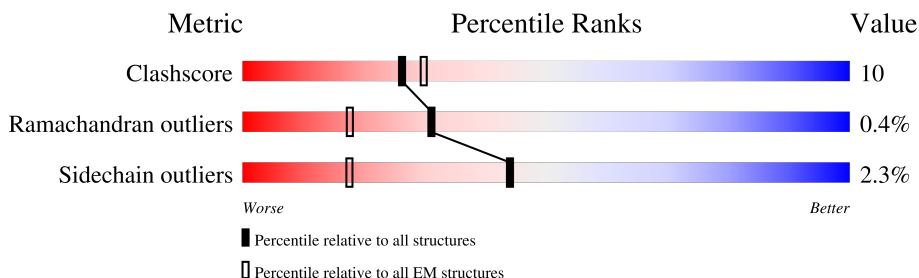
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1503	83% 64% 23% • 11%
1	B	1503	89% 65% 23% • 11%
1	C	1503	89% 64% 23% • 11%
1	D	1503	88% 65% 23% • 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 43120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transient receptor potential cation channel subfamily M member 2.

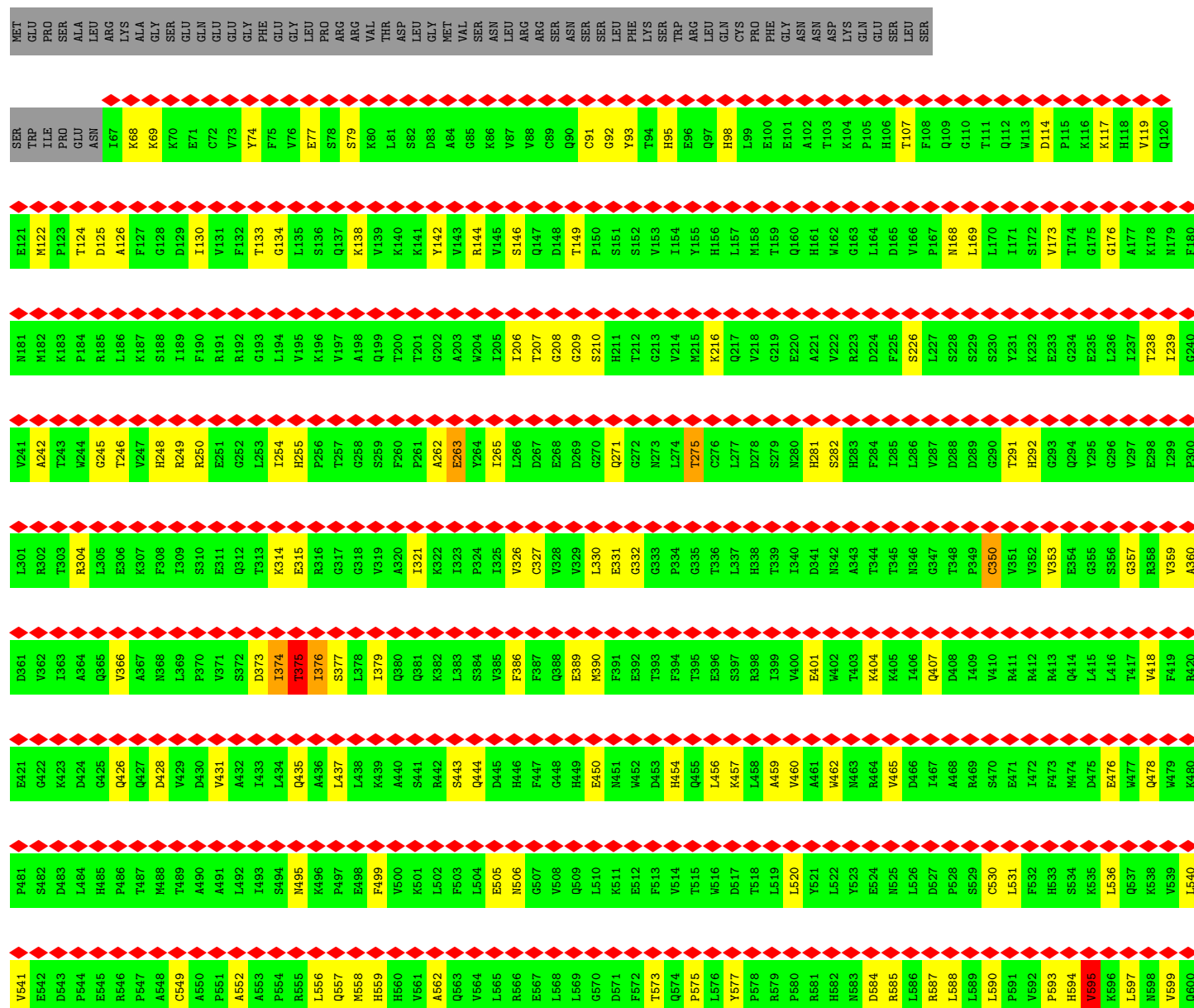
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		
1	B	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		
1	C	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		
1	D	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		



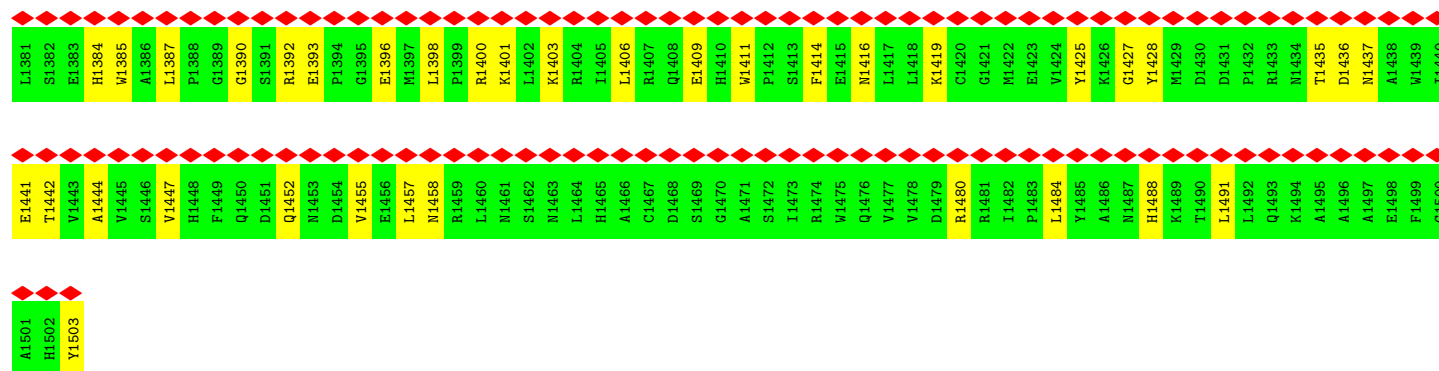


- Molecule 1: Transient receptor potential cation channel subfamily M member 2

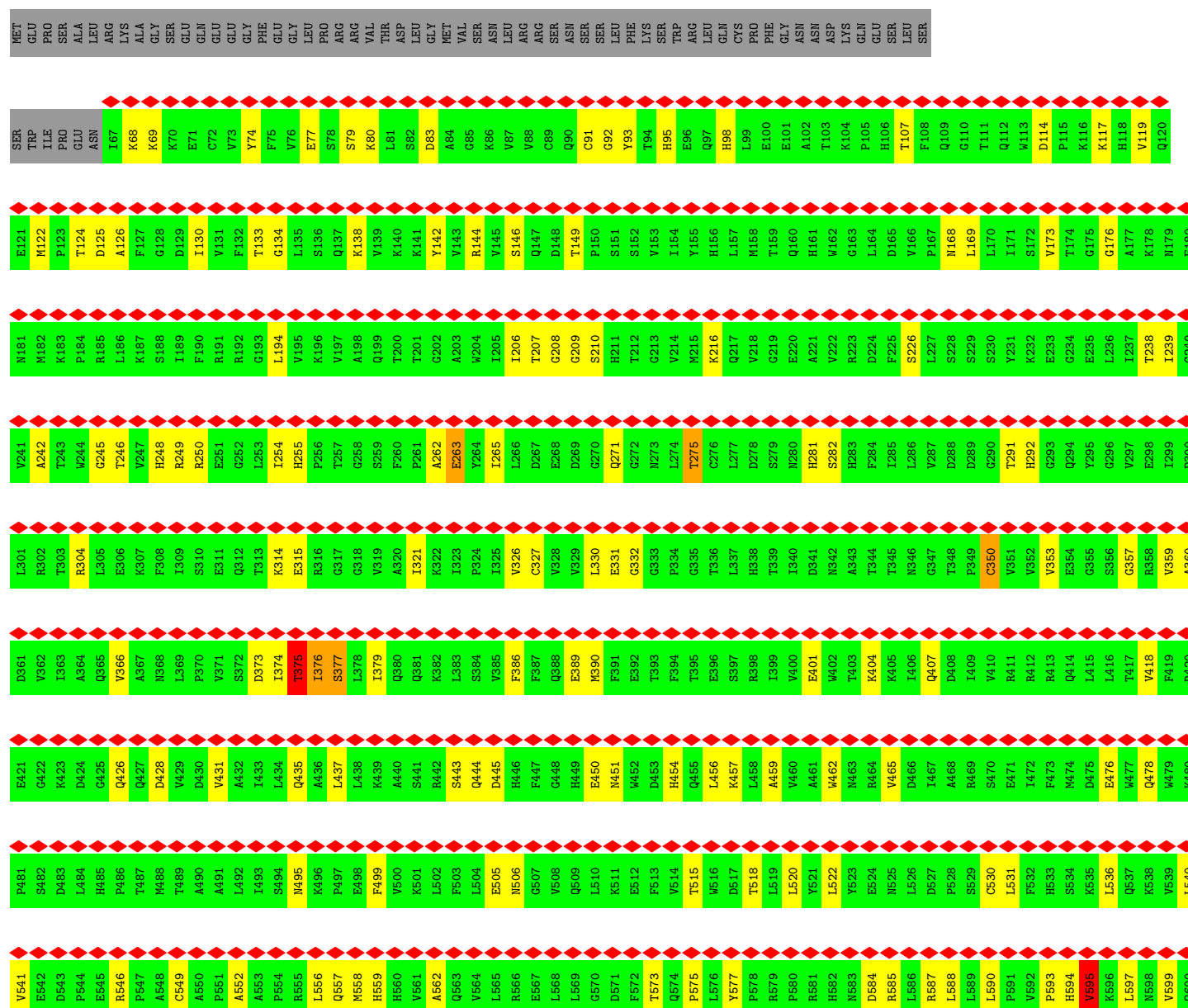
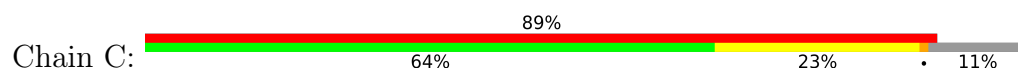
Chain B: 65% 89% 23% 11%



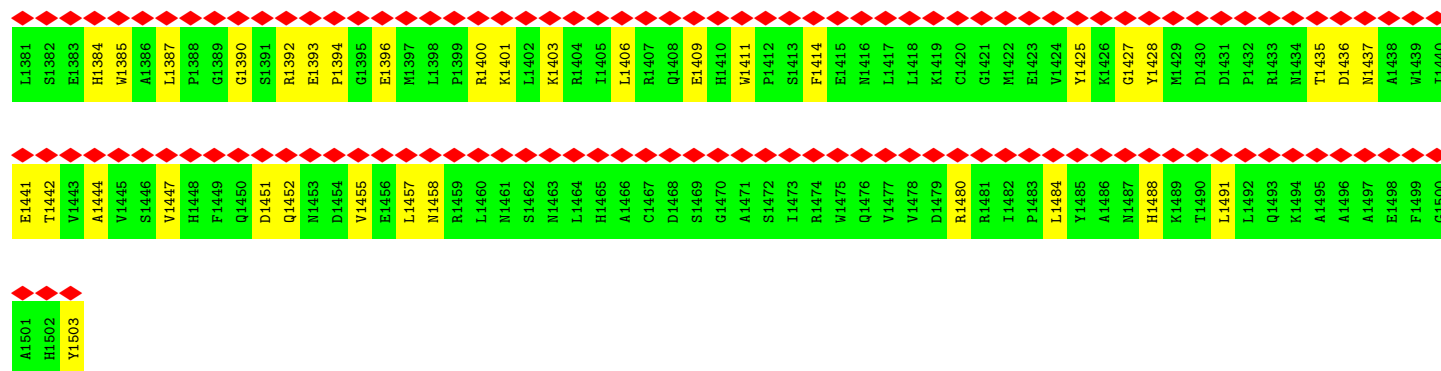
A1321	G1322	L1323	P1324	L1325	N1326	P1327	M1328	G1329	R1330	T1331	G1332	L1333	R1334	G1335	R1336	G1337	S1338	L1339	S1340	C1341	F1342	G1343	P1344	N1345	H1346	T1347	L1348	P1349	M1350	M1351	V1352	L1353	R1354	W1355	R1356	R1357	N1358	E1359	D1360	G1361	I1362	I1363	C1364	R1365	K1366	S1367	T1368	K1369	L1370	M1371	L1372	E1373	V1374	L1375	V1376	V1377	K1378	L1379	P1380																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
K1261	V1262	P1263	W1264	E1265	T1266	E1267	F1268	L1269	I1270	Y1271	D1272	P1273	L1274	F1275	Y1276	T1277	A1278	E1279	K1280	R1281	G1282	A1283	A1284	D1285	M1286	D1287	P1288	M1289	G1290	D1291	T1292	L1293	E1294	P1295	L1296	S1297	L1298	I1299	Q1300	Y1301	M1302	V1303	V1304	D1305	G1306	L1307	R1308	D1309	R1310	R1311	S1312	F1313	H1314	G1315	P1316	Y1317	T1318	V1319	Q1320																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
SER	GLY	PHE	SER	GLU	ALA	ASP	PRO	THR	LEU	ALA	SER	GLN	LYS	ALA	GLU	PRO	ASP	ALA	GLU	PRO	GLY	GLY	ARG	LYS	LYS	GLN	VAL	ALA	GLU	GLU	GLN	VAL	ALA	LEU	SER	LEU	GLU	GLU	GLN	VAL	ALA	GLN	THR	ALA	LEU	HIS	TRP	ILE	VAL	ARG	THR	LEU	ARG	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G1235	D1236	S1237	H1238	H1239	V1240	N1241	A1242	R1243	H1244	L1245	L1246	Y1247	P1248	N1249	C1250	P1251	V1252	T1253	F1254	R1255	P1256	V1257	N1258	M1259	E1260																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</



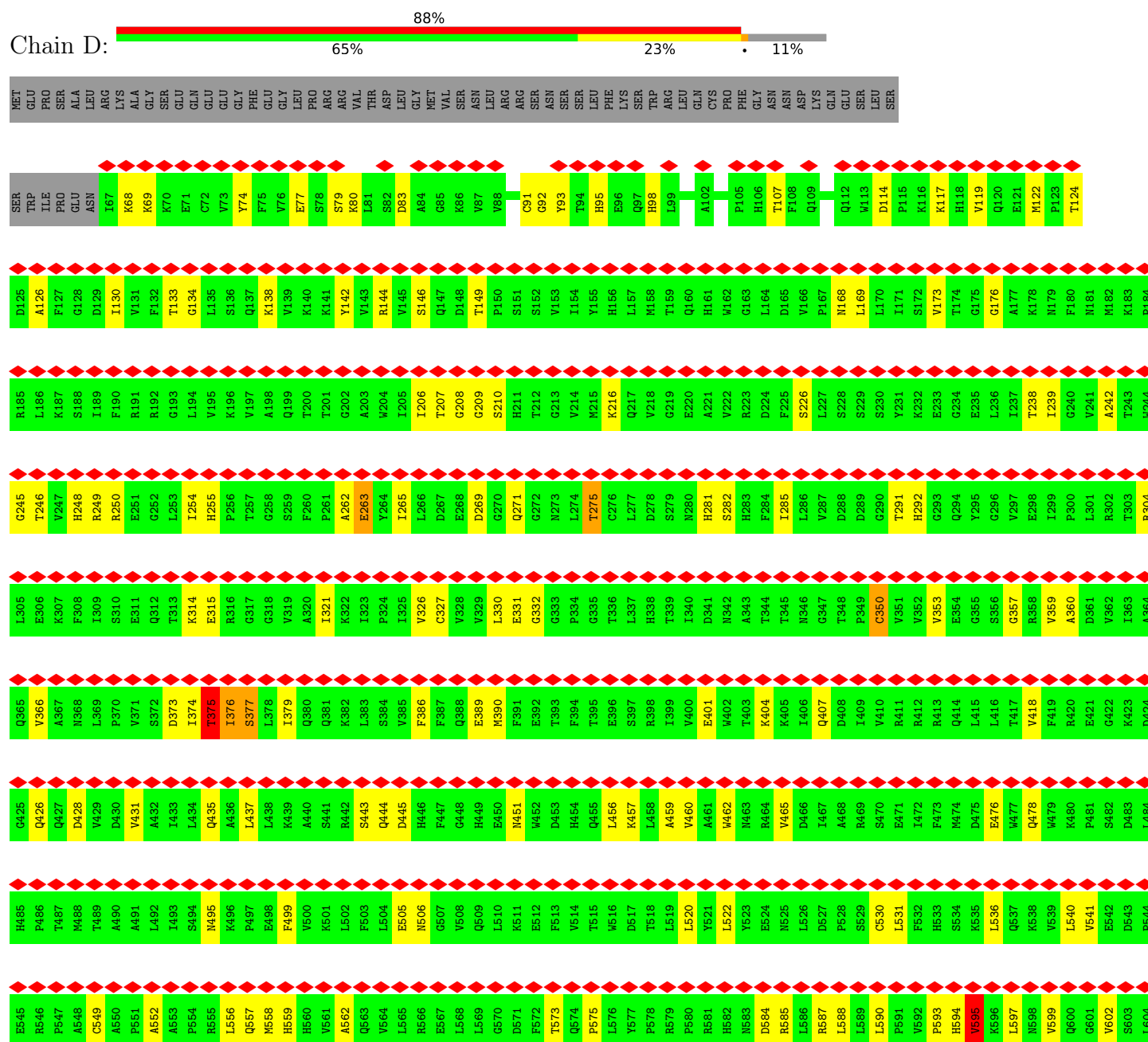
- Molecule 1: Transient receptor potential cation channel subfamily M member 2







- Molecule 1: Transient receptor potential cation channel subfamily M member 2



L1325	E1265	SER	E1145	I1085	T1025	W965	L905	R945	A785	K725	E665	R605
N1326	T1266	GLU	Q1146	L1086	V1026	L966	F906	Q946	A786	D726	E666	S606
P1327	E1267	ALA	K1147	L1087	L1027	F967	C907	L947	R787	M727	E667	L607
M1328	F1268	VAL	I1148	S1088	L1028	R968	L908	F948	A788	K728	D668	Y608
G1329	L1269	PRO	E1149	H1089	C1030	G969	R909	Y949	R789	F729	T669	K609
R1330	I1270	THR	D1150	L1090	L1030	A970	L910	D950	A790	V730	D670	R610
T1331	I1271	LEU	I1151	Q1091	L1031	V971	M911	P951	F791	S731	S611	S612
G1332	D1272	ALA	S1152	L1092	Y1032	Y972	H912	D952	F792	H732	S672	S613
L1333	P1273	SER	M1153	F1093	L1033	H973	I913	E953	T793	G733	E673	G614
R1334	P1274	LVS	K1154	I1094	L1034	S974	F914	C954	A794	G734	E674	H615
G1335	F1275	ALA	V1155	K1095	F1035	Y975	T915	G955	P795	I735	M675	V615
R1336	Y1276	GLU	D1156	R1096	T1036	L976	I916	L956	V796	Q736	L676	T616
G1337	T1277	GLU	A1157	V1097	N1037	T977	S917	M957	A797	A737	A677	F617
S1338	ASP	PRO	M1158	V1098	I1038	I978	K918	K958	F798	F738	L678	T618
L1339	E1279	ALA	V1159	L1099	L1039	F979	T919	K959	F799	L739	A679	M619
S1340	R1280	GLU	D1160	K1100	L1040	G980	L920	A960	H800	T740	E680	D620
C1341	K1281	PRO	L1161	P1101	L1041	Q981	G921	A961	L901	K741	E681	P621
F1342	D1282	GLY	L1162	T1102	N1042	I982	P922	L962	N902	V742	E682	I622
A1283	A1283	ARG	D1163	A1103	L1043	P983	K923	Y963	I903	W743	E683	R623
A1284	A1284	LVS	L1164	K1104	L1044	G984	I924	F964	L904	W744	H684	D624
A1285	A1285	LVS	D1165	R1105	I1045	Y985	I925	S965	S905	G745	R685	L625
H1346	M1286	THR	PRO	H1106	A1046	I986	I926	D966	Y906	Q746	A686	L626
T1347	D1287	GLU	LEU	K1107	M1047	D987	V927	F967	F907	L747	I627	I627
L1348	P1288	LYS	ARG	Q1108	F1048	W988	K928	W968	A908	S748	W628	W628
Y1349	M1289	SER	GLY	L1109	N1049	N989	R929	N969	F909	V749	A629	A629
P1350	G1290	SER	K1110	K1110	Y1050	PHE	M930	K970	L910	D750	F690	I630
M1351	D1291	MET	M1111	M1111	T1051	ASN	M931	L871	C911	N751	T691	V631
V1352	T1292	GLU	GLN	K1112	F1052	PRO	K932	D972	L912	G752	E692	Q632
L1353	L1293	ARG	L1113	L1113	Q1053	GLU	D933	W973	F913	L753	C693	M633
R1354	E1294	ARG	E1114	E1114	Q1054	HIS	V934	G974	A814	W754	Y694	R634
W1355	P1295	LEU	K1115	K1115	V1055	CYS	F935	A975	Y915	R755	R695	R635
R1356	L1296	ALA	SER	M1116	Q1056	PRO	F936	I976	V916	V756	E636	E636
R1357	S1297	LEU	LEU	E1117	E1057	ASN	F937	L977	L917	T757	K637	L637
N1358	H1244	GLU	GLU	E1118	H1058	THR	L938	L978	M918	L758	D697	A638
E1359	L1245	GLN	GLN	A1119	T1059	ASP	F939	F979	V919	C759	E699	G639
D1360	L1246	VAL	VAL	A1120	D1060	PRO	L940	W980	R700	M760	R700	I640
G1361	Y1247	ALA	L1121	L1121	Q1061	TYR	L941	A981	F921	L761	A701	I641
I1363	P1248	GLN	L1122	L1122	I1062	LYS	G942	G982	Q922	A762	Q702	W642
V1303	N1249	ALA	S1123	S1123	W1063	LYS	V943	L983	P923	F763	K703	A643
V1304	P1251	GLN	W1124	W1124	K1064	CYS	N944	T984	V924	P764	L704	Q644
D1305	V1252	LEU	E1125	E1125	F1065	GLU	V945	C985	P925	L765	L705	S645
G1306	T1253	LEU	I1126	I1126	Q1066	SER	V946	S926	S926	L766	T706	S646
L1307	R1254	TRP	Y1127	Y1127	R1067	ASP	S947	L987	W927	L767	R707	D647
R1308	F1255	ILE	L1128	L1128	H1068	ALA	F948	I988	C928	T768	R707	D647
D1309	P1256	VAL	VAL	K1129	D1069	THR	G949	P989	E929	T769	W708	C648
R1310	V1257	ARG	THR	E1130	L1070	GLN	V950	A990	C930	G769	S709	I649
R1311	T1258	LEU	LEU	M1131	I1071	ARG	A951	T991	A831	I771	A711	A651
S1312	N1259	ALA	Y1132	Y1132	E1072	PRO	K952	L992	I932	S772	W712	A652
H1313	F1313	SER	L1133	L1133	Y1073	ALA	Q953	Y993	I933	F773	G713	L653
G1315	G1315	GLY	Q1134	Q1134	Y1074	P1021	A954	P994	L934	W774	K714	A654
P1316	V1262	PHE	N1135	N1135	H1075	E1022	I955	G995	W935	E775	T715	C655
Y1317	P1263	SER	R1136	R1136	G1076	W1023	L956	R996	L936	K776	T716	S656
T1318	Y1317		Q1137	Q1137	R1077	W1024	I957	V997	F937	R777	C717	K657
V1319	T1318		F1138	F1138	P1078	H958	H958	I998	S938	L778	L718	I658
P1320	V1319		Q1139	Q1139	A1079	N959	N959	L999	L939	Q779	Q719	L659
L1381	Q1320		Q1140	Q1140	A1080	E960	E960	S900	V940	D780	L720	K660
A1321	A1321		K1141	K1141	P1081	R961	R961	L901	C941	V781	A721	E661
S1382	L1322		Q1142	Q1142	P1082	R962	R962	S902	E942	L782	L722	L662
E1383	L1323		R1143	R1143	P1083	V963	V963	F903	E943	T783	E723	S663
H1384	P1324		P1144	P1144	F1084	D964	D964	I904	M944	P784	A724	K664

W1385	A1386	L1387	P1388	G1389	G1390	S1391	R1392	E1393	P1394	G1395	E1396	M1397	L1398	P1399	R1400	K1401	L1402	K1403	R1404	I1405	L1406	R1407	Q1408	E1409	H1410	W1411	P1412	S1413	F1414	E1415	N1416	L1417	L1418	K1419	C1420	G1421	M1422	E1423	V1424	Y1425	K1426	G1427	Y1428	M1429	D1430	D1431	P1432	R1433	N1434	T1435	D1436	N1437	A1438	W1439	I1440	E1441	T1442	V1443	A1444
V1445	S1446	V1447	H1448	F1449	Q1450	D1451	Q1452	N1453	D1454	V1455	E1456	L1457	N1458	R1459	L1460	N1461	S1462	N1463	L1464	H1465	A1466	C1467	D1468	S1469	G1470	A1471	S1472	I1473	R1474	W1475	Q1476	V1477	V1478	D1479	R1480	R1481	I1482	P1483	L1484	Y1485	A1486	N1487	H1488	K1489	T1490	L1491	L1492	Q1493	K1494	A1495	A1496	A1497	E1498	F1499	G1500	A1501	H1502	Y1503	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34477	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.12	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.431	Depositor
Minimum map value	-7.266	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	0.522	Depositor
Recommended contour level	1.7	Depositor
Map size ($\text{\AA}$)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

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	0.31	1/11050 (0.0%)	0.68	9/14990 (0.1%)
1	B	0.31	1/11050 (0.0%)	0.68	13/14990 (0.1%)
1	C	0.31	0/11050	0.68	13/14990 (0.1%)
1	D	0.31	1/11050 (0.0%)	0.68	11/14990 (0.1%)
All	All	0.31	3/44200 (0.0%)	0.68	46/59960 (0.1%)

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	12
1	B	0	12
1	C	0	12
1	D	0	12
All	All	0	48

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1398	LEU	C-N	5.80	1.38	1.33
1	D	1398	LEU	C-N	5.77	1.38	1.33
1	B	1398	LEU	C-N	5.71	1.38	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1055	VAL	N-CA-C	-6.64	104.86	111.77
1	D	495	ASN	CA-C-N	6.61	133.60	121.70
1	D	495	ASN	C-N-CA	6.61	133.60	121.70
1	A	495	ASN	CA-C-N	6.60	133.58	121.70
1	A	495	ASN	C-N-CA	6.60	133.58	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	495	ASN	CA-C-N	6.59	133.56	121.70
1	C	495	ASN	C-N-CA	6.59	133.56	121.70
1	B	495	ASN	CA-C-N	6.58	133.55	121.70
1	B	495	ASN	C-N-CA	6.58	133.55	121.70
1	C	350	CYS	CA-CB-SG	6.06	128.34	114.40
1	D	350	CYS	CA-CB-SG	6.04	128.30	114.40
1	A	350	CYS	CA-CB-SG	6.04	128.29	114.40
1	B	350	CYS	CA-CB-SG	6.03	128.26	114.40
1	C	667	GLU	CA-C-N	5.92	132.85	121.54
1	C	667	GLU	C-N-CA	5.92	132.85	121.54
1	A	315	GLU	CA-CB-CG	5.35	124.79	114.10
1	C	375	THR	CA-C-N	5.34	131.59	121.97
1	C	375	THR	C-N-CA	5.34	131.59	121.97
1	C	315	GLU	CA-CB-CG	5.34	124.78	114.10
1	A	375	THR	CA-C-N	5.33	131.56	121.97
1	A	375	THR	C-N-CA	5.33	131.56	121.97
1	B	315	GLU	CA-CB-CG	5.33	124.75	114.10
1	D	375	THR	CA-C-N	5.33	131.56	121.97
1	D	375	THR	C-N-CA	5.33	131.56	121.97
1	C	925	ILE	CG1-CB-CG2	-5.33	94.72	110.70
1	A	925	ILE	CG1-CB-CG2	-5.32	94.74	110.70
1	D	315	GLU	CA-CB-CG	5.32	124.73	114.10
1	D	925	ILE	CG1-CB-CG2	-5.32	94.75	110.70
1	B	925	ILE	CG1-CB-CG2	-5.31	94.76	110.70
1	B	375	THR	CA-C-N	5.31	131.53	121.97
1	B	375	THR	C-N-CA	5.31	131.53	121.97
1	A	1277	THR	CA-C-N	5.27	131.60	121.54
1	A	1277	THR	C-N-CA	5.27	131.60	121.54
1	D	1277	THR	CA-C-N	5.26	131.59	121.54
1	D	1277	THR	C-N-CA	5.26	131.59	121.54
1	C	1277	THR	CA-C-N	5.25	131.56	121.54
1	C	1277	THR	C-N-CA	5.25	131.56	121.54
1	B	1277	THR	CA-C-N	5.25	131.56	121.54
1	B	1277	THR	C-N-CA	5.25	131.56	121.54
1	D	669	THR	CA-C-N	5.04	131.17	121.54
1	D	669	THR	C-N-CA	5.04	131.17	121.54
1	B	669	THR	CA-C-N	5.03	131.15	121.54
1	B	669	THR	C-N-CA	5.03	131.15	121.54
1	C	669	THR	CA-C-N	5.02	131.13	121.54
1	C	669	THR	C-N-CA	5.02	131.13	121.54
1	B	315	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1109	LEU	Peptide
1	A	1247	TYR	Peptide
1	A	1333	LEU	Peptide
1	A	1355	TRP	Peptide
1	A	374	ILE	Peptide
1	A	375	THR	Peptide
1	A	549	CYS	Peptide
1	A	615	VAL	Peptide
1	A	666	GLU	Peptide
1	A	669	THR	Peptide
1	A	713	GLY	Peptide
1	A	725	LYS	Peptide
1	B	1109	LEU	Peptide
1	B	1247	TYR	Peptide
1	B	1333	LEU	Peptide
1	B	1355	TRP	Peptide
1	B	374	ILE	Peptide
1	B	375	THR	Peptide
1	B	549	CYS	Peptide
1	B	615	VAL	Peptide
1	B	666	GLU	Peptide
1	B	669	THR	Peptide
1	B	713	GLY	Peptide
1	B	725	LYS	Peptide
1	C	1109	LEU	Peptide
1	C	1247	TYR	Peptide
1	C	1333	LEU	Peptide
1	C	1355	TRP	Peptide
1	C	374	ILE	Peptide
1	C	375	THR	Peptide
1	C	549	CYS	Peptide
1	C	615	VAL	Peptide
1	C	666	GLU	Peptide
1	C	669	THR	Peptide
1	C	713	GLY	Peptide
1	C	725	LYS	Peptide
1	D	1109	LEU	Peptide
1	D	1247	TYR	Peptide
1	D	1333	LEU	Peptide
1	D	1355	TRP	Peptide
1	D	374	ILE	Peptide
1	D	375	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	549	CYS	Peptide
1	D	615	VAL	Peptide
1	D	666	GLU	Peptide
1	D	669	THR	Peptide
1	D	713	GLY	Peptide
1	D	725	LYS	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	10780	0	10822	234	0
1	B	10780	0	10822	233	0
1	C	10780	0	10822	234	0
1	D	10780	0	10822	222	0
All	All	43120	0	43288	873	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 10.

All (873) 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:923:LYS:HD2	1:D:1047:MET:HG2	1.67	0.77
1:A:984:GLY:O	1:B:968:ARG:NH2	2.21	0.72
1:D:968:ARG:HA	1:D:972:TYR:HB3	1.72	0.72
1:B:968:ARG:HA	1:B:972:TYR:HB3	1.72	0.71
1:C:968:ARG:HA	1:C:972:TYR:HB3	1.72	0.71
1:A:968:ARG:HA	1:A:972:TYR:HB3	1.72	0.71
1:B:74:TYR:HB2	1:B:122:MET:H	1.56	0.70
1:B:1029:LEU:HG	1:C:975:TYR:CE2	2.27	0.70
1:C:74:TYR:HB2	1:C:122:MET:H	1.56	0.70
1:D:74:TYR:HB2	1:D:122:MET:H	1.56	0.69
1:B:988:GLY:O	1:C:968:ARG:NH2	2.25	0.69
1:A:1254:ARG:HH21	1:A:1334:ARG:HD2	1.58	0.69
1:D:1254:ARG:HH21	1:D:1334:ARG:HD2	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TYR:HB2	1:A:122:MET:H	1.56	0.68
1:B:176:GLY:H	1:B:331:GLU:HB2	1.58	0.68
1:D:176:GLY:H	1:D:331:GLU:HB2	1.58	0.68
1:B:1254:ARG:HH21	1:B:1334:ARG:HD2	1.58	0.68
1:C:1276:TYR:H	1:C:1334:ARG:HB3	1.58	0.68
1:B:1042:ASN:HB3	1:C:1045:ILE:HG12	1.75	0.68
1:A:976:LEU:HB3	1:A:981:GLN:HB3	1.75	0.68
1:A:176:GLY:H	1:A:331:GLU:HB2	1.58	0.68
1:D:1276:TYR:H	1:D:1334:ARG:HB3	1.58	0.68
1:C:176:GLY:H	1:C:331:GLU:HB2	1.58	0.68
1:A:1276:TYR:H	1:A:1334:ARG:HB3	1.58	0.67
1:B:976:LEU:HB3	1:B:981:GLN:HB3	1.75	0.67
1:B:982:ILE:O	1:C:981:GLN:NE2	2.27	0.67
1:C:1254:ARG:HH21	1:C:1334:ARG:HD2	1.58	0.67
1:A:1039:LEU:HA	1:A:1043:LEU:HD13	1.77	0.67
1:C:976:LEU:HB3	1:C:981:GLN:HB3	1.75	0.67
1:D:976:LEU:HB3	1:D:981:GLN:HB3	1.75	0.67
1:A:962:ARG:HB2	1:A:965:TRP:HB2	1.77	0.67
1:B:1039:LEU:HA	1:B:1043:LEU:HD13	1.77	0.67
1:B:1276:TYR:H	1:B:1334:ARG:HB3	1.58	0.67
1:C:962:ARG:HB2	1:C:965:TRP:HB2	1.77	0.66
1:D:962:ARG:HB2	1:D:965:TRP:HB2	1.77	0.66
1:A:270:GLY:O	1:B:1365:ARG:NH1	2.28	0.66
1:D:1039:LEU:HA	1:D:1043:LEU:HD13	1.77	0.65
1:B:962:ARG:HB2	1:B:965:TRP:HB2	1.77	0.65
1:C:1039:LEU:HA	1:C:1043:LEU:HD13	1.77	0.65
1:B:1286:MET:HB3	1:B:1289:MET:HB2	1.79	0.64
1:C:1286:MET:HB3	1:C:1289:MET:HB2	1.79	0.64
1:A:95:HIS:O	1:A:98:HIS:ND1	2.31	0.64
1:A:1286:MET:HB3	1:A:1289:MET:HB2	1.79	0.63
1:C:95:HIS:O	1:C:98:HIS:ND1	2.31	0.63
1:B:95:HIS:O	1:B:98:HIS:ND1	2.31	0.62
1:C:1047:MET:HG2	1:D:923:LYS:HD2	1.81	0.62
1:D:95:HIS:O	1:D:98:HIS:ND1	2.31	0.62
1:A:327:CYS:H	1:A:350:CYS:HB3	1.65	0.62
1:A:786:ALA:HA	1:A:789:ARG:HB2	1.82	0.62
1:C:327:CYS:H	1:C:350:CYS:HB3	1.65	0.62
1:D:386:PHE:HB3	1:D:389:GLU:HA	1.81	0.62
1:D:327:CYS:H	1:D:350:CYS:HB3	1.65	0.62
1:D:786:ALA:HA	1:D:789:ARG:HB2	1.82	0.62
1:D:1286:MET:HB3	1:D:1289:MET:HB2	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ALA:HA	1:B:789:ARG:HB2	1.82	0.62
1:B:327:CYS:H	1:B:350:CYS:HB3	1.65	0.62
1:B:1029:LEU:HG	1:C:975:TYR:HE2	1.64	0.61
1:C:1028:LEU:HA	1:C:1031:LEU:HB2	1.82	0.61
1:A:386:PHE:HB3	1:A:389:GLU:HA	1.81	0.61
1:C:786:ALA:HA	1:C:789:ARG:HB2	1.82	0.61
1:B:386:PHE:HB3	1:B:389:GLU:HA	1.82	0.61
1:B:536:LEU:HD13	1:B:556:LEU:HD11	1.83	0.61
1:A:1028:LEU:HA	1:A:1031:LEU:HB2	1.82	0.61
1:D:1028:LEU:HA	1:D:1031:LEU:HB2	1.82	0.61
1:B:357:GLY:HA3	1:B:360:ALA:HB3	1.83	0.61
1:A:536:LEU:HD13	1:A:556:LEU:HD11	1.83	0.61
1:A:1277:THR:HA	1:A:1336:ARG:HA	1.83	0.61
1:B:1028:LEU:HA	1:B:1031:LEU:HB2	1.82	0.61
1:D:536:LEU:HD13	1:D:556:LEU:HD11	1.83	0.60
1:B:984:GLY:O	1:C:968:ARG:NH2	2.34	0.60
1:A:904:ILE:HD11	1:D:951:ALA:HB2	1.83	0.60
1:C:386:PHE:HB3	1:C:389:GLU:HA	1.81	0.60
1:A:357:GLY:HA3	1:A:360:ALA:HB3	1.83	0.60
1:C:357:GLY:HA3	1:C:360:ALA:HB3	1.83	0.60
1:C:593:PRO:HB2	1:C:597:LEU:HB2	1.84	0.60
1:D:1277:THR:HA	1:D:1336:ARG:HA	1.83	0.60
1:C:536:LEU:HD13	1:C:556:LEU:HD11	1.83	0.60
1:B:126:ALA:HB3	1:B:144:ARG:HG2	1.84	0.60
1:A:1047:MET:HG2	1:B:923:LYS:HD2	1.84	0.59
1:B:593:PRO:HB2	1:B:597:LEU:HB2	1.84	0.59
1:B:1043:LEU:HD12	1:C:1048:PHE:CD2	2.37	0.59
1:D:593:PRO:HB2	1:D:597:LEU:HB2	1.84	0.59
1:B:952:LYS:NZ	1:B:973:HIS:O	2.36	0.59
1:C:1277:THR:HA	1:C:1336:ARG:HA	1.83	0.59
1:B:1277:THR:HA	1:B:1336:ARG:HA	1.83	0.59
1:D:357:GLY:HA3	1:D:360:ALA:HB3	1.83	0.59
1:C:952:LYS:NZ	1:C:973:HIS:O	2.36	0.59
1:A:245:GLY:HA2	1:A:250:ARG:HH21	1.68	0.59
1:A:593:PRO:HB2	1:A:597:LEU:HB2	1.84	0.59
1:A:952:LYS:NZ	1:A:973:HIS:O	2.36	0.59
1:A:126:ALA:HB3	1:A:144:ARG:HG2	1.84	0.58
1:A:530:CYS:SG	1:A:531:LEU:N	2.76	0.58
1:C:245:GLY:HA2	1:C:250:ARG:HH21	1.68	0.58
1:C:149:THR:O	1:C:304:ARG:NH2	2.37	0.58
1:B:245:GLY:HA2	1:B:250:ARG:HH21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:CYS:SG	1:D:531:LEU:N	2.76	0.58
1:B:74:TYR:HA	1:B:144:ARG:HH12	1.68	0.58
1:C:74:TYR:HA	1:C:144:ARG:HH12	1.68	0.58
1:C:126:ALA:HB3	1:C:144:ARG:HG2	1.84	0.58
1:D:245:GLY:HA2	1:D:250:ARG:HH21	1.68	0.58
1:B:1038:ILE:HG23	1:C:1044:LEU:HD21	1.85	0.58
1:D:74:TYR:HA	1:D:144:ARG:HH12	1.68	0.58
1:B:530:CYS:SG	1:B:531:LEU:N	2.76	0.58
1:C:428:ASP:HB3	1:C:431:VAL:H	1.69	0.58
1:A:459:ALA:HA	1:A:462:TRP:HD1	1.69	0.58
1:D:149:THR:O	1:D:304:ARG:NH2	2.37	0.58
1:B:149:THR:O	1:B:304:ARG:NH2	2.37	0.58
1:A:74:TYR:HA	1:A:144:ARG:HH12	1.68	0.57
1:A:149:THR:O	1:A:304:ARG:NH2	2.36	0.57
1:B:459:ALA:HA	1:B:462:TRP:HD1	1.69	0.57
1:D:431:VAL:O	1:D:435:GLN:N	2.37	0.57
1:D:952:LYS:NZ	1:D:973:HIS:O	2.36	0.57
1:B:428:ASP:HB3	1:B:431:VAL:H	1.69	0.57
1:C:530:CYS:SG	1:C:531:LEU:N	2.76	0.57
1:D:459:ALA:HA	1:D:462:TRP:HD1	1.69	0.57
1:C:777:ARG:NH2	1:C:777:ARG:O	2.37	0.57
1:D:126:ALA:HB3	1:D:144:ARG:HG2	1.84	0.57
1:D:1406:LEU:HA	1:D:1409:GLU:HG2	1.86	0.57
1:A:1406:LEU:HA	1:A:1409:GLU:HG2	1.86	0.57
1:D:428:ASP:HB3	1:D:431:VAL:H	1.69	0.57
1:D:777:ARG:O	1:D:777:ARG:NH2	2.37	0.57
1:C:459:ALA:HA	1:C:462:TRP:HD1	1.69	0.57
1:B:1249:ASN:HB2	1:B:1336:ARG:HH12	1.70	0.57
1:A:431:VAL:O	1:A:435:GLN:N	2.37	0.57
1:A:777:ARG:O	1:A:777:ARG:NH2	2.37	0.56
1:B:271:GLN:O	1:C:1365:ARG:NH1	2.38	0.56
1:B:777:ARG:O	1:B:777:ARG:NH2	2.37	0.56
1:A:404:LYS:NZ	1:A:1243:ARG:O	2.38	0.56
1:A:428:ASP:HB3	1:A:431:VAL:H	1.69	0.56
1:A:934:VAL:HG13	1:D:1034:LEU:HD21	1.88	0.56
1:A:1278:ALA:H	1:A:1337:GLY:H	1.53	0.56
1:C:1406:LEU:HA	1:C:1409:GLU:HG2	1.86	0.56
1:A:1480:ARG:NH1	1:A:1503:TYR:O	2.39	0.56
1:D:1249:ASN:HB2	1:D:1336:ARG:HH12	1.70	0.56
1:A:977:THR:HG22	1:A:982:ILE:HA	1.88	0.56
1:B:1406:LEU:HA	1:B:1409:GLU:HG2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1480:ARG:NH1	1:B:1503:TYR:O	2.39	0.56
1:C:1048:PHE:O	1:C:1052:PHE:N	2.38	0.56
1:A:1249:ASN:HB2	1:A:1336:ARG:HH12	1.70	0.56
1:B:249:ARG:NH1	1:B:265:ILE:O	2.39	0.56
1:C:941:LEU:O	1:C:945:VAL:N	2.39	0.56
1:C:1278:ALA:H	1:C:1337:GLY:H	1.53	0.56
1:D:1278:ALA:H	1:D:1337:GLY:H	1.53	0.56
1:D:1480:ARG:NH1	1:D:1503:TYR:O	2.39	0.56
1:B:1278:ALA:H	1:B:1337:GLY:H	1.53	0.56
1:D:941:LEU:O	1:D:945:VAL:N	2.39	0.55
1:A:625:LEU:HB3	1:A:641:ILE:HD13	1.88	0.55
1:C:249:ARG:NH1	1:C:265:ILE:O	2.39	0.55
1:D:1384:HIS:HB2	1:D:1484:LEU:HA	1.89	0.55
1:A:941:LEU:O	1:A:945:VAL:N	2.39	0.55
1:B:404:LYS:NZ	1:B:1243:ARG:O	2.38	0.55
1:B:431:VAL:O	1:B:435:GLN:N	2.38	0.55
1:B:476:GLU:O	1:B:478:GLN:NE2	2.39	0.55
1:C:977:THR:HG22	1:C:982:ILE:HA	1.88	0.55
1:C:1480:ARG:NH1	1:C:1503:TYR:O	2.39	0.55
1:C:404:LYS:NZ	1:C:1243:ARG:O	2.38	0.55
1:D:249:ARG:NH1	1:D:265:ILE:O	2.39	0.55
1:A:1384:HIS:HB2	1:A:1484:LEU:HA	1.89	0.55
1:B:1384:HIS:HB2	1:B:1484:LEU:HA	1.89	0.55
1:D:625:LEU:HB3	1:D:641:ILE:HD13	1.88	0.55
1:A:1158:MET:HB2	1:B:1158:MET:HE1	1.89	0.55
1:B:977:THR:HG22	1:B:982:ILE:HA	1.87	0.55
1:C:625:LEU:HB3	1:C:641:ILE:HD13	1.88	0.55
1:D:168:ASN:OD1	1:D:314:LYS:NZ	2.36	0.55
1:D:476:GLU:O	1:D:478:GLN:NE2	2.39	0.55
1:A:249:ARG:NH1	1:A:265:ILE:O	2.39	0.55
1:B:1048:PHE:O	1:B:1052:PHE:N	2.38	0.55
1:C:1249:ASN:HB2	1:C:1336:ARG:HH12	1.70	0.55
1:C:1384:HIS:HB2	1:C:1484:LEU:HA	1.89	0.55
1:D:977:THR:HG22	1:D:982:ILE:HA	1.87	0.54
1:B:625:LEU:HB3	1:B:641:ILE:HD13	1.88	0.54
1:C:1311:ARG:NH1	1:C:1312:SER:O	2.41	0.54
1:C:431:VAL:O	1:C:435:GLN:N	2.37	0.54
1:A:1312:SER:OG	1:A:1313:PHE:N	2.41	0.54
1:B:1311:ARG:NH1	1:B:1312:SER:O	2.41	0.54
1:D:531:LEU:HD21	1:D:665:GLU:HB3	1.90	0.54
1:D:404:LYS:NZ	1:D:1243:ARG:O	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1311:ARG:NH1	1:D:1312:SER:O	2.41	0.54
1:C:531:LEU:HD21	1:C:665:GLU:HB3	1.90	0.54
1:C:1312:SER:OG	1:C:1313:PHE:N	2.41	0.54
1:C:930:MET:O	1:C:934:VAL:N	2.41	0.54
1:D:1312:SER:OG	1:D:1313:PHE:N	2.41	0.54
1:A:1311:ARG:NH1	1:A:1312:SER:O	2.40	0.54
1:B:941:LEU:O	1:B:945:VAL:N	2.39	0.54
1:B:1428:TYR:HA	1:B:1441:GLU:HA	1.91	0.53
1:D:930:MET:O	1:D:934:VAL:N	2.41	0.53
1:D:1048:PHE:O	1:D:1052:PHE:N	2.38	0.53
1:A:955:ILE:HG23	1:B:897:VAL:HG12	1.90	0.53
1:C:69:LYS:NZ	1:C:124:THR:O	2.41	0.53
1:A:930:MET:O	1:A:934:VAL:N	2.41	0.53
1:A:1058:HIS:O	1:A:1062:ILE:N	2.34	0.53
1:B:520:LEU:HD11	1:B:557:GLN:HA	1.90	0.53
1:A:1299:ILE:O	1:A:1310:ARG:NH1	2.42	0.53
1:D:971:VAL:O	1:D:974:SER:OG	2.24	0.53
1:D:1428:TYR:HA	1:D:1441:GLU:HA	1.91	0.53
1:A:476:GLU:O	1:A:478:GLN:NE2	2.39	0.53
1:A:1428:TYR:HA	1:A:1441:GLU:HA	1.91	0.53
1:C:330:LEU:HD13	1:C:353:VAL:HG21	1.91	0.53
1:A:401:GLU:HG2	1:A:1256:PRO:HG3	1.91	0.53
1:A:929:ARG:HE	1:A:1055:VAL:HG21	1.73	0.53
1:B:597:LEU:HG	1:B:599:VAL:H	1.74	0.53
1:B:1312:SER:OG	1:B:1313:PHE:N	2.41	0.53
1:A:520:LEU:HD11	1:A:557:GLN:HA	1.90	0.53
1:A:531:LEU:HD21	1:A:665:GLU:HB3	1.90	0.53
1:C:1428:TYR:HA	1:C:1441:GLU:HA	1.91	0.53
1:A:138:LYS:NZ	1:A:226:SER:OG	2.42	0.53
1:B:330:LEU:HD13	1:B:353:VAL:HG21	1.91	0.53
1:D:520:LEU:HD11	1:D:557:GLN:HA	1.90	0.53
1:A:1042:ASN:HA	1:A:1045:ILE:HD12	1.91	0.52
1:B:401:GLU:HG2	1:B:1256:PRO:HG3	1.91	0.52
1:C:401:GLU:HG2	1:C:1256:PRO:HG3	1.91	0.52
1:C:597:LEU:HG	1:C:599:VAL:H	1.74	0.52
1:C:929:ARG:HE	1:C:1055:VAL:HG21	1.73	0.52
1:D:597:LEU:HG	1:D:599:VAL:H	1.74	0.52
1:B:531:LEU:HD21	1:B:665:GLU:HB3	1.90	0.52
1:D:401:GLU:HG2	1:D:1256:PRO:HG3	1.91	0.52
1:D:1042:ASN:HA	1:D:1045:ILE:HD12	1.91	0.52
1:D:1299:ILE:O	1:D:1310:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:THR:OG1	1:A:292:HIS:N	2.42	0.52
1:B:1042:ASN:HA	1:B:1045:ILE:HD12	1.91	0.52
1:C:476:GLU:O	1:C:478:GLN:NE2	2.39	0.52
1:C:1299:ILE:O	1:C:1310:ARG:NH1	2.42	0.52
1:C:1042:ASN:HA	1:C:1045:ILE:HD12	1.91	0.52
1:A:951:ALA:HB2	1:B:904:ILE:HD11	1.91	0.52
1:A:207:THR:OG1	1:A:208:GLY:N	2.43	0.52
1:C:209:GLY:HA3	1:C:242:ALA:HB2	1.92	0.52
1:D:573:THR:HG21	1:D:714:LYS:HG2	1.91	0.52
1:A:426:GLN:HE22	1:A:1164:LEU:HB3	1.75	0.52
1:A:573:THR:HG21	1:A:714:LYS:HG2	1.92	0.52
1:B:332:GLY:HA3	1:B:359:VAL:HG12	1.92	0.52
1:B:929:ARG:HE	1:B:1055:VAL:HG21	1.73	0.52
1:C:138:LYS:NZ	1:C:226:SER:OG	2.42	0.52
1:D:138:LYS:NZ	1:D:226:SER:OG	2.42	0.52
1:D:209:GLY:HA3	1:D:242:ALA:HB2	1.92	0.52
1:D:291:THR:OG1	1:D:292:HIS:N	2.42	0.52
1:A:584:ASP:OD2	1:A:587:ARG:NH1	2.43	0.52
1:C:291:THR:OG1	1:C:292:HIS:N	2.42	0.52
1:D:584:ASP:OD2	1:D:587:ARG:NH1	2.43	0.52
1:A:866:ASP:HB2	1:A:869:ASN:HB2	1.92	0.52
1:A:1048:PHE:O	1:A:1052:PHE:N	2.38	0.52
1:B:138:LYS:NZ	1:B:226:SER:OG	2.42	0.52
1:B:930:MET:O	1:B:934:VAL:N	2.41	0.52
1:B:1299:ILE:O	1:B:1310:ARG:NH1	2.42	0.52
1:B:209:GLY:HA3	1:B:242:ALA:HB2	1.92	0.52
1:C:520:LEU:HD11	1:C:557:GLN:HA	1.90	0.52
1:C:1140:GLN:OE1	1:C:1143:ARG:NH2	2.40	0.52
1:D:1330:ARG:HG2	1:D:1332:GLY:H	1.75	0.52
1:A:1330:ARG:HG2	1:A:1332:GLY:H	1.75	0.51
1:C:332:GLY:HA3	1:C:359:VAL:HG12	1.92	0.51
1:C:1348:LEU:HG	1:C:1390:GLY:HA3	1.92	0.51
1:D:866:ASP:HB2	1:D:869:ASN:HB2	1.92	0.51
1:A:597:LEU:HG	1:A:599:VAL:H	1.74	0.51
1:B:1330:ARG:HG2	1:B:1332:GLY:H	1.75	0.51
1:C:216:LYS:NZ	1:D:476:GLU:OE1	2.40	0.51
1:A:897:VAL:HG12	1:D:955:ILE:HG23	1.93	0.51
1:D:332:GLY:HA3	1:D:359:VAL:HG12	1.92	0.51
1:D:929:ARG:HE	1:D:1055:VAL:HG21	1.73	0.51
1:A:330:LEU:HD13	1:A:353:VAL:HG21	1.91	0.51
1:B:426:GLN:HE22	1:B:1164:LEU:HB3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1330:ARG:HG2	1:C:1332:GLY:H	1.75	0.51
1:C:271:GLN:H	1:D:1358:ASN:HD22	1.58	0.51
1:A:168:ASN:OD1	1:A:314:LYS:NZ	2.36	0.51
1:B:1262:VAL:HG23	1:B:1263:PRO:HD3	1.92	0.51
1:C:426:GLN:HE22	1:C:1164:LEU:HB3	1.75	0.51
1:A:797:VAL:HA	1:A:800:HIS:HB2	1.93	0.51
1:A:1348:LEU:HG	1:A:1390:GLY:HA3	1.92	0.51
1:B:797:VAL:HA	1:B:800:HIS:HB2	1.93	0.51
1:C:573:THR:HG21	1:C:714:LYS:HG2	1.92	0.51
1:B:573:THR:HG21	1:B:714:LYS:HG2	1.92	0.51
1:D:330:LEU:HD13	1:D:353:VAL:HG21	1.91	0.51
1:A:209:GLY:HA3	1:A:242:ALA:HB2	1.92	0.51
1:A:332:GLY:HA3	1:A:359:VAL:HG12	1.92	0.51
1:A:1262:VAL:HG23	1:A:1263:PRO:HD3	1.92	0.51
1:C:456:LEU:HD12	1:C:459:ALA:HB3	1.93	0.51
1:D:1262:VAL:HG23	1:D:1263:PRO:HD3	1.92	0.51
1:B:207:THR:OG1	1:B:208:GLY:N	2.43	0.51
1:B:584:ASP:OD2	1:B:587:ARG:NH1	2.43	0.51
1:B:1396:GLU:HB3	1:B:1400:ARG:HD2	1.93	0.51
1:D:1348:LEU:HG	1:D:1390:GLY:HA3	1.92	0.51
1:D:1396:GLU:HB3	1:D:1400:ARG:HD2	1.93	0.51
1:B:456:LEU:HD12	1:B:459:ALA:HB3	1.93	0.50
1:B:866:ASP:HB2	1:B:869:ASN:HB2	1.92	0.50
1:B:1042:ASN:HD22	1:B:1045:ILE:HD12	1.77	0.50
1:C:866:ASP:HB2	1:C:869:ASN:HB2	1.92	0.50
1:C:1058:HIS:O	1:C:1062:ILE:N	2.34	0.50
1:C:1262:VAL:HG23	1:C:1263:PRO:HD3	1.92	0.50
1:A:803:ILE:O	1:A:807:PHE:N	2.43	0.50
1:B:321:ILE:HG22	1:B:457:LYS:HB3	1.94	0.50
1:B:1348:LEU:HG	1:B:1390:GLY:HA3	1.92	0.50
1:B:1393:GLU:H	1:B:1401:LYS:HB2	1.77	0.50
1:C:797:VAL:HA	1:C:800:HIS:HB2	1.93	0.50
1:D:616:THR:OG1	1:D:617:PHE:N	2.44	0.50
1:A:456:LEU:HD12	1:A:459:ALA:HB3	1.93	0.50
1:A:1036:THR:HA	1:A:1040:LEU:HD12	1.93	0.50
1:B:616:THR:OG1	1:B:617:PHE:N	2.44	0.50
1:C:584:ASP:OD2	1:C:587:ARG:NH1	2.43	0.50
1:C:1036:THR:HA	1:C:1040:LEU:HD12	1.93	0.50
1:C:1393:GLU:H	1:C:1401:LYS:HB2	1.77	0.50
1:D:426:GLN:HE22	1:D:1164:LEU:HB3	1.75	0.50
1:D:456:LEU:HD12	1:D:459:ALA:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:803:ILE:O	1:D:807:PHE:N	2.43	0.50
1:A:1046:ALA:HB2	1:B:1049:ASN:OD1	2.11	0.50
1:A:1393:GLU:H	1:A:1401:LYS:HB2	1.77	0.50
1:B:985:TYR:HA	1:C:968:ARG:HH22	1.77	0.50
1:B:1021:PRO:O	1:B:1025:THR:OG1	2.27	0.50
1:D:321:ILE:HG22	1:D:457:LYS:HB3	1.94	0.50
1:D:734:GLY:HA2	1:D:737:ALA:HB3	1.94	0.50
1:D:1393:GLU:H	1:D:1401:LYS:HB2	1.77	0.50
1:C:207:THR:OG1	1:C:208:GLY:N	2.43	0.50
1:C:1042:ASN:HD22	1:C:1045:ILE:HD12	1.77	0.50
1:A:734:GLY:HA2	1:A:737:ALA:HB3	1.94	0.50
1:C:114:ASP:O	1:C:117:LYS:N	2.45	0.50
1:C:321:ILE:HG22	1:C:457:LYS:HB3	1.94	0.50
1:A:1396:GLU:HB3	1:A:1400:ARG:HD2	1.93	0.50
1:C:540:LEU:HD11	1:C:556:LEU:HB2	1.94	0.50
1:D:207:THR:OG1	1:D:208:GLY:N	2.43	0.50
1:A:249:ARG:HH12	1:A:265:ILE:HB	1.77	0.50
1:B:1058:HIS:O	1:B:1062:ILE:N	2.34	0.50
1:D:797:VAL:HA	1:D:800:HIS:HB2	1.93	0.50
1:A:321:ILE:HG22	1:A:457:LYS:HB3	1.94	0.50
1:A:620:ASP:HB2	1:A:623:ARG:HB2	1.94	0.50
1:B:1036:THR:HA	1:B:1040:LEU:HD12	1.93	0.50
1:D:620:ASP:HB2	1:D:623:ARG:HB2	1.94	0.50
1:A:616:THR:OG1	1:A:617:PHE:N	2.44	0.49
1:B:540:LEU:HD11	1:B:556:LEU:HB2	1.94	0.49
1:B:1282:ASP:HB3	1:B:1285:ALA:HB3	1.94	0.49
1:C:762:ALA:HB1	1:C:765:LEU:HD13	1.94	0.49
1:A:920:LEU:HB2	1:D:936:PHE:CE1	2.47	0.49
1:A:1261:LYS:HD2	1:A:1269:LEU:HG	1.94	0.49
1:C:620:ASP:HB2	1:C:623:ARG:HB2	1.94	0.49
1:D:1042:ASN:HD22	1:D:1045:ILE:HD12	1.76	0.49
1:A:1335:GLY:HA2	1:A:1437:ASN:HB2	1.95	0.49
1:C:1352:VAL:HA	1:C:1447:VAL:HG23	1.93	0.49
1:D:114:ASP:O	1:D:117:LYS:N	2.44	0.49
1:D:1140:GLN:OE1	1:D:1143:ARG:NH2	2.41	0.49
1:A:1042:ASN:HD22	1:A:1045:ILE:HD12	1.77	0.49
1:B:620:ASP:HB2	1:B:623:ARG:HB2	1.94	0.49
1:B:1261:LYS:HD2	1:B:1269:LEU:HG	1.94	0.49
1:C:616:THR:OG1	1:C:617:PHE:N	2.44	0.49
1:D:1036:THR:HA	1:D:1040:LEU:HD12	1.93	0.49
1:D:1335:GLY:HA2	1:D:1437:ASN:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:O	1:A:117:LYS:N	2.45	0.49
1:B:762:ALA:HB1	1:B:765:LEU:HD13	1.94	0.49
1:C:1261:LYS:HD2	1:C:1269:LEU:HG	1.95	0.49
1:D:1261:LYS:HD2	1:D:1269:LEU:HG	1.94	0.49
1:A:1034:LEU:HD21	1:B:934:VAL:HG13	1.95	0.49
1:A:1336:ARG:NH2	1:A:1338:SER:OG	2.44	0.49
1:B:1352:VAL:HA	1:B:1447:VAL:HG23	1.93	0.49
1:C:1396:GLU:HB3	1:C:1400:ARG:HD2	1.93	0.49
1:B:114:ASP:O	1:B:117:LYS:N	2.44	0.49
1:B:249:ARG:HH12	1:B:265:ILE:HB	1.77	0.49
1:C:1335:GLY:HA2	1:C:1437:ASN:HB2	1.95	0.49
1:C:1336:ARG:NH2	1:C:1338:SER:OG	2.44	0.49
1:A:953:GLN:HB3	1:A:958:HIS:CD2	2.48	0.49
1:A:968:ARG:HG3	1:A:972:TYR:HD2	1.78	0.49
1:D:249:ARG:HH12	1:D:265:ILE:HB	1.77	0.49
1:D:1165:ASP:OD1	1:D:1165:ASP:N	2.46	0.49
1:D:1387:LEU:HD12	1:D:1488:HIS:HD2	1.77	0.49
1:A:271:GLN:O	1:B:1365:ARG:NH1	2.46	0.49
1:A:762:ALA:HB1	1:A:765:LEU:HD13	1.94	0.49
1:A:985:TYR:HD1	1:B:968:ARG:HH22	1.60	0.49
1:C:953:GLN:HB3	1:C:958:HIS:CD2	2.48	0.49
1:C:968:ARG:HG3	1:C:972:TYR:HD2	1.78	0.49
1:D:540:LEU:HD11	1:D:556:LEU:HB2	1.94	0.49
1:D:968:ARG:HG3	1:D:972:TYR:HD2	1.78	0.49
1:B:953:GLN:HB3	1:B:958:HIS:CD2	2.48	0.49
1:B:1335:GLY:HA2	1:B:1437:ASN:HB2	1.95	0.49
1:C:249:ARG:HH12	1:C:265:ILE:HB	1.77	0.49
1:C:734:GLY:HA2	1:C:737:ALA:HB3	1.94	0.49
1:D:937:PHE:HZ	1:D:1040:LEU:HB3	1.78	0.49
1:A:1140:GLN:OE1	1:A:1143:ARG:NH2	2.40	0.48
1:D:1336:ARG:NH2	1:D:1338:SER:OG	2.44	0.48
1:D:1352:VAL:HA	1:D:1447:VAL:HG23	1.94	0.48
1:D:1356:ARG:O	1:D:1452:GLN:NE2	2.46	0.48
1:B:1046:ALA:HB2	1:C:1049:ASN:OD1	2.13	0.48
1:C:1282:ASP:HB3	1:C:1285:ALA:HB3	1.94	0.48
1:C:1436:ASP:OD1	1:C:1436:ASP:N	2.46	0.48
1:A:520:LEU:HD13	1:A:558:MET:HG2	1.95	0.48
1:A:1282:ASP:HB3	1:A:1285:ALA:HB3	1.94	0.48
1:A:1352:VAL:HA	1:A:1447:VAL:HG23	1.93	0.48
1:B:1436:ASP:N	1:B:1436:ASP:OD1	2.47	0.48
1:C:937:PHE:HZ	1:C:1040:LEU:HB3	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:762:ALA:HB1	1:D:765:LEU:HD13	1.94	0.48
1:A:552:ALA:HB2	1:A:590:LEU:HD13	1.95	0.48
1:B:168:ASN:OD1	1:B:314:LYS:NZ	2.36	0.48
1:B:734:GLY:HA2	1:B:737:ALA:HB3	1.94	0.48
1:B:1272:ASP:OD1	1:B:1272:ASP:N	2.46	0.48
1:A:1356:ARG:O	1:A:1452:GLN:NE2	2.46	0.48
1:B:520:LEU:HD13	1:B:558:MET:HG2	1.95	0.48
1:B:552:ALA:HB2	1:B:590:LEU:HD13	1.95	0.48
1:B:1392:ARG:NH1	1:B:1396:GLU:O	2.47	0.48
1:C:168:ASN:OD1	1:C:314:LYS:NZ	2.36	0.48
1:D:552:ALA:HB2	1:D:590:LEU:HD13	1.95	0.48
1:D:614:HIS:NE2	1:D:616:THR:O	2.47	0.48
1:A:540:LEU:HD11	1:A:556:LEU:HB2	1.94	0.48
1:B:130:ILE:HG23	1:B:263:GLU:HA	1.96	0.48
1:C:552:ALA:HB2	1:C:590:LEU:HD13	1.95	0.48
1:D:1455:VAL:HA	1:D:1458:ASN:HB2	1.96	0.48
1:A:605:ARG:HE	1:A:615:VAL:HG22	1.79	0.48
1:A:968:ARG:NH2	1:D:984:GLY:O	2.43	0.48
1:B:937:PHE:HZ	1:B:1040:LEU:HB3	1.78	0.48
1:B:1165:ASP:OD1	1:B:1165:ASP:N	2.46	0.48
1:C:1356:ARG:O	1:C:1452:GLN:NE2	2.46	0.48
1:D:69:LYS:NZ	1:D:124:THR:O	2.41	0.48
1:D:953:GLN:HB3	1:D:958:HIS:CD2	2.48	0.48
1:A:937:PHE:HZ	1:A:1040:LEU:HB3	1.78	0.48
1:A:1042:ASN:HB2	1:B:1048:PHE:HE2	1.79	0.48
1:A:1387:LEU:HD12	1:A:1488:HIS:HD2	1.78	0.48
1:B:746:GLN:OE1	1:B:774:ARG:NH1	2.47	0.48
1:B:968:ARG:HG3	1:B:972:TYR:HD2	1.78	0.48
1:B:1387:LEU:HD12	1:B:1488:HIS:HD2	1.77	0.48
1:C:331:GLU:HA	1:C:357:GLY:HA2	1.96	0.48
1:C:614:HIS:NE2	1:C:616:THR:O	2.47	0.48
1:D:331:GLU:HA	1:D:357:GLY:HA2	1.96	0.48
1:D:605:ARG:HE	1:D:615:VAL:HG22	1.79	0.48
1:B:653:LEU:O	1:B:656:SER:OG	2.28	0.48
1:B:1336:ARG:NH2	1:B:1338:SER:OG	2.44	0.48
1:C:133:THR:HA	1:C:134:GLY:HA2	1.61	0.48
1:C:1387:LEU:HD12	1:C:1488:HIS:HD2	1.78	0.48
1:D:520:LEU:HD13	1:D:558:MET:HG2	1.95	0.48
1:B:1356:ARG:O	1:B:1452:GLN:NE2	2.46	0.48
1:C:130:ILE:HG23	1:C:263:GLU:HA	1.96	0.48
1:C:520:LEU:HD13	1:C:558:MET:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1392:ARG:NH1	1:C:1396:GLU:O	2.47	0.48
1:D:1272:ASP:OD1	1:D:1272:ASP:N	2.46	0.48
1:A:1455:VAL:HA	1:A:1458:ASN:HB2	1.96	0.47
1:B:1455:VAL:HA	1:B:1458:ASN:HB2	1.96	0.47
1:C:605:ARG:HE	1:C:615:VAL:HG22	1.79	0.47
1:A:1165:ASP:N	1:A:1165:ASP:OD1	2.46	0.47
1:C:1264:TRP:HB3	1:C:1330:ARG:HB2	1.96	0.47
1:D:1264:TRP:HB3	1:D:1330:ARG:HB2	1.96	0.47
1:A:331:GLU:HA	1:A:357:GLY:HA2	1.96	0.47
1:A:618:THR:O	1:A:618:THR:OG1	2.28	0.47
1:A:1021:PRO:O	1:A:1025:THR:OG1	2.27	0.47
1:D:1392:ARG:NH1	1:D:1396:GLU:O	2.47	0.47
1:A:407:GLN:HE22	1:A:1259:ASN:HB2	1.80	0.47
1:A:614:HIS:NE2	1:A:616:THR:O	2.47	0.47
1:B:614:HIS:NE2	1:B:616:THR:O	2.47	0.47
1:B:1047:MET:HG2	1:C:923:LYS:HD2	1.96	0.47
1:D:1282:ASP:HB3	1:D:1285:ALA:HB3	1.94	0.47
1:D:1436:ASP:OD1	1:D:1436:ASP:N	2.46	0.47
1:B:407:GLN:HE22	1:B:1259:ASN:HB2	1.80	0.47
1:B:693:CYS:HA	1:B:1128:LEU:HD13	1.97	0.47
1:B:1105:ARG:HH21	1:B:1106:HIS:H	1.62	0.47
1:D:746:GLN:OE1	1:D:774:ARG:NH1	2.47	0.47
1:A:1264:TRP:HB3	1:A:1330:ARG:HB2	1.96	0.47
1:B:1140:GLN:OE1	1:B:1143:ARG:NH2	2.40	0.47
1:B:1264:TRP:HB3	1:B:1330:ARG:HB2	1.96	0.47
1:B:1340:SER:O	1:B:1340:SER:OG	2.28	0.47
1:B:1358:ASN:OD1	1:B:1361:GLY:N	2.48	0.47
1:C:407:GLN:HE22	1:C:1259:ASN:HB2	1.79	0.47
1:D:465:VAL:HA	1:D:499:PHE:HE1	1.80	0.47
1:A:1392:ARG:NH1	1:A:1396:GLU:O	2.47	0.47
1:B:605:ARG:HE	1:B:615:VAL:HG22	1.79	0.47
1:B:669:THR:OG1	1:B:670:ASP:N	2.47	0.47
1:D:130:ILE:HG23	1:D:263:GLU:HA	1.96	0.47
1:D:1358:ASN:OD1	1:D:1361:GLY:N	2.48	0.47
1:A:669:THR:OG1	1:A:670:ASP:N	2.47	0.47
1:A:1358:ASN:OD1	1:A:1361:GLY:N	2.48	0.47
1:C:1272:ASP:OD1	1:C:1272:ASP:N	2.46	0.47
1:C:1358:ASN:OD1	1:C:1361:GLY:N	2.48	0.47
1:D:663:SER:O	1:D:672:SER:OG	2.33	0.47
1:B:133:THR:HA	1:B:134:GLY:HA2	1.61	0.47
1:B:465:VAL:HA	1:B:499:PHE:HE1	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HG23	1:A:263:GLU:HA	1.96	0.46
1:B:331:GLU:HA	1:B:357:GLY:HA2	1.96	0.46
1:B:971:VAL:O	1:B:974:SER:OG	2.24	0.46
1:A:693:CYS:HA	1:A:1128:LEU:HD13	1.97	0.46
1:C:663:SER:O	1:C:672:SER:OG	2.33	0.46
1:C:1411:TRP:NE1	1:C:1414:PHE:O	2.43	0.46
1:D:407:GLN:HE22	1:D:1259:ASN:HB2	1.80	0.46
1:A:734:GLY:O	1:A:738:PHE:N	2.47	0.46
1:A:746:GLN:OE1	1:A:774:ARG:NH1	2.47	0.46
1:C:1105:ARG:HH21	1:C:1106:HIS:H	1.62	0.46
1:C:1455:VAL:HA	1:C:1458:ASN:HB2	1.96	0.46
1:D:635:ARG:HG3	1:D:678:LEU:HD13	1.97	0.46
1:A:1435:THR:OG1	1:A:1436:ASP:N	2.49	0.46
1:B:635:ARG:HG3	1:B:678:LEU:HD13	1.97	0.46
1:D:1435:THR:OG1	1:D:1436:ASP:N	2.49	0.46
1:D:618:THR:O	1:D:618:THR:OG1	2.29	0.46
1:A:465:VAL:HA	1:A:499:PHE:HE1	1.80	0.46
1:B:77:GLU:HB2	1:B:119:VAL:HA	1.98	0.46
1:B:1020:PHE:HA	1:C:964:ASP:HB3	1.98	0.46
1:C:1165:ASP:N	1:C:1165:ASP:OD1	2.46	0.46
1:D:1058:HIS:O	1:D:1062:ILE:N	2.34	0.46
1:A:1272:ASP:OD1	1:A:1272:ASP:N	2.46	0.46
1:B:851:PRO:HB3	1:B:859:LYS:HD2	1.98	0.46
1:B:1435:THR:OG1	1:B:1436:ASP:N	2.49	0.46
1:C:515:THR:OG1	1:C:518:THR:OG1	2.30	0.46
1:D:1393:GLU:HB3	1:D:1396:GLU:HB2	1.98	0.46
1:B:91:CYS:SG	1:B:92:GLY:N	2.89	0.46
1:B:1254:ARG:HB3	1:B:1274:PRO:HD2	1.98	0.46
1:B:1277:THR:OG1	1:B:1283:ALA:O	2.30	0.46
1:C:91:CYS:SG	1:C:92:GLY:N	2.89	0.46
1:C:669:THR:OG1	1:C:670:ASP:N	2.47	0.46
1:D:91:CYS:SG	1:D:92:GLY:N	2.89	0.46
1:D:1400:ARG:HG2	1:D:1403:LYS:HZ3	1.81	0.46
1:A:1254:ARG:HB3	1:A:1274:PRO:HD2	1.98	0.46
1:B:443:SER:O	1:B:444:GLN:NE2	2.49	0.46
1:C:505:GLU:OE2	1:C:506:ASN:ND2	2.49	0.46
1:C:693:CYS:HA	1:C:1128:LEU:HD13	1.97	0.46
1:D:376:ILE:O	1:D:379:ILE:N	2.39	0.46
1:D:1021:PRO:O	1:D:1025:THR:OG1	2.27	0.46
1:A:77:GLU:HB2	1:A:119:VAL:HA	1.98	0.46
1:A:505:GLU:OE2	1:A:506:ASN:ND2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:ARG:HH21	1:A:1106:HIS:H	1.62	0.46
1:A:1290:GLY:O	1:A:1308:ARG:NE	2.49	0.46
1:A:1411:TRP:HD1	1:A:1414:PHE:H	1.65	0.46
1:B:505:GLU:OE2	1:B:506:ASN:ND2	2.49	0.46
1:B:663:SER:O	1:B:672:SER:OG	2.33	0.46
1:C:851:PRO:HB3	1:C:859:LYS:HD2	1.98	0.46
1:C:1290:GLY:O	1:C:1308:ARG:NE	2.49	0.46
1:C:1393:GLU:HB3	1:C:1396:GLU:HB2	1.98	0.46
1:D:868:TRP:HA	1:D:871:LEU:HB2	1.98	0.46
1:A:80:LYS:NZ	1:A:83:ASP:O	2.40	0.45
1:A:91:CYS:SG	1:A:92:GLY:N	2.89	0.45
1:A:443:SER:O	1:A:444:GLN:NE2	2.49	0.45
1:A:851:PRO:HB3	1:A:859:LYS:HD2	1.98	0.45
1:B:1034:LEU:HD22	1:C:938:LEU:HB2	1.97	0.45
1:C:77:GLU:HB2	1:C:119:VAL:HA	1.98	0.45
1:C:465:VAL:HA	1:C:499:PHE:HE1	1.80	0.45
1:A:663:SER:O	1:A:672:SER:OG	2.33	0.45
1:A:1358:ASN:HD22	1:D:271:GLN:H	1.62	0.45
1:B:983:PRO:HB2	1:B:986:ILE:HB	1.98	0.45
1:C:795:PRO:HA	1:C:798:VAL:HG12	1.98	0.45
1:D:77:GLU:HB2	1:D:119:VAL:HA	1.98	0.45
1:D:1254:ARG:HB3	1:D:1274:PRO:HD2	1.98	0.45
1:D:1411:TRP:HD1	1:D:1414:PHE:H	1.65	0.45
1:A:635:ARG:HG3	1:A:678:LEU:HD13	1.97	0.45
1:A:653:LEU:O	1:A:656:SER:OG	2.28	0.45
1:A:783:THR:HG22	1:A:786:ALA:H	1.81	0.45
1:A:920:LEU:HB2	1:D:936:PHE:HE1	1.81	0.45
1:B:825:PRO:HA	1:B:829:GLU:HG2	1.98	0.45
1:C:783:THR:HG22	1:C:786:ALA:H	1.81	0.45
1:D:708:VAL:HG21	1:D:1112:LYS:HD2	1.99	0.45
1:D:1105:ARG:HH21	1:D:1106:HIS:H	1.62	0.45
1:A:825:PRO:HA	1:A:829:GLU:HG2	1.98	0.45
1:A:971:VAL:O	1:A:974:SER:OG	2.24	0.45
1:B:238:THR:N	1:B:282:SER:OG	2.50	0.45
1:B:1104:LYS:H	1:B:1104:LYS:HG2	1.55	0.45
1:C:746:GLN:OE1	1:C:774:ARG:NH1	2.47	0.45
1:C:868:TRP:HA	1:C:871:LEU:HB2	1.98	0.45
1:D:443:SER:O	1:D:444:GLN:NE2	2.49	0.45
1:D:505:GLU:OE2	1:D:506:ASN:ND2	2.49	0.45
1:D:557:GLN:HB3	1:D:585:ARG:HB3	1.98	0.45
1:D:1290:GLY:O	1:D:1308:ARG:NE	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:LYS:H	1:A:1104:LYS:HG2	1.55	0.45
1:C:708:VAL:HG21	1:C:1112:LYS:HD2	1.98	0.45
1:C:917:SER:O	1:C:921:GLY:N	2.42	0.45
1:C:1411:TRP:HD1	1:C:1414:PHE:H	1.65	0.45
1:A:708:VAL:HG21	1:A:1112:LYS:HD2	1.98	0.45
1:B:1411:TRP:HD1	1:B:1414:PHE:H	1.64	0.45
1:C:327:CYS:HB2	1:C:350:CYS:HB2	1.89	0.45
1:C:983:PRO:HB2	1:C:986:ILE:HB	1.98	0.45
1:C:1400:ARG:HG2	1:C:1403:LYS:HZ3	1.82	0.45
1:D:238:THR:N	1:D:282:SER:OG	2.50	0.45
1:D:825:PRO:HA	1:D:829:GLU:HG2	1.98	0.45
1:D:983:PRO:HB2	1:D:986:ILE:HB	1.98	0.45
1:A:238:THR:N	1:A:282:SER:OG	2.50	0.45
1:A:868:TRP:HA	1:A:871:LEU:HB2	1.98	0.45
1:B:783:THR:HG22	1:B:786:ALA:H	1.81	0.45
1:C:443:SER:O	1:C:444:GLN:NE2	2.49	0.45
1:C:445:ASP:OD2	1:C:451:ASN:ND2	2.33	0.45
1:D:783:THR:HG22	1:D:786:ALA:H	1.81	0.45
1:D:795:PRO:HA	1:D:798:VAL:HG12	1.98	0.45
1:A:1393:GLU:HB3	1:A:1396:GLU:HB2	1.98	0.45
1:B:1290:GLY:O	1:B:1308:ARG:NE	2.49	0.45
1:B:1393:GLU:HB3	1:B:1396:GLU:HB2	1.98	0.45
1:A:1052:PHE:CD2	1:D:1046:ALA:HB1	2.51	0.45
1:B:803:ILE:O	1:B:807:PHE:N	2.43	0.45
1:C:825:PRO:HA	1:C:829:GLU:HG2	1.98	0.45
1:D:669:THR:OG1	1:D:670:ASP:N	2.47	0.45
1:A:557:GLN:HB3	1:A:585:ARG:HB3	1.98	0.45
1:A:1436:ASP:N	1:A:1436:ASP:OD1	2.46	0.45
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.83	0.45
1:B:734:GLY:O	1:B:738:PHE:N	2.47	0.45
1:B:1257:VAL:HA	1:B:1258:PRO:HD3	1.84	0.45
1:C:635:ARG:HG3	1:C:678:LEU:HD13	1.97	0.45
1:C:1254:ARG:HB3	1:C:1274:PRO:HD2	1.98	0.45
1:D:693:CYS:HA	1:D:1128:LEU:HD13	1.97	0.45
1:D:1059:THR:HA	1:D:1062:ILE:HB	1.99	0.45
1:A:671:SER:HA	1:A:674:GLU:HB2	1.98	0.44
1:C:1055:VAL:HA	1:C:1058:HIS:HD2	1.83	0.44
1:D:851:PRO:HB3	1:D:859:LYS:HD2	1.98	0.44
1:D:1425:TYR:H	1:D:1444:ALA:HB3	1.82	0.44
1:A:795:PRO:HA	1:A:798:VAL:HG12	1.98	0.44
1:A:860:ALA:HA	1:A:863:TYR:HD1	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:PRO:HB2	1:A:986:ILE:HB	1.98	0.44
1:B:1444:ALA:HB2	1:B:1491:LEU:HD11	2.00	0.44
1:C:450:GLU:O	1:C:454:HIS:N	2.50	0.44
1:C:1059:THR:HA	1:C:1062:ILE:HB	1.99	0.44
1:D:285:ILE:HD13	1:D:285:ILE:HA	1.86	0.44
1:D:671:SER:HA	1:D:674:GLU:HB2	1.98	0.44
1:A:376:ILE:O	1:A:379:ILE:N	2.39	0.44
1:B:327:CYS:HB2	1:B:350:CYS:HB2	1.89	0.44
1:B:1400:ARG:HG2	1:B:1403:LYS:HZ3	1.82	0.44
1:C:557:GLN:HB3	1:C:585:ARG:HB3	1.98	0.44
1:C:1444:ALA:HB2	1:C:1491:LEU:HD11	2.00	0.44
1:D:445:ASP:OD2	1:D:451:ASN:ND2	2.33	0.44
1:D:917:SER:O	1:D:921:GLY:N	2.42	0.44
1:B:291:THR:OG1	1:B:292:HIS:N	2.42	0.44
1:B:868:TRP:HA	1:B:871:LEU:HB2	1.98	0.44
1:B:1038:ILE:HG22	1:C:1048:PHE:HZ	1.83	0.44
1:B:1411:TRP:NE1	1:B:1414:PHE:O	2.43	0.44
1:C:671:SER:HA	1:C:674:GLU:HB2	1.98	0.44
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.83	0.44
1:A:831:ALA:O	1:A:835:TRP:N	2.51	0.44
1:A:917:SER:O	1:A:921:GLY:N	2.42	0.44
1:B:254:ILE:O	1:B:255:HIS:ND1	2.51	0.44
1:B:831:ALA:O	1:B:835:TRP:N	2.51	0.44
1:B:1118:GLU:HG3	1:B:1122:LEU:HD23	2.00	0.44
1:C:1305:ASP:HA	1:C:1306:GLY:HA2	1.74	0.44
1:A:1118:GLU:HG3	1:A:1122:LEU:HD23	2.00	0.44
1:A:1444:ALA:HB2	1:A:1491:LEU:HD11	2.00	0.44
1:B:557:GLN:HE22	1:B:588:LEU:HB2	1.82	0.44
1:C:1425:TYR:H	1:C:1444:ALA:HB3	1.82	0.44
1:D:327:CYS:HB2	1:D:350:CYS:HB2	1.89	0.44
1:D:557:GLN:HE22	1:D:588:LEU:HB2	1.82	0.44
1:D:785:ALA:O	1:D:789:ARG:N	2.49	0.44
1:D:1105:ARG:HD2	1:D:1105:ARG:HA	1.81	0.44
1:A:450:GLU:O	1:A:454:HIS:N	2.50	0.44
1:A:1425:TYR:H	1:A:1444:ALA:HB3	1.82	0.44
1:B:1425:TYR:H	1:B:1444:ALA:HB3	1.82	0.44
1:C:248:HIS:HD2	1:C:271:GLN:HG3	1.83	0.44
1:C:376:ILE:O	1:C:379:ILE:N	2.39	0.44
1:D:859:LYS:NZ	1:D:863:TYR:OH	2.51	0.44
1:D:860:ALA:HA	1:D:863:TYR:HD1	1.83	0.44
1:A:130:ILE:HG12	1:A:262:ALA:C	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:O	1:A:255:HIS:ND1	2.51	0.44
1:A:1055:VAL:HA	1:A:1058:HIS:HD2	1.83	0.44
1:B:557:GLN:HB3	1:B:585:ARG:HB3	1.98	0.44
1:B:795:PRO:HA	1:B:798:VAL:HG12	1.98	0.44
1:B:1055:VAL:HA	1:B:1058:HIS:HD2	1.83	0.44
1:C:859:LYS:NZ	1:C:863:TYR:OH	2.51	0.44
1:D:1444:ALA:HB2	1:D:1491:LEU:HD11	2.00	0.44
1:A:785:ALA:O	1:A:789:ARG:N	2.49	0.44
1:A:859:LYS:NZ	1:A:863:TYR:OH	2.51	0.44
1:B:708:VAL:HG21	1:B:1112:LYS:HD2	1.99	0.44
1:C:734:GLY:O	1:C:738:PHE:N	2.47	0.44
1:D:1055:VAL:HA	1:D:1058:HIS:HD2	1.83	0.44
1:D:1305:ASP:HA	1:D:1306:GLY:HA2	1.75	0.44
1:A:327:CYS:HB2	1:A:350:CYS:HB2	1.89	0.43
1:A:1042:ASN:HB2	1:B:1048:PHE:CE2	2.53	0.43
1:B:130:ILE:HG12	1:B:262:ALA:C	2.43	0.43
1:B:216:LYS:NZ	1:C:476:GLU:OE1	2.49	0.43
1:B:671:SER:HA	1:B:674:GLU:HB2	1.98	0.43
1:B:859:LYS:NZ	1:B:863:TYR:OH	2.51	0.43
1:C:1286:MET:O	1:C:1290:GLY:N	2.43	0.43
1:A:207:THR:HG21	1:A:281:HIS:CE1	2.54	0.43
1:A:557:GLN:HE22	1:A:588:LEU:HB2	1.82	0.43
1:A:961:ARG:HA	1:A:966:LEU:HB2	2.00	0.43
1:B:248:HIS:HD2	1:B:271:GLN:HG3	1.83	0.43
1:B:1305:ASP:HA	1:B:1306:GLY:HA2	1.75	0.43
1:C:238:THR:N	1:C:282:SER:OG	2.50	0.43
1:C:254:ILE:O	1:C:255:HIS:ND1	2.51	0.43
1:C:546:ARG:HA	1:C:546:ARG:HD3	1.87	0.43
1:C:803:ILE:O	1:C:807:PHE:N	2.43	0.43
1:C:1118:GLU:HG3	1:C:1122:LEU:HD23	2.00	0.43
1:C:1393:GLU:HA	1:C:1394:PRO:HD3	1.90	0.43
1:D:1036:THR:OG1	1:D:1037:ASN:N	2.52	0.43
1:D:1352:VAL:HG21	1:D:1375:LEU:HD12	2.00	0.43
1:A:1059:THR:HA	1:A:1062:ILE:HB	1.99	0.43
1:A:1240:VAL:N	1:A:1430:ASP:OD2	2.42	0.43
1:A:1352:VAL:HG21	1:A:1375:LEU:HD12	2.00	0.43
1:A:1427:GLY:O	1:A:1442:THR:N	2.40	0.43
1:B:69:LYS:NZ	1:B:124:THR:O	2.41	0.43
1:C:831:ALA:O	1:C:835:TRP:N	2.51	0.43
1:D:831:ALA:O	1:D:835:TRP:N	2.51	0.43
1:B:248:HIS:CD2	1:B:271:GLN:HG3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:GLN:HE22	1:C:588:LEU:HB2	1.82	0.43
1:C:577:TYR:OH	1:C:624:ASP:OD1	2.28	0.43
1:C:1158:MET:HB2	1:D:1158:MET:HE1	2.00	0.43
1:C:1269:LEU:HD23	1:C:1269:LEU:HA	1.86	0.43
1:D:248:HIS:HD2	1:D:271:GLN:HG3	1.83	0.43
1:D:961:ARG:HA	1:D:966:LEU:HB2	2.00	0.43
1:A:1286:MET:O	1:A:1290:GLY:N	2.43	0.43
1:A:1323:LEU:HD23	1:A:1323:LEU:HA	1.88	0.43
1:B:860:ALA:HA	1:B:863:TYR:HD1	1.83	0.43
1:C:785:ALA:O	1:C:789:ARG:N	2.49	0.43
1:C:1435:THR:OG1	1:C:1436:ASP:N	2.49	0.43
1:D:68:LYS:HD3	1:D:68:LYS:HA	1.88	0.43
1:D:662:LEU:HD23	1:D:662:LEU:HA	1.91	0.43
1:D:1277:THR:OG1	1:D:1283:ALA:O	2.30	0.43
1:A:1360:ASP:OD1	1:A:1360:ASP:N	2.51	0.43
1:B:1036:THR:OG1	1:B:1037:ASN:N	2.52	0.43
1:B:1059:THR:HA	1:B:1062:ILE:HB	1.99	0.43
1:B:207:THR:HG21	1:B:281:HIS:CE1	2.54	0.43
1:B:326:VAL:HB	1:B:437:LEU:HD21	2.01	0.43
1:A:79:SER:HB3	1:A:93:TYR:CE2	2.54	0.43
1:B:1352:VAL:HG21	1:B:1375:LEU:HD12	2.00	0.43
1:C:117:LYS:HD2	1:C:117:LYS:HA	1.86	0.43
1:C:130:ILE:HG12	1:C:262:ALA:C	2.43	0.43
1:C:618:THR:O	1:C:618:THR:OG1	2.28	0.43
1:C:643:ALA:O	1:C:1129:LYS:NZ	2.49	0.43
1:D:1118:GLU:HG3	1:D:1122:LEU:HD23	2.00	0.43
1:B:618:THR:O	1:B:618:THR:OG1	2.28	0.43
1:B:1046:ALA:HB2	1:C:1049:ASN:CG	2.44	0.43
1:C:207:THR:HG21	1:C:281:HIS:CE1	2.54	0.43
1:C:326:VAL:HB	1:C:437:LEU:HD21	2.01	0.43
1:D:207:THR:HG21	1:D:281:HIS:CE1	2.54	0.43
1:D:254:ILE:O	1:D:255:HIS:ND1	2.51	0.43
1:D:559:HIS:H	1:D:585:ARG:HB2	1.84	0.43
1:A:248:HIS:HD2	1:A:271:GLN:HG3	1.83	0.43
1:A:690:PHE:O	1:A:694:TYR:N	2.52	0.43
1:A:1393:GLU:HA	1:A:1394:PRO:HD3	1.90	0.43
1:C:248:HIS:CD2	1:C:271:GLN:HG3	2.54	0.43
1:C:375:THR:O	1:C:377:SER:N	2.50	0.43
1:C:961:ARG:HA	1:C:966:LEU:HB2	2.01	0.43
1:C:1352:VAL:HG21	1:C:1375:LEU:HD12	2.00	0.43
1:D:130:ILE:HG12	1:D:262:ALA:C	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HB	1:A:142:TYR:CZ	2.54	0.42
1:B:79:SER:HB3	1:B:93:TYR:CE2	2.54	0.42
1:B:625:LEU:HD23	1:B:625:LEU:HA	1.87	0.42
1:C:80:LYS:NZ	1:C:83:ASP:O	2.40	0.42
1:C:559:HIS:H	1:C:585:ARG:HB2	1.84	0.42
1:C:1451:ASP:OD1	1:C:1451:ASP:N	2.52	0.42
1:D:79:SER:HB3	1:D:93:TYR:CE2	2.54	0.42
1:D:80:LYS:NZ	1:D:83:ASP:O	2.40	0.42
1:A:927:VAL:HG12	1:D:1039:LEU:HD12	2.01	0.42
1:A:1036:THR:OG1	1:A:1037:ASN:N	2.52	0.42
1:B:785:ALA:O	1:B:789:ARG:N	2.49	0.42
1:B:1360:ASP:N	1:B:1360:ASP:OD1	2.51	0.42
1:A:692:GLU:HG3	1:A:1132:TYR:HB2	2.02	0.42
1:B:585:ARG:HH12	1:B:602:VAL:HG12	1.85	0.42
1:B:961:ARG:HA	1:B:966:LEU:HB2	2.00	0.42
1:C:79:SER:HB3	1:C:93:TYR:CE2	2.54	0.42
1:C:271:GLN:O	1:D:1365:ARG:NH1	2.52	0.42
1:C:690:PHE:O	1:C:694:TYR:N	2.52	0.42
1:D:246:THR:O	1:D:275:THR:N	2.53	0.42
1:D:1451:ASP:OD1	1:D:1451:ASP:N	2.53	0.42
1:A:248:HIS:CD2	1:A:271:GLN:HG3	2.54	0.42
1:B:450:GLU:O	1:B:454:HIS:N	2.50	0.42
1:B:1331:THR:O	1:B:1331:THR:OG1	2.37	0.42
1:C:246:THR:O	1:C:275:THR:N	2.53	0.42
1:C:1360:ASP:OD1	1:C:1360:ASP:N	2.51	0.42
1:A:326:VAL:HB	1:A:437:LEU:HD21	2.01	0.42
1:A:585:ARG:HH12	1:A:602:VAL:HG12	1.85	0.42
1:A:1378:LYS:HB2	1:A:1385:TRP:CD2	2.55	0.42
1:B:130:ILE:HB	1:B:142:TYR:CZ	2.54	0.42
1:C:130:ILE:HB	1:C:142:TYR:CZ	2.54	0.42
1:D:248:HIS:CD2	1:D:271:GLN:HG3	2.54	0.42
1:D:734:GLY:O	1:D:738:PHE:N	2.47	0.42
1:D:803:ILE:HD13	1:D:803:ILE:HA	1.94	0.42
1:A:559:HIS:H	1:A:585:ARG:HB2	1.84	0.42
1:D:130:ILE:HB	1:D:142:TYR:CZ	2.54	0.42
1:A:1269:LEU:HD23	1:A:1269:LEU:HA	1.86	0.42
1:C:921:GLY:O	1:C:925:ILE:HG12	2.20	0.42
1:C:1036:THR:OG1	1:C:1037:ASN:N	2.52	0.42
1:C:1104:LYS:H	1:C:1104:LYS:HG2	1.55	0.42
1:A:476:GLU:OE1	1:D:216:LYS:NZ	2.53	0.42
1:A:888:ILE:HA	1:A:889:PRO:HD3	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:O	1:B:275:THR:N	2.53	0.42
1:C:125:ASP:O	1:C:255:HIS:N	2.49	0.42
1:C:585:ARG:HH12	1:C:602:VAL:HG12	1.85	0.42
1:C:860:ALA:HA	1:C:863:TYR:HD1	1.83	0.42
1:C:1366:LYS:HZ2	1:C:1371:MET:HE2	1.85	0.42
1:C:1378:LYS:HB2	1:C:1385:TRP:CD2	2.55	0.42
1:A:125:ASP:O	1:A:255:HIS:N	2.49	0.42
1:B:562:ALA:HB1	1:B:575:PRO:HB2	2.02	0.42
1:C:68:LYS:HD3	1:C:68:LYS:HA	1.88	0.42
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.83	0.42
1:D:375:THR:O	1:D:377:SER:N	2.50	0.42
1:D:692:GLU:HG3	1:D:1132:TYR:HB2	2.01	0.42
1:D:921:GLY:O	1:D:925:ILE:HG12	2.20	0.42
1:B:376:ILE:O	1:B:379:ILE:N	2.39	0.42
1:B:559:HIS:H	1:B:585:ARG:HB2	1.84	0.42
1:B:692:GLU:HG3	1:B:1132:TYR:HB2	2.02	0.42
1:B:1378:LYS:HB2	1:B:1385:TRP:CD2	2.55	0.42
1:C:562:ALA:HB1	1:C:575:PRO:HB2	2.02	0.42
1:D:133:THR:HA	1:D:134:GLY:HA2	1.61	0.41
1:D:206:ILE:HD13	1:D:239:ILE:HB	2.02	0.41
1:D:562:ALA:HB1	1:D:575:PRO:HB2	2.02	0.41
1:A:1411:TRP:NE1	1:A:1414:PHE:O	2.43	0.41
1:B:593:PRO:HD2	1:B:597:LEU:HD22	2.03	0.41
1:C:520:LEU:HD12	1:C:520:LEU:HA	1.88	0.41
1:D:326:VAL:HB	1:D:437:LEU:HD21	2.01	0.41
1:D:593:PRO:HD2	1:D:597:LEU:HD22	2.03	0.41
1:D:1049:ASN:HA	1:D:1052:PHE:HB3	2.03	0.41
1:A:1366:LYS:HZ2	1:A:1371:MET:HE2	1.85	0.41
1:C:743:TRP:HB2	1:C:1071:ILE:HD12	2.03	0.41
1:D:1411:TRP:NE1	1:D:1414:PHE:O	2.43	0.41
1:A:373:ASP:CG	1:A:375:THR:H	2.29	0.41
1:A:593:PRO:HD2	1:A:597:LEU:HD22	2.03	0.41
1:A:620:ASP:HB2	1:A:623:ARG:HD3	2.03	0.41
1:A:921:GLY:O	1:A:925:ILE:HG12	2.20	0.41
1:A:1400:ARG:HG2	1:A:1403:LYS:HZ3	1.84	0.41
1:A:1419:LYS:HE3	1:A:1419:LYS:HB2	1.93	0.41
1:B:917:SER:O	1:B:921:GLY:N	2.42	0.41
1:B:1416:ASN:HB3	1:B:1419:LYS:HB3	2.03	0.41
1:C:590:LEU:O	1:C:608:TYR:OH	2.36	0.41
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.92	0.41
1:A:246:THR:O	1:A:275:THR:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:HD23	1:A:662:LEU:HA	1.91	0.41
1:A:1052:PHE:CG	1:D:1046:ALA:HB1	2.56	0.41
1:B:743:TRP:HB2	1:B:1071:ILE:HD12	2.03	0.41
1:B:984:GLY:H	1:C:981:GLN:NE2	2.18	0.41
1:A:1277:THR:OG1	1:A:1283:ALA:O	2.30	0.41
1:A:1340:SER:O	1:A:1340:SER:OG	2.28	0.41
1:B:620:ASP:HB2	1:B:623:ARG:HD3	2.03	0.41
1:B:921:GLY:O	1:B:925:ILE:HG12	2.20	0.41
1:C:593:PRO:HD2	1:C:597:LEU:HD22	2.02	0.41
1:C:882:GLY:HA3	1:C:899:LEU:HD21	2.03	0.41
1:D:968:ARG:HG3	1:D:972:TYR:CD2	2.55	0.41
1:A:206:ILE:HD13	1:A:239:ILE:HB	2.02	0.41
1:A:314:LYS:HA	1:A:314:LYS:HD3	1.92	0.41
1:C:206:ILE:HD13	1:C:239:ILE:HB	2.02	0.41
1:C:692:GLU:HG3	1:C:1132:TYR:HB2	2.01	0.41
1:D:1104:LYS:H	1:D:1104:LYS:HG2	1.55	0.41
1:A:730:VAL:HG11	1:A:1065:PHE:HD1	1.86	0.41
1:B:882:GLY:HA3	1:B:899:LEU:HD21	2.03	0.41
1:C:194:LEU:HD12	1:C:194:LEU:HA	1.92	0.41
1:C:630:ILE:HD13	1:C:630:ILE:HA	1.87	0.41
1:D:1378:LYS:HB2	1:D:1385:TRP:CD2	2.55	0.41
1:A:562:ALA:HB1	1:A:575:PRO:HB2	2.02	0.41
1:A:936:PHE:HE1	1:B:920:LEU:HB2	1.86	0.41
1:A:1305:ASP:HA	1:A:1306:GLY:HA2	1.75	0.41
1:A:1451:ASP:OD1	1:A:1451:ASP:N	2.52	0.41
1:B:373:ASP:CG	1:B:375:THR:H	2.29	0.41
1:B:577:TYR:OH	1:B:624:ASP:OD1	2.28	0.41
1:B:937:PHE:CD1	1:B:940:LEU:HD23	2.56	0.41
1:B:1427:GLY:O	1:B:1442:THR:N	2.40	0.41
1:C:642:TRP:HE1	1:C:652:ALA:HB2	1.86	0.41
1:C:1021:PRO:O	1:C:1025:THR:OG1	2.27	0.41
1:C:1105:ARG:HD2	1:C:1105:ARG:HA	1.81	0.41
1:D:269:ASP:OD1	1:D:269:ASP:N	2.54	0.41
1:D:743:TRP:HB2	1:D:1071:ILE:HD12	2.03	0.41
1:D:1427:GLY:O	1:D:1442:THR:N	2.40	0.41
1:A:460:VAL:HA	1:A:499:PHE:HE2	1.86	0.41
1:A:743:TRP:HB2	1:A:1071:ILE:HD12	2.03	0.41
1:A:968:ARG:HG3	1:A:972:TYR:CD2	2.55	0.41
1:B:460:VAL:HA	1:B:499:PHE:HE2	1.86	0.41
1:D:314:LYS:HD3	1:D:314:LYS:HA	1.91	0.41
1:D:642:TRP:HE1	1:D:652:ALA:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:GLY:HA3	1:D:899:LEU:HD21	2.03	0.41
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.86	0.40
1:C:373:ASP:CG	1:C:375:THR:H	2.29	0.40
1:C:925:ILE:HD12	1:C:925:ILE:HG23	1.94	0.40
1:C:1427:GLY:O	1:C:1442:THR:N	2.40	0.40
1:D:373:ASP:CG	1:D:375:THR:H	2.29	0.40
1:D:643:ALA:O	1:D:1129:LYS:NZ	2.49	0.40
1:A:375:THR:O	1:A:377:SER:N	2.50	0.40
1:A:937:PHE:CD1	1:A:940:LEU:HD23	2.56	0.40
1:A:1416:ASN:HB3	1:A:1419:LYS:HB3	2.03	0.40
1:B:117:LYS:HD2	1:B:117:LYS:HA	1.86	0.40
1:B:125:ASP:O	1:B:255:HIS:N	2.49	0.40
1:C:522:LEU:HD12	1:C:522:LEU:HA	1.83	0.40
1:C:730:VAL:HG11	1:C:1065:PHE:HD1	1.86	0.40
1:D:460:VAL:HA	1:D:499:PHE:HE2	1.86	0.40
1:D:620:ASP:HB2	1:D:623:ARG:HD3	2.03	0.40
1:D:625:LEU:HD23	1:D:625:LEU:HA	1.87	0.40
1:A:558:MET:HE3	1:A:558:MET:HB3	1.96	0.40
1:A:648:CYS:SG	1:A:1129:LYS:HD3	2.61	0.40
1:B:374:ILE:HB	1:B:376:ILE:HA	2.03	0.40
1:B:594:HIS:ND1	1:B:595:VAL:HG23	2.36	0.40
1:B:1049:ASN:HA	1:B:1052:PHE:HB3	2.03	0.40
1:C:594:HIS:ND1	1:C:595:VAL:HG23	2.36	0.40
1:C:1049:ASN:HA	1:C:1052:PHE:HB3	2.03	0.40
1:D:522:LEU:HD12	1:D:522:LEU:HA	1.84	0.40
1:D:585:ARG:HH12	1:D:602:VAL:HG12	1.85	0.40
1:D:1416:ASN:HB3	1:D:1419:LYS:HB3	2.03	0.40
1:A:1105:ARG:HA	1:A:1105:ARG:HD2	1.81	0.40
1:B:648:CYS:SG	1:B:1129:LYS:HD3	2.61	0.40
1:B:988:GLY:C	1:C:968:ARG:HE	2.30	0.40
1:B:1029:LEU:HG	1:C:975:TYR:CD2	2.56	0.40
1:C:620:ASP:HB2	1:C:623:ARG:HD3	2.03	0.40
1:D:594:HIS:ND1	1:D:595:VAL:HG23	2.36	0.40
1:A:1331:THR:O	1:A:1331:THR:OG1	2.37	0.40
1:B:68:LYS:HD3	1:B:68:LYS:HA	1.88	0.40
1:B:206:ILE:HD13	1:B:239:ILE:HB	2.02	0.40
1:D:520:LEU:HD12	1:D:520:LEU:HA	1.88	0.40
1:D:648:CYS:SG	1:D:1129:LYS:HD3	2.61	0.40
1:D:730:VAL:HG11	1:D:1065:PHE:HD1	1.86	0.40
1:D:1364:CYS:HA	1:D:1371:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	61
1	B	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	61
1	C	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	61
1	D	1331/1503 (89%)	1133 (85%)	193 (14%)	5 (0%)	30	61
All	All	5324/6012 (89%)	4526 (85%)	778 (15%)	20 (0%)	31	61

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ILE
1	A	377	SER
1	B	376	ILE
1	B	377	SER
1	C	376	ILE
1	C	377	SER
1	D	376	ILE
1	D	377	SER
1	A	714	LYS
1	B	714	LYS
1	C	714	LYS
1	D	714	LYS
1	A	670	ASP
1	B	670	ASP
1	C	670	ASP
1	D	670	ASP
1	A	595	VAL
1	B	595	VAL
1	C	595	VAL
1	D	595	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 PDB entries followed by that with respect to all EM entries.

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	1176/1318 (89%)	1149 (98%)	27 (2%)	44	64
1	B	1176/1318 (89%)	1149 (98%)	27 (2%)	44	64
1	C	1176/1318 (89%)	1149 (98%)	27 (2%)	44	64
1	D	1176/1318 (89%)	1149 (98%)	27 (2%)	44	64
All	All	4704/5272 (89%)	4596 (98%)	108 (2%)	44	64

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	THR
1	A	146	SER
1	A	169	LEU
1	A	173	VAL
1	A	210	SER
1	A	263	GLU
1	A	275	THR
1	A	366	VAL
1	A	390	MET
1	A	418	VAL
1	A	541	VAL
1	A	595	VAL
1	A	606	SER
1	A	607	LEU
1	A	612	SER
1	A	618	THR
1	A	624	ASP
1	A	698	GLU
1	A	759	CYS
1	A	878	LEU
1	A	927	VAL
1	A	1253	THR
1	A	1262	VAL
1	A	1331	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1352	VAL
1	A	1372	LEU
1	A	1457	LEU
1	B	107	THR
1	B	146	SER
1	B	169	LEU
1	B	173	VAL
1	B	210	SER
1	B	263	GLU
1	B	275	THR
1	B	366	VAL
1	B	390	MET
1	B	418	VAL
1	B	541	VAL
1	B	595	VAL
1	B	606	SER
1	B	607	LEU
1	B	612	SER
1	B	618	THR
1	B	624	ASP
1	B	698	GLU
1	B	759	CYS
1	B	878	LEU
1	B	927	VAL
1	B	1253	THR
1	B	1262	VAL
1	B	1331	THR
1	B	1352	VAL
1	B	1372	LEU
1	B	1457	LEU
1	C	107	THR
1	C	146	SER
1	C	169	LEU
1	C	173	VAL
1	C	210	SER
1	C	263	GLU
1	C	275	THR
1	C	366	VAL
1	C	390	MET
1	C	418	VAL
1	C	541	VAL
1	C	595	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	606	SER
1	C	607	LEU
1	C	612	SER
1	C	618	THR
1	C	624	ASP
1	C	698	GLU
1	C	759	CYS
1	C	878	LEU
1	C	927	VAL
1	C	1253	THR
1	C	1262	VAL
1	C	1331	THR
1	C	1352	VAL
1	C	1372	LEU
1	C	1457	LEU
1	D	107	THR
1	D	146	SER
1	D	169	LEU
1	D	173	VAL
1	D	210	SER
1	D	263	GLU
1	D	275	THR
1	D	366	VAL
1	D	390	MET
1	D	418	VAL
1	D	541	VAL
1	D	595	VAL
1	D	606	SER
1	D	607	LEU
1	D	612	SER
1	D	618	THR
1	D	624	ASP
1	D	698	GLU
1	D	759	CYS
1	D	878	LEU
1	D	927	VAL
1	D	1253	THR
1	D	1262	VAL
1	D	1331	THR
1	D	1352	VAL
1	D	1372	LEU
1	D	1457	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	137	GLN
1	A	156	HIS
1	A	161	HIS
1	A	181	ASN
1	A	248	HIS
1	A	280	ASN
1	A	380	GLN
1	A	381	GLN
1	A	506	ASN
1	A	509	GLN
1	A	557	GLN
1	A	646	GLN
1	A	736	GLN
1	A	958	HIS
1	A	1042	ASN
1	A	1058	HIS
1	A	1249	ASN
1	A	1476	GLN
1	B	90	GLN
1	B	156	HIS
1	B	161	HIS
1	B	181	ASN
1	B	248	HIS
1	B	280	ASN
1	B	380	GLN
1	B	381	GLN
1	B	506	ASN
1	B	509	GLN
1	B	557	GLN
1	B	646	GLN
1	B	736	GLN
1	B	958	HIS
1	B	959	ASN
1	B	1037	ASN
1	B	1042	ASN
1	B	1058	HIS
1	B	1066	GLN
1	B	1249	ASN
1	B	1476	GLN
1	C	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	156	HIS
1	C	161	HIS
1	C	181	ASN
1	C	248	HIS
1	C	280	ASN
1	C	380	GLN
1	C	381	GLN
1	C	506	ASN
1	C	509	GLN
1	C	557	GLN
1	C	646	GLN
1	C	736	GLN
1	C	958	HIS
1	C	959	ASN
1	C	981	GLN
1	C	1042	ASN
1	C	1058	HIS
1	C	1249	ASN
1	C	1476	GLN
1	D	90	GLN
1	D	156	HIS
1	D	161	HIS
1	D	181	ASN
1	D	248	HIS
1	D	280	ASN
1	D	380	GLN
1	D	381	GLN
1	D	506	ASN
1	D	509	GLN
1	D	557	GLN
1	D	646	GLN
1	D	736	GLN
1	D	958	HIS
1	D	1042	ASN
1	D	1058	HIS
1	D	1249	ASN
1	D	1384	HIS
1	D	1476	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

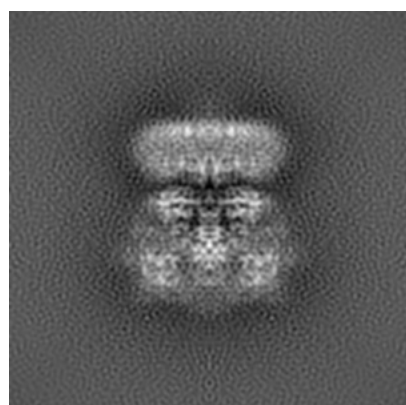
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9132. These allow visual inspection of the internal detail of the map and identification of artifacts.

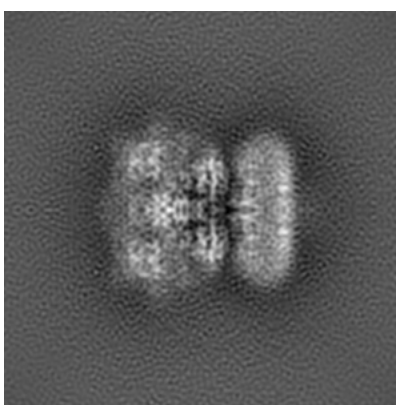
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

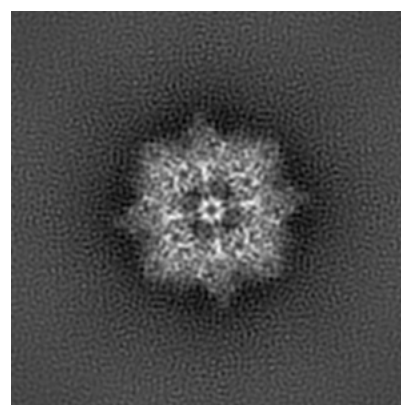
6.1.1 Primary map



X



Y

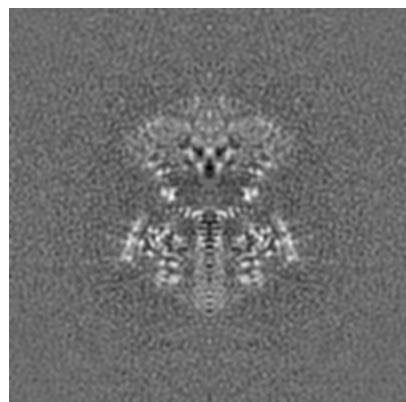


Z

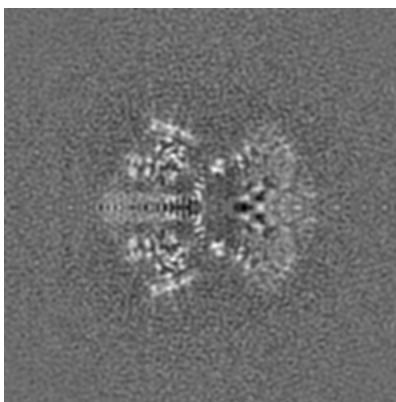
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

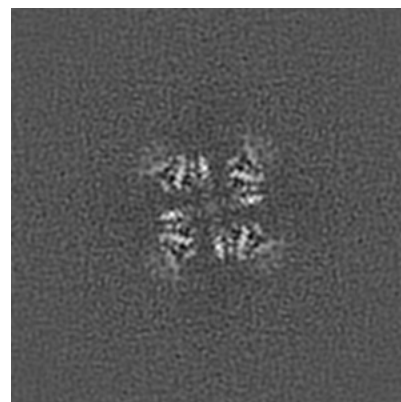
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

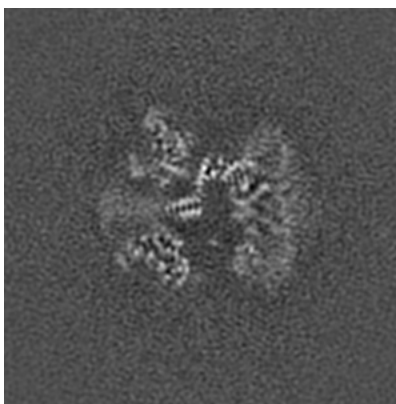
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

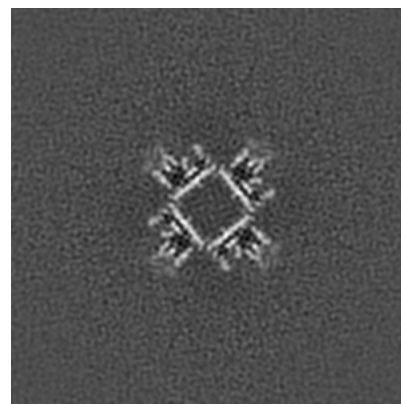
6.3.1 Primary map



X Index: 193



Y Index: 207

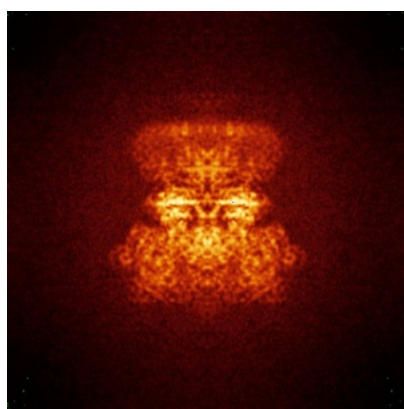


Z Index: 208

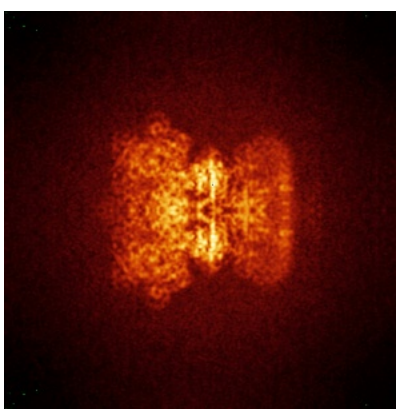
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

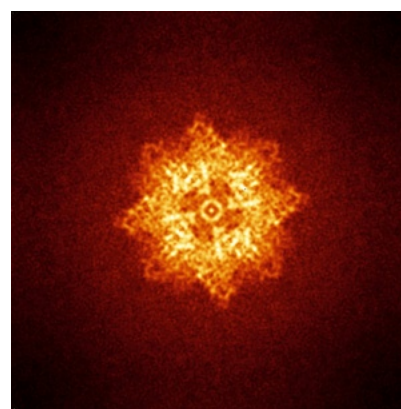
6.4.1 Primary map



X



Y

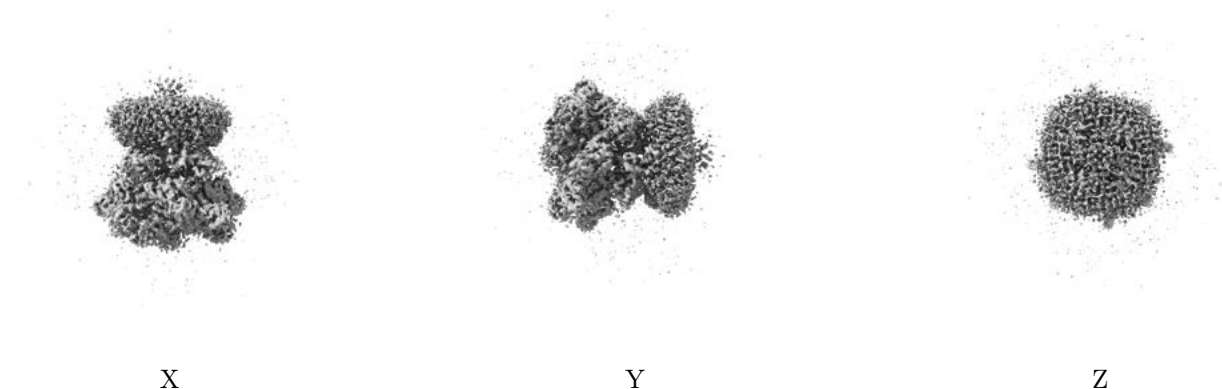


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

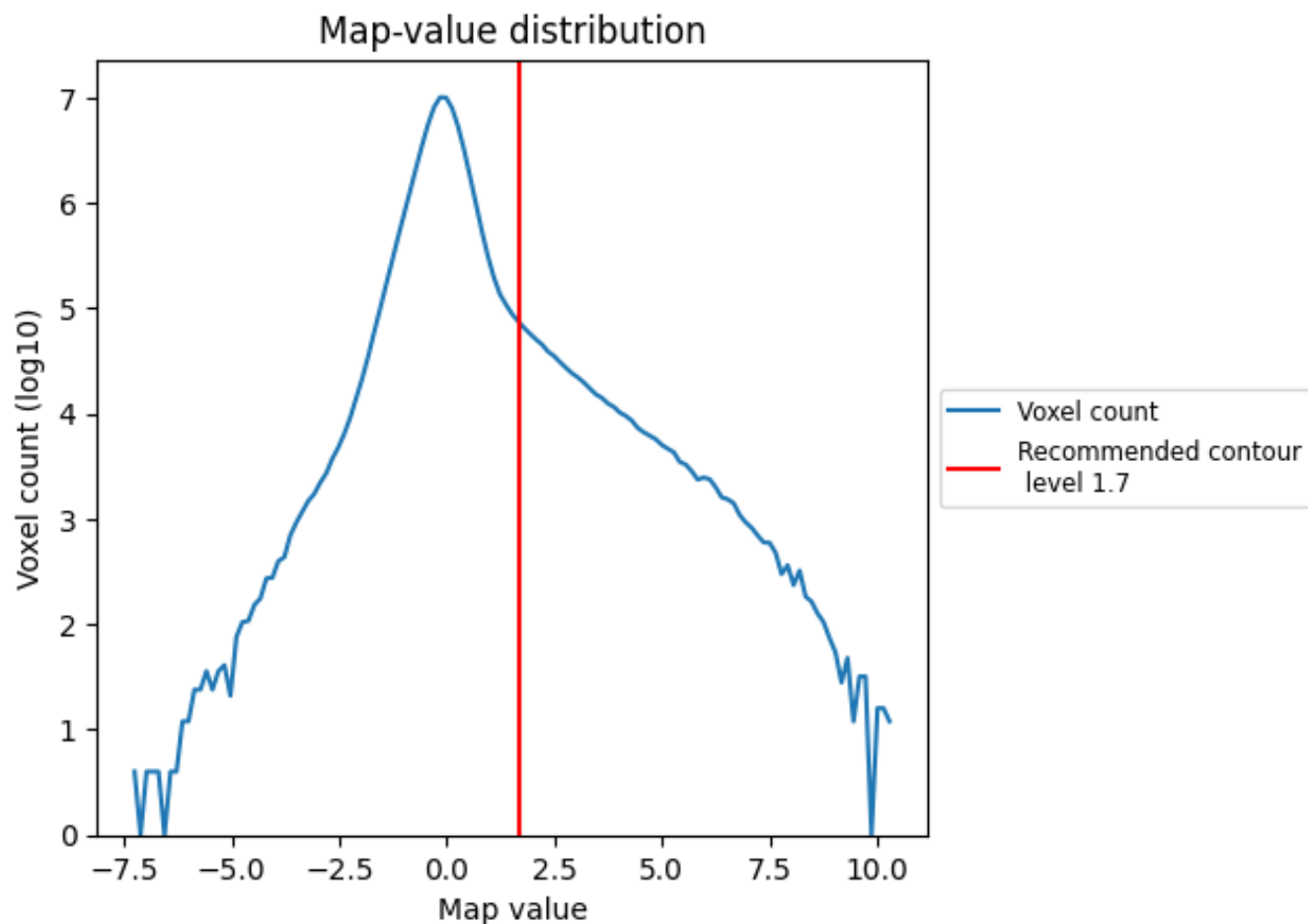
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

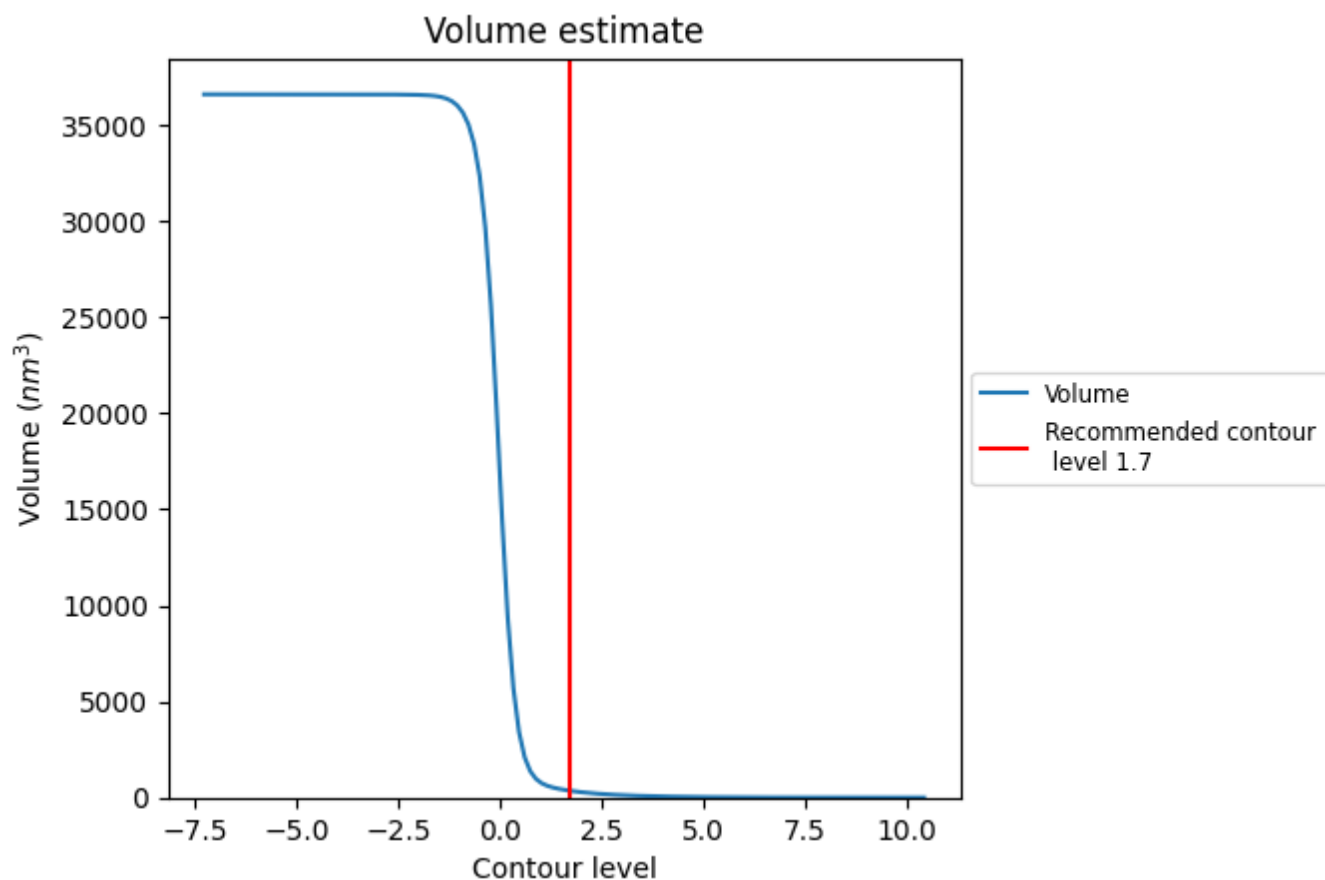
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

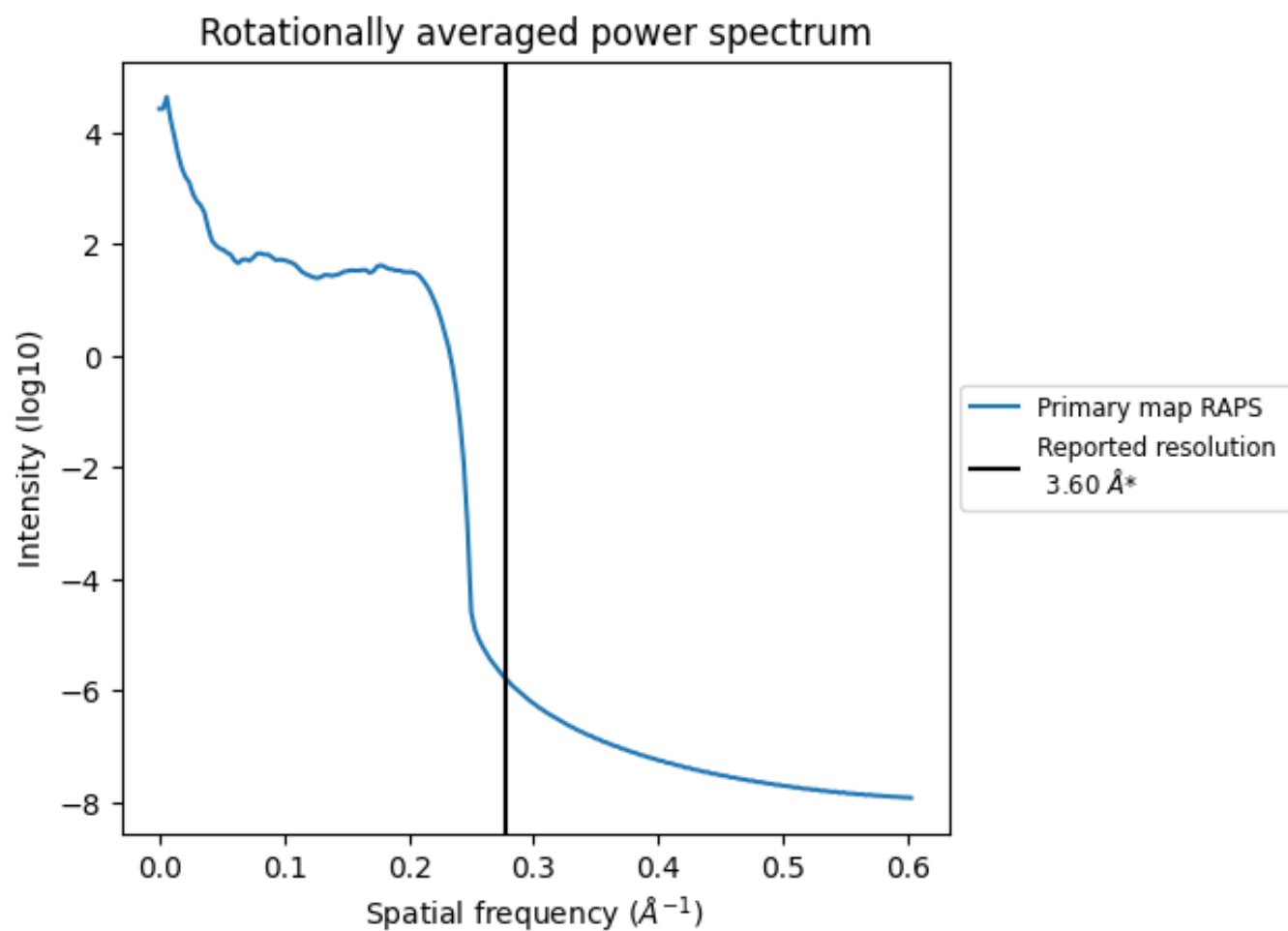
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 364 nm³; this corresponds to an approximate mass of 328 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

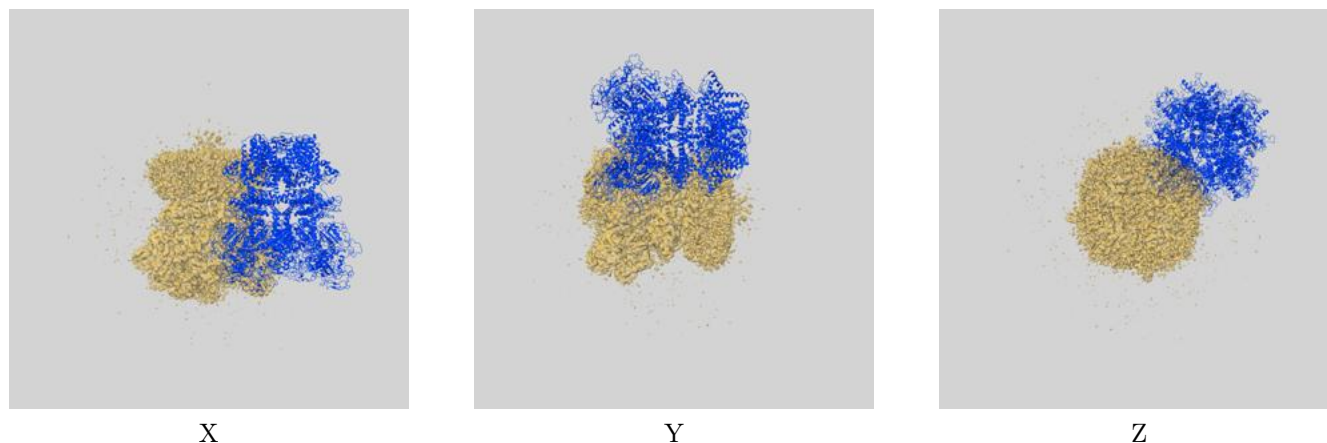
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

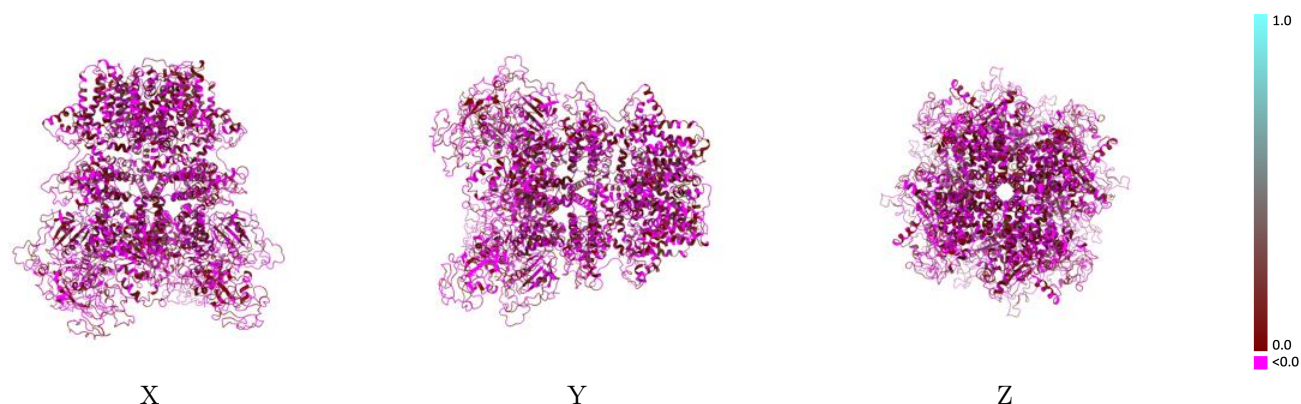
This section contains information regarding the fit between EMDB map EMD-9132 and PDB model 6MIX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



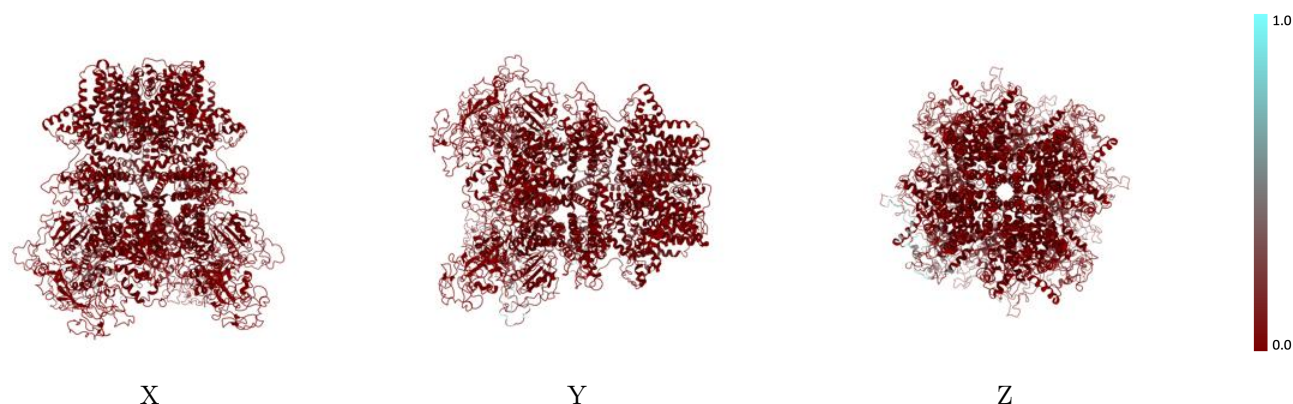
The images above show the 3D surface view of the map at the recommended contour level 1.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



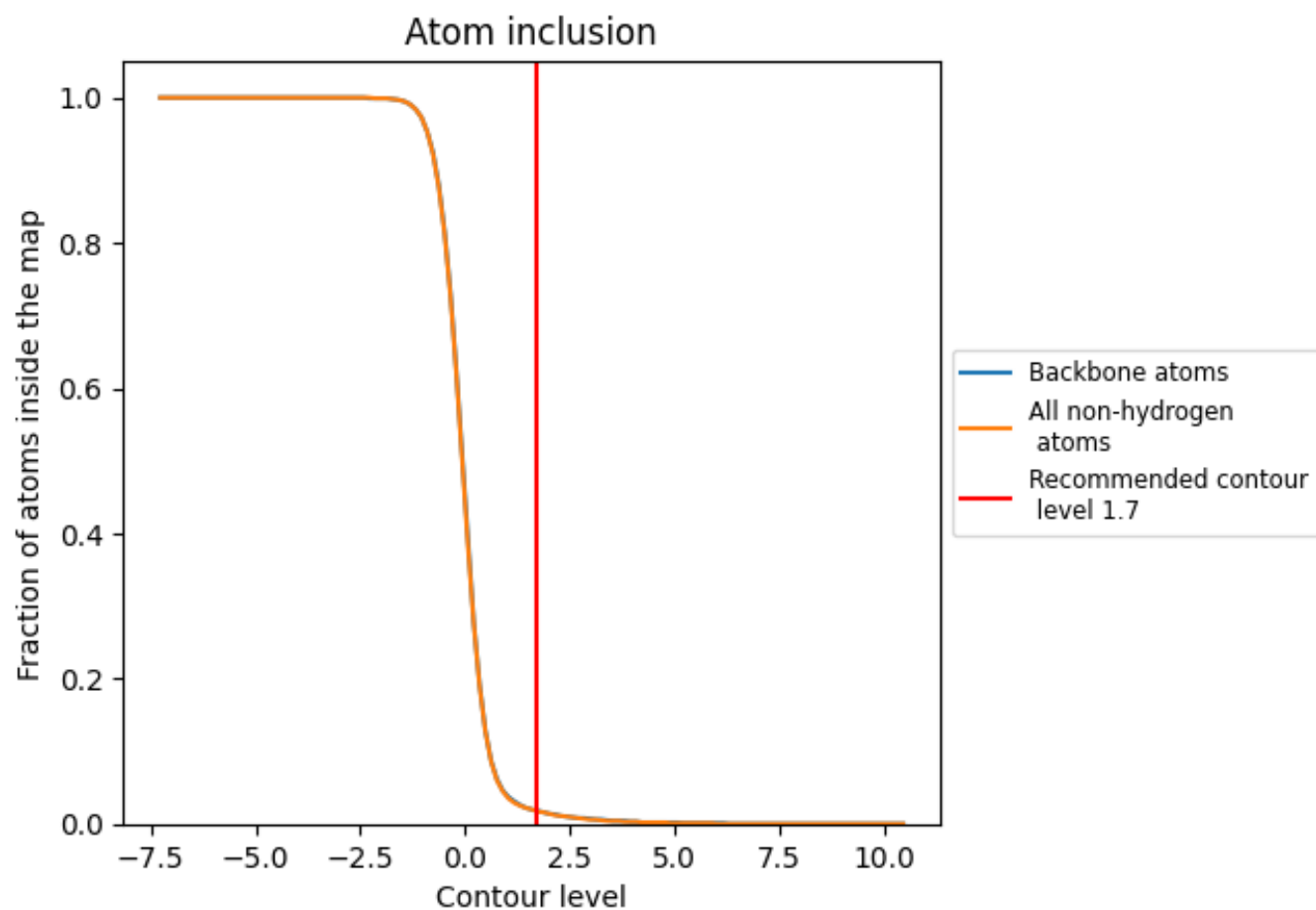
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 2% of all backbone atoms, 2% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0180	-0.0010
A	0.0610	-0.0020
B	0.0000	-0.0000
C	0.0000	0.0070
D	0.0090	-0.0080

