Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 01:19 PM EST

PDB ID	:	6MJ2
EMDB ID	:	EMD-9134
Title	:	Human TRPM2 ion channel in a calcium- and ADPR-bound state
Authors	:	Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on	:	2018-09-20
Resolution	:	6.36 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:

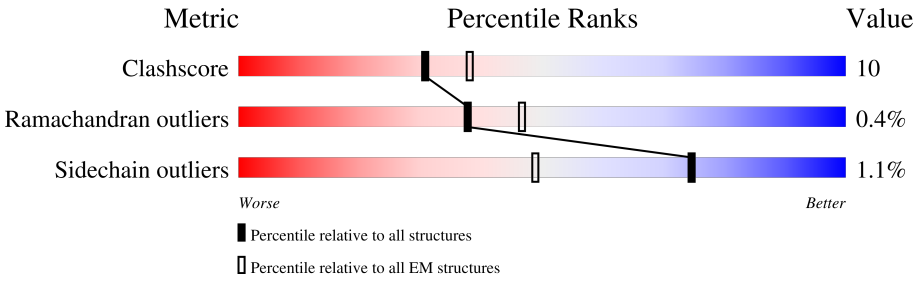
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.36 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	84% 65% 23% • 11%
1	B	1503	89% 65% 23% • 11%
1	C	1503	89% 65% 23% • 11%
1	D	1503	88% 65% 23% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43124 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 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

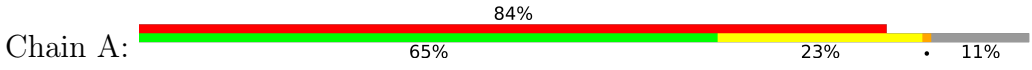
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	

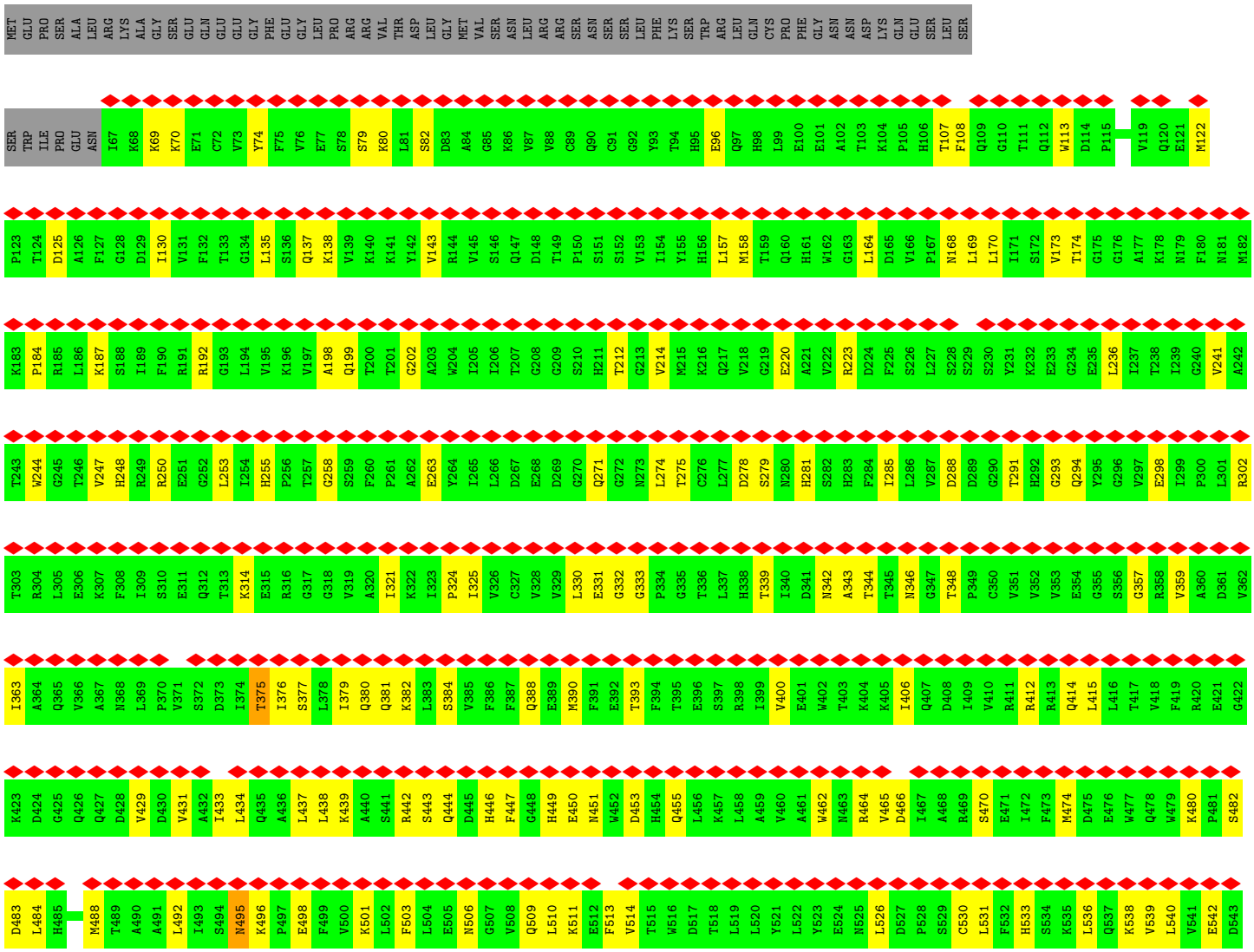
3 Residue-property plots (i)

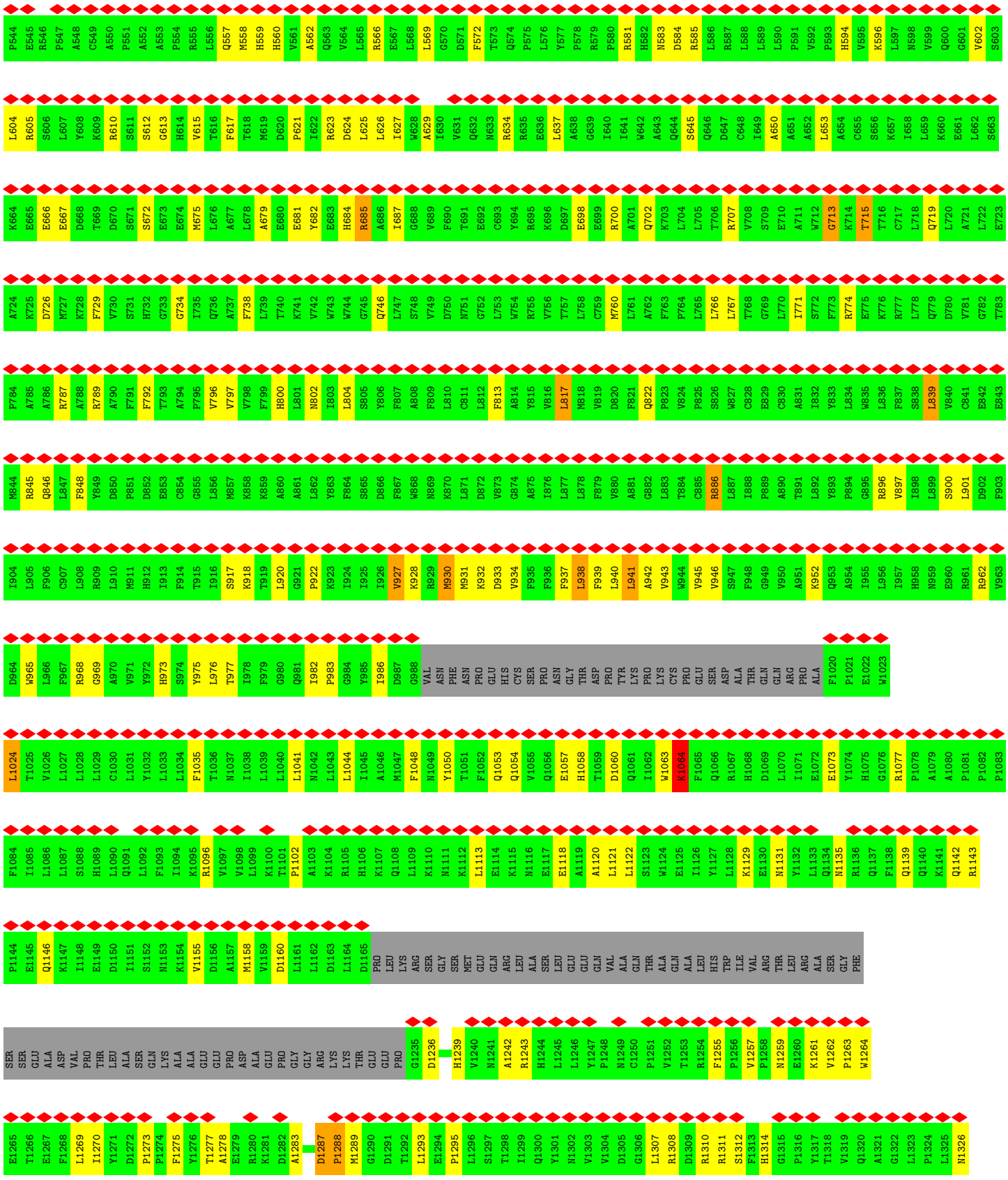
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Transient receptor potential cation channel subfamily M member 2

Chain A:



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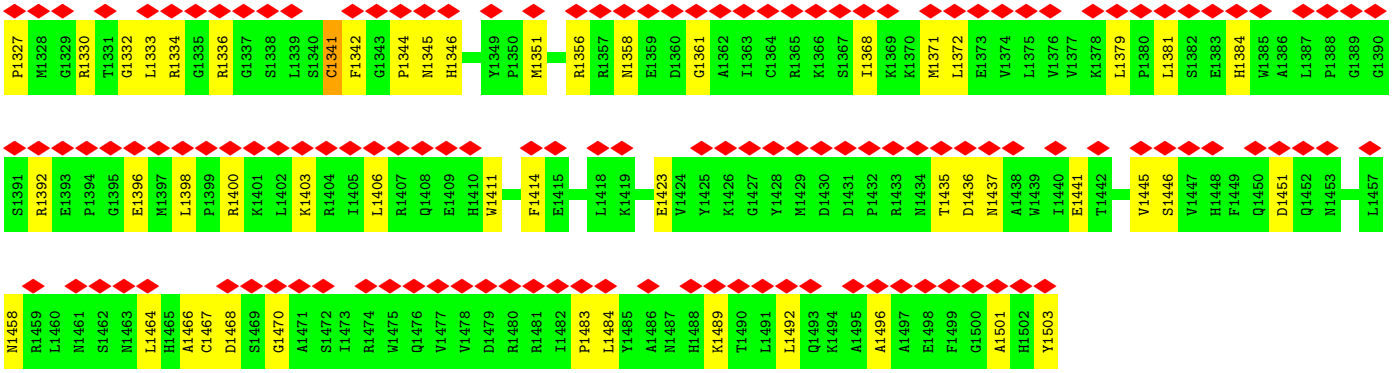
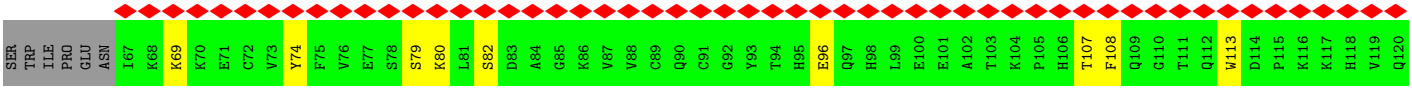
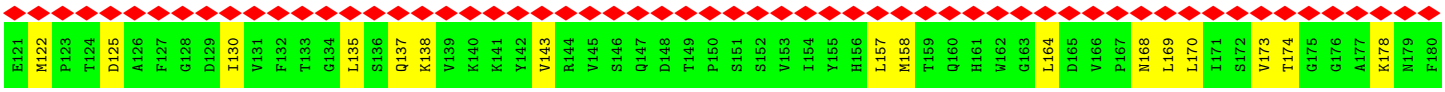
L604 R605 S606 L607 Y608 K609 R610 S611 S612 G613 H614 V615 T616 F617 T618 M619 D620 P621 I622 R623 D624 L625 L626 I627 W628 A629 I630 V631 Q632 N633 R634 R635 E636 L637 A638 G639 I640 I641 W642 A643 Q644 S645 Q646 D647 C648 I649 A650 A651 A652 L653 A654 C655 S656 K657 I658 L659 K660 E661 L662 S663
K664 E665 E666 E667 D668 T669 D670 S671 S672 E673 E674 M675 L676 A677 L678 A679 E680 E681 Y682 E683 H684 R685 A686 I687 G688 V689 F690 T691 E692 C693 Y694 R695 K696 D697 E698 E699 R700 A701 Q702 K703 L704 L705 T706 R707 V708 S709 E710 A711 W712 G713 K714 T715 T716 C717 L718 Q719 L720 A721 L722 E723
A724 K725 D726 M727 K728 F729 V730 S731 H732 G733 G734 I735 Q736 A737 F738 L739 T740 K741 V742 W743 W744 G745 Q746 L747 S748 V749 D750 N751 G752 L753 W754 R755 V756 T757 L758 C759 M760 L761 A762 F763 P764 L765 L766 L767 T768 G769 L770 I771 S772 F773 R774 E775 K776 R777 L778 Q779 D780 V781 G782 T783
P784 A785 A786 R787 A788 R789 A790 F791 F792 T793 A794 P795 V796 V797 V798 F799 H800 L801 N802 I803 L804 S805 Y806 F807 A808 F809 L810 C811 L812 F813 A814 Y815 V816 L817 M818 V819 D820 F821 Q822 P823 V824 P825 S826 W827 C828 E829 C830 A831 I832 Y833 L834 W835 L836 F837 S838 L839 V840 C841 E842 E843
M844 R845 Q846 L847 F848 Y849 D850 P851 D852 E853 C854 G855 L856 M857 K858 K859 A860 A861 L862 Y863 F864 S865 D866 F867 W868 N869 K870 L871 D872 V873 G874 A875 I876 L877 L878 F879 V880 A881 G882 L883 T884 C885 R886 L887 I888 P889 A890 T891 L892 Y893 P894 G895 R896 V897 I898 L899 S900 L901 D902 F903
I904 L905 F906 C907 L908 R909 L910 M911 H912 I913 F914 P915 I916 S917 K918 T919 L920 G921 P922 K923 I924 I925 I926 V927 K928 R929 M930 M931 K932 D933 V934 F935 F936 F937 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 F948 G949 V950 A951 K952 Q953 A954 I955 L956 I957 H958 N959 E960 R961 R962 V963
D964 W965 L966 F967 R968 G969 A970 V971 Y972 H973 S974 Y975 L976 T977 I978 F979 G980 Q981 I982 P983 G984 Y985 I986 D987 G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA F1020 P1021 E1022 W1023
L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 I1045 A1046 M1047 F1048 N1049 Y1050 T1051 F1052 Q1053 Q1054 V1055 Q1056 E1057 H1058 T1059 D1060 Q1061 I1062 W1063 K1064 F1065 Q1066 R1067 H1068 D1069 L1070 I1071 E1072 E1073 Y1074 H1075 G1076 R1077 P1078 A1079 A1080 P1081 P1082 P1083
F1084 I1085 L1086 L1087 S1088 H1089 L1090 Q1091 L1092 F1093 I1094 K1095 R1096 V1097 V1098 L1099 K1100 T1101 P1102 A1103 K1104 R1105 H1106 K1107 Q1108 L1109 K1110 N1111 K1112 L1113 E1114 K1115 N1116 E1117 E1118 A1119 A1120 L1121 L1122 S1123 W1124 E1125 I1126 Y1127 L1128 K1129 E1130 N1131 Y1132 L1133 Q1134 N1135 R1136 Q1137 F1138 Q1139 Q1140 K1141 Q1142 R1143
P1144 E1145 Q1146 K1147 I1148 E1149 D1150 I1151 S1152 N1153 K1154 V1155 D1156 A1157 M1158 V1159 D1160 L1161 L1162 D1163 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE
SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 D1236 H1239 Y1240 N1241 A1242 R1243 H1244 L1245 L1246 Y1247 P1248 N1249 C1250 P1251 V1252 T1253 R1254 F1255 P1256 V1257 P1258 N1259 E1260 K1261 V1262 P1263 W1264
E1265 T1266 E1267 F1268 L1269 I1270 Y1271 D1272 P1273 P1274 F1275 Y1276 T1277 A1278 E1279 R1280 K1281 D1282 A1283 D1287 P1288 M1289 G1290 D1291 T1292 L1293 E1294 P1295 L1296 S1297 T1298 I1299 Q1300 Y1301 N1302 V1303 V1304 D1305 G1306 L1307 R1308 D1309 R1310 R1311 S1312 F1313 H1314 G1315 P1316 Y1317 T1318 V1319 Q1320 A1321 G1322 L1323 P1324 L1325 N1326

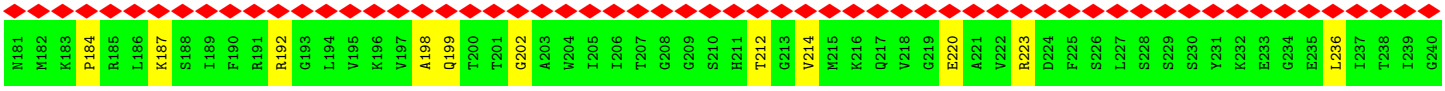


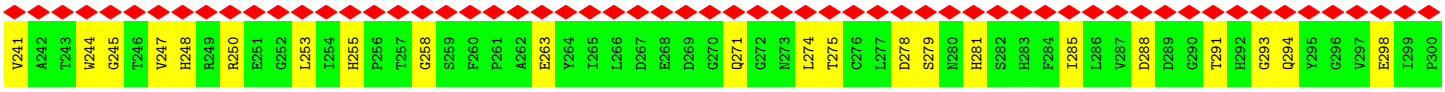
• Molecule 1: Transient receptor potential cation channel subfamily M member 2

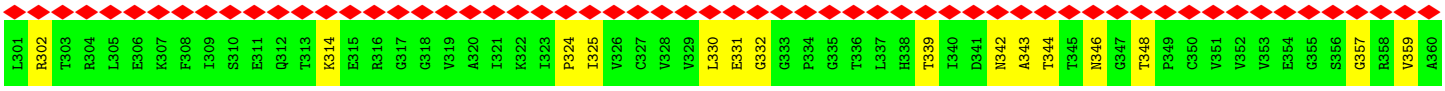
Chain B:

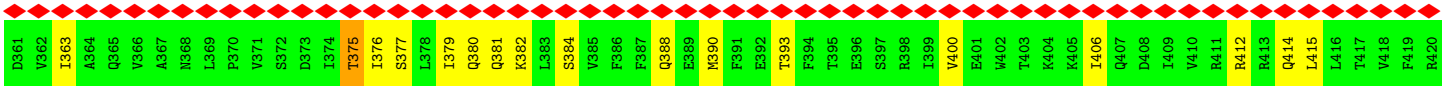


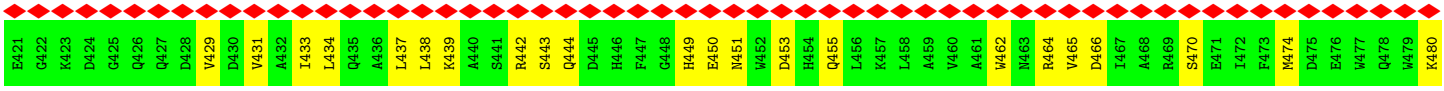


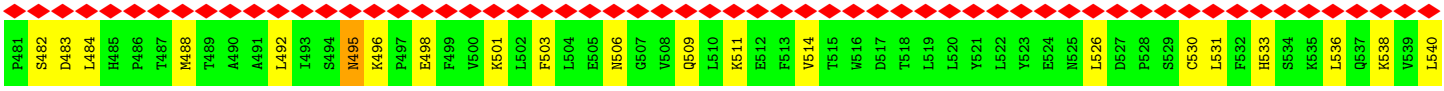


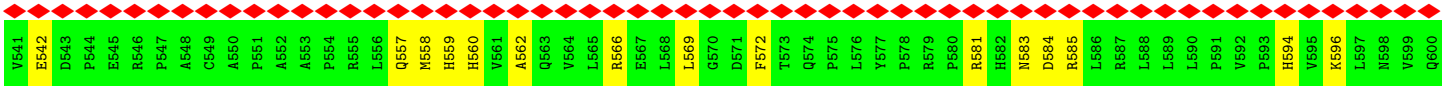


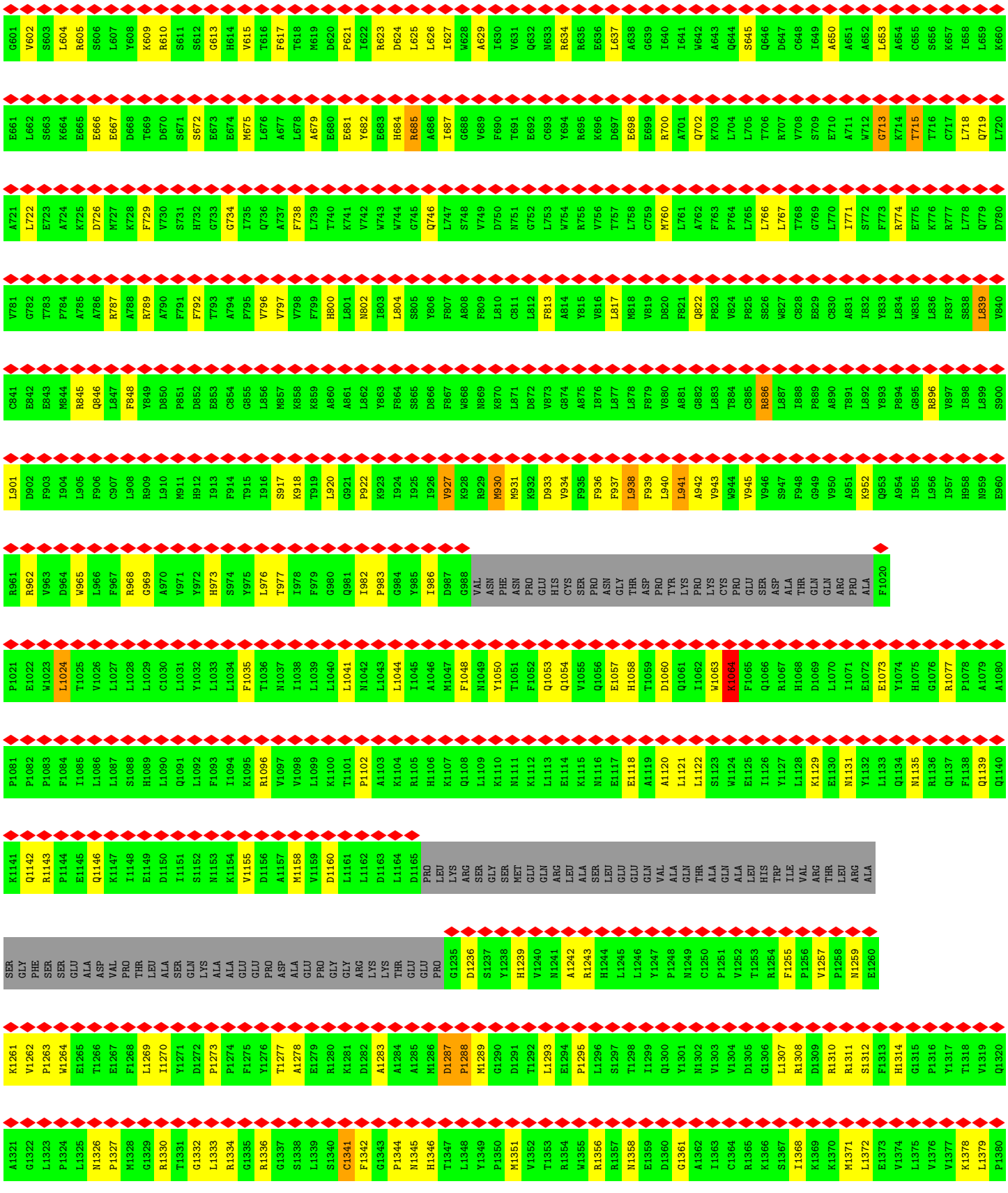








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V781 G782 T783 P784 A785 A786 R787 A788 R789 A790 F791 F792 T793 A794 P795 V796 V797 V798 F799 H800 L801 N802 I803 L804 S805 Y806 F807 A808 F809 L810 C811 L812 F813 A814 Y815 V816 L817 M818 V819 D820 F821 Q822 P823 V824 P825 S826 W827 C828 E829 C830 A831 I832 Y833 L834 W835 L836 F837 S838 L839 V840
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P1081 P1082 P1083 F1084 I1085 L1086 L1087 S1088 H1089 L1090 Q1091 L1092 F1093 I1094 K1095 R1096 V1097 V1098 L1099 K1100 T1101 P1102 A1103 K1104 R1105 H1106 K1107 Q1108 L1109 K1110 N1111 K1112 L1113 E1114 K1115 N1116 E1117 E1118 A1119 A1120 L1121 L1122 S1123 W1124 E1125 I1126 Y1127 L1128 K1129 E1130 N1131 Y1132 L1133 Q1134 N1135 R1136 Q137 F1138 Q1139 Q1140
K1141 Q1142 R1143 P1144 E1145 Q1146 K1147 I1148 E1149 D1150 I1151 S1152 N1153 K1154 V1155 D1156 A1157 M1158 V1159 D1160 L1161 L1162 D1163 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA
SER GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 D1236 S1237 Y1238 H1239 V1240 N1241 A1242 R1243 H1244 L1245 L1246 Y1247 P1248 N1249 C1250 P1251 V1252 T1253 R1254 F1255 P1256 V1257 P1258 N1259 E1260
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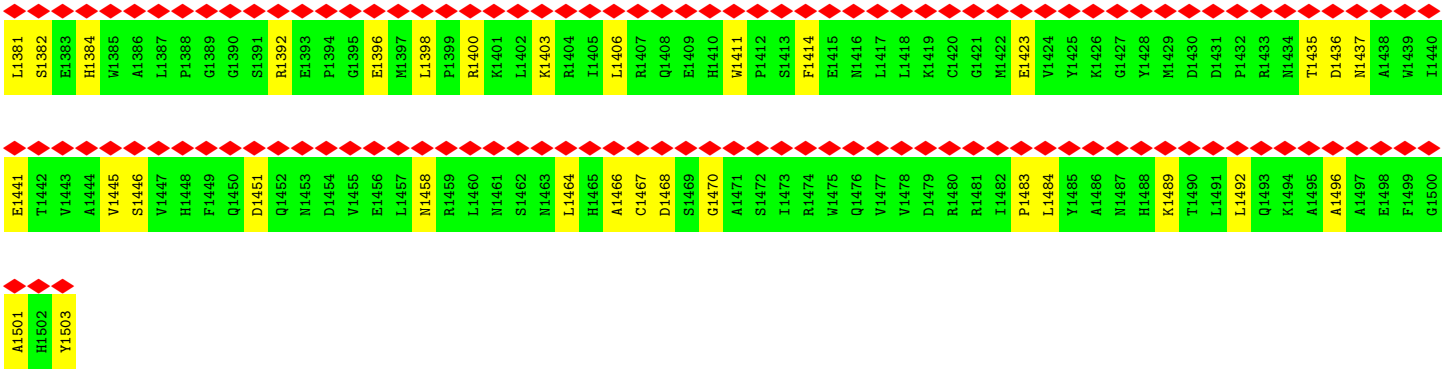
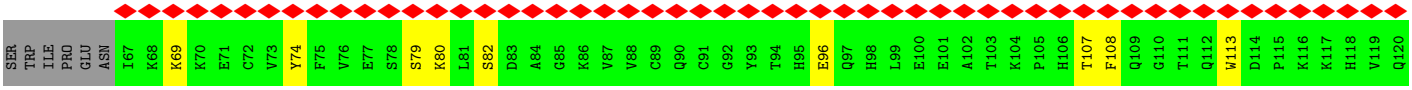
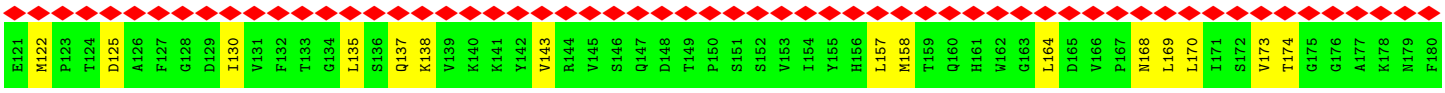
A1321 G1322 L1323 P1324 L1325 N1326 P1327 M1328 G1329 R1330 T1331 G1332 L1333 R1334 G1335 R1336 G1337 S1338 L1339 S1340 C1341 F1342 G1343 P1344 N1345 H1346 T1347 L1348 Y1349 P1350 M1351 V1352 T1353 R1354 W1355 R1356 R1357 N1358 E1359 D1360 G1361 A1362 I1363 C1364 R1365 K1366 S1367 I1368 K1369 K1370 M1371 L1372 E1373 V1374 L1375 V1376 V1377 K1378 L1379 P1380

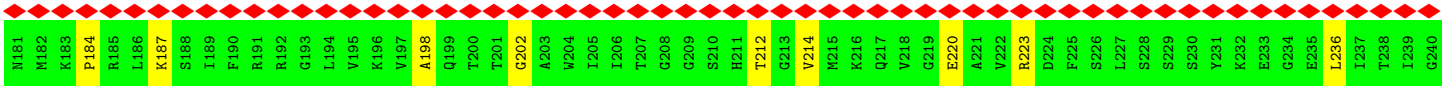


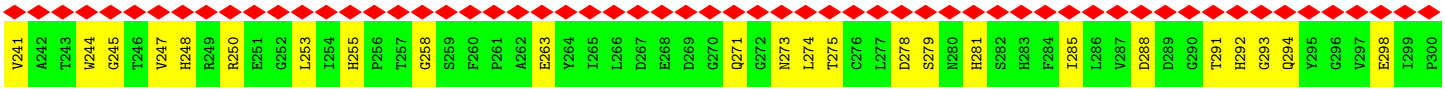
• Molecule 1: Transient receptor potential cation channel subfamily M member 2

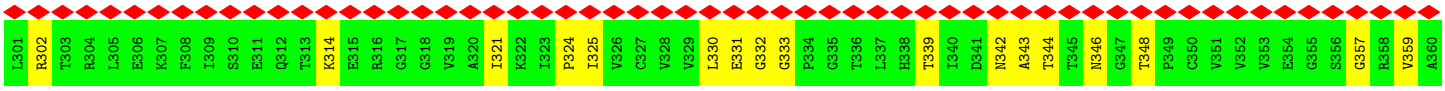
Chain C:

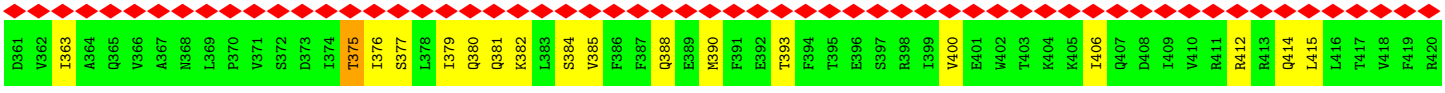


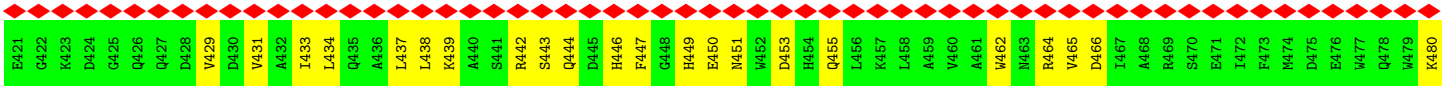


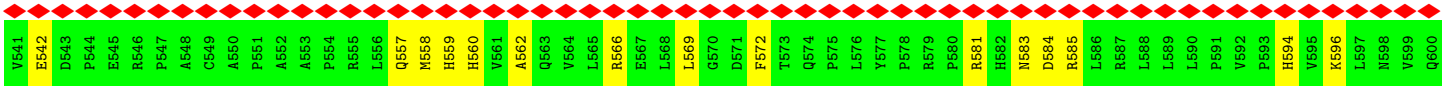


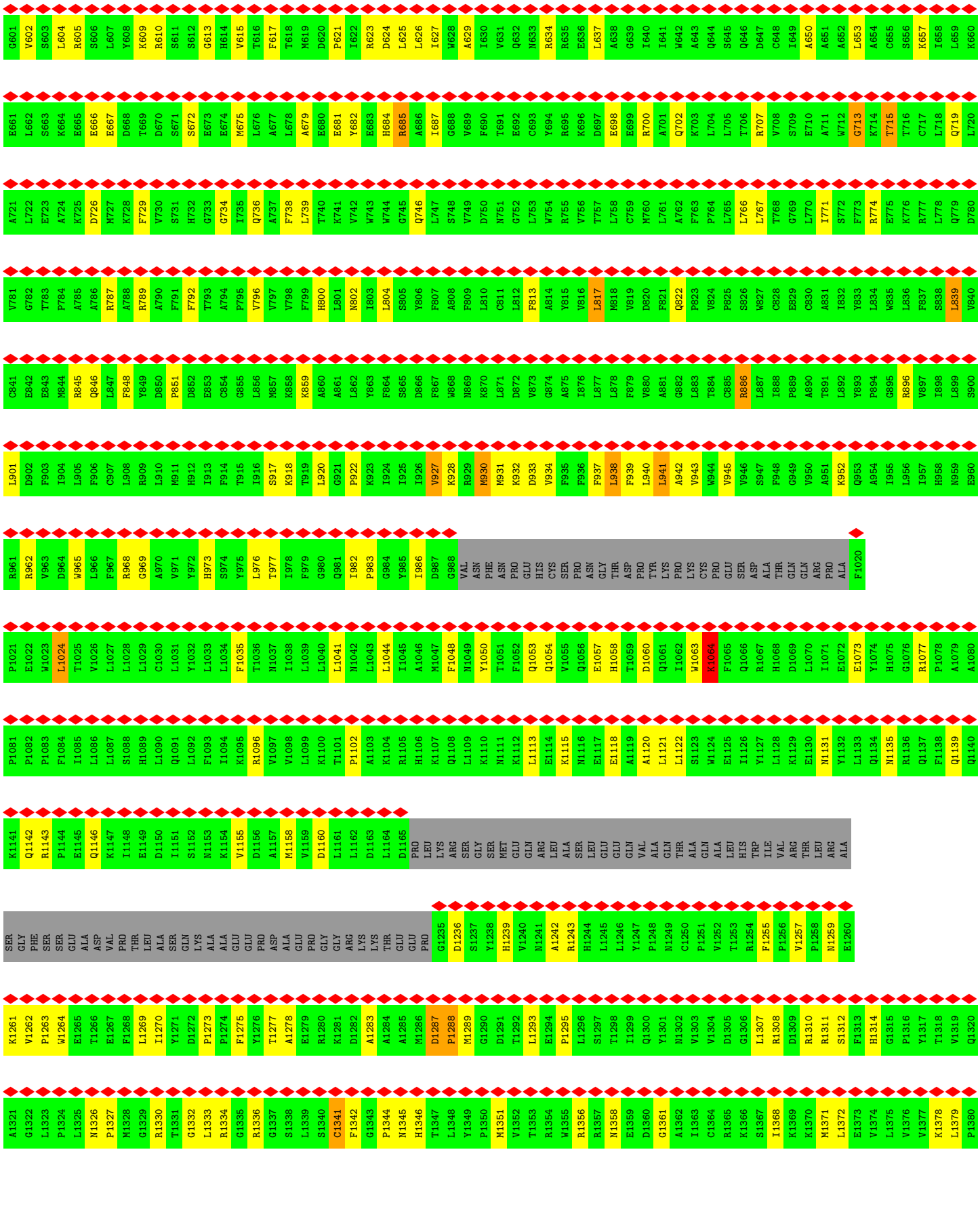








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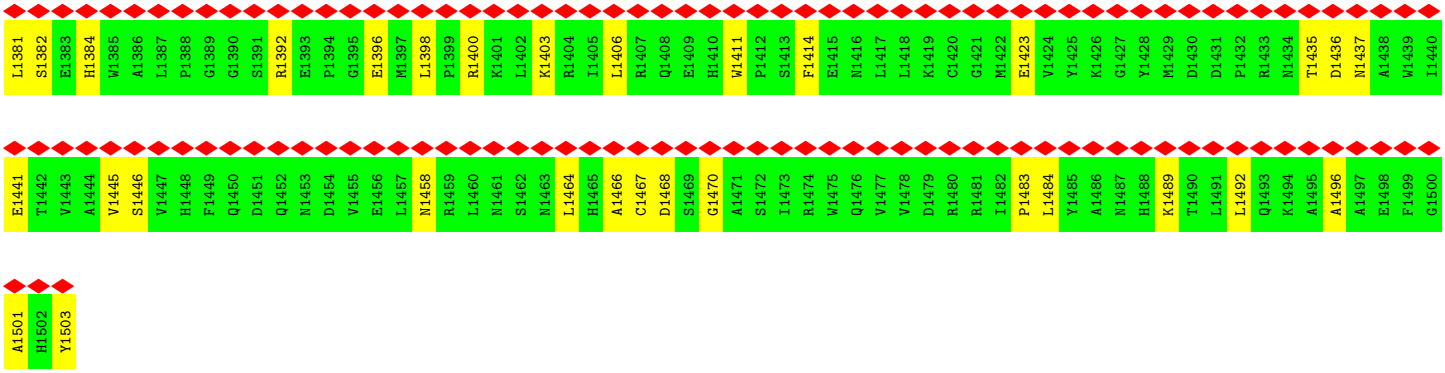
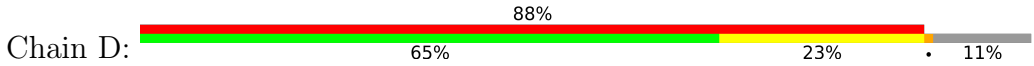
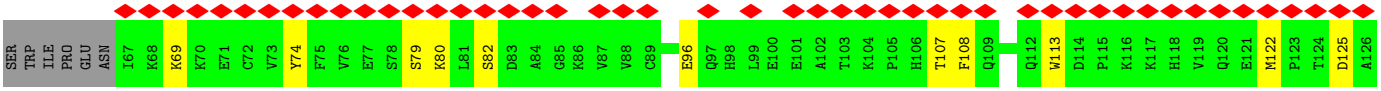
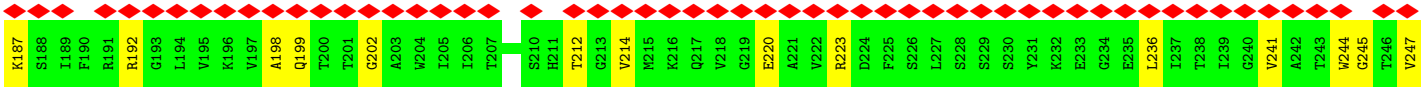
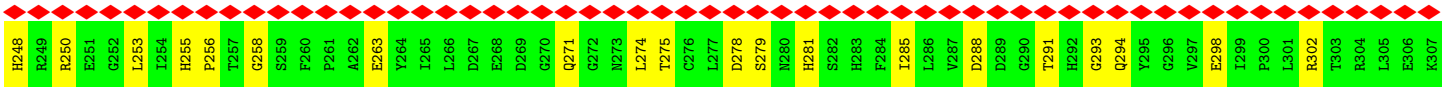


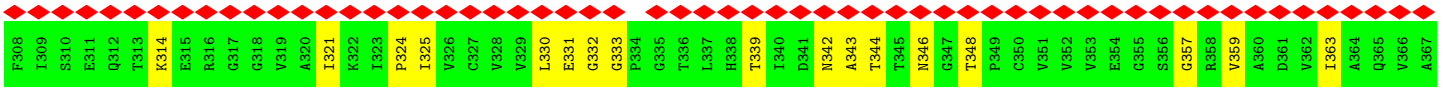
• Molecule 1: Transient receptor potential cation channel subfamily M member 2

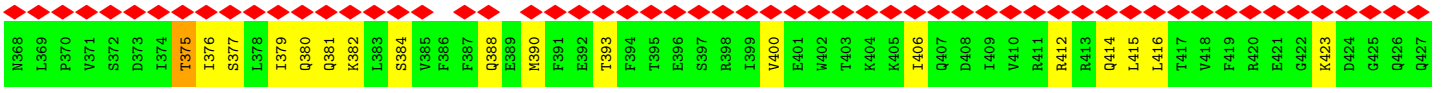


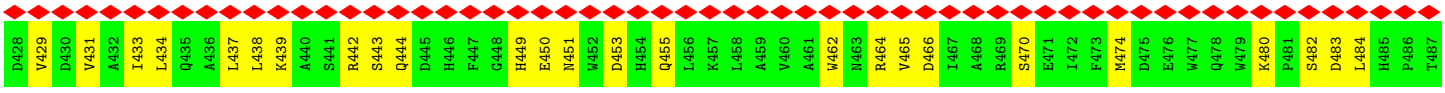


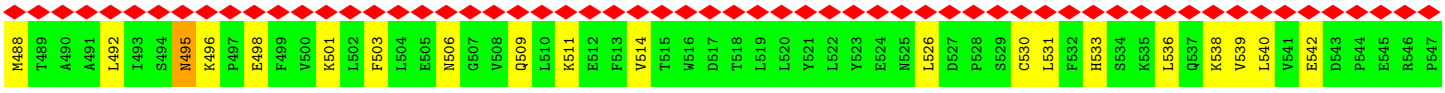


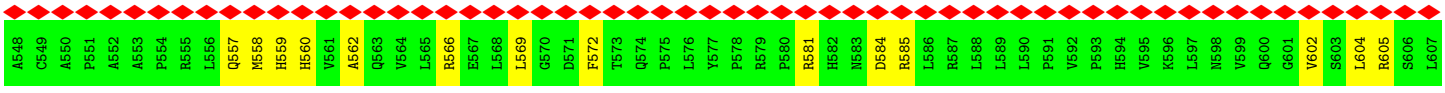


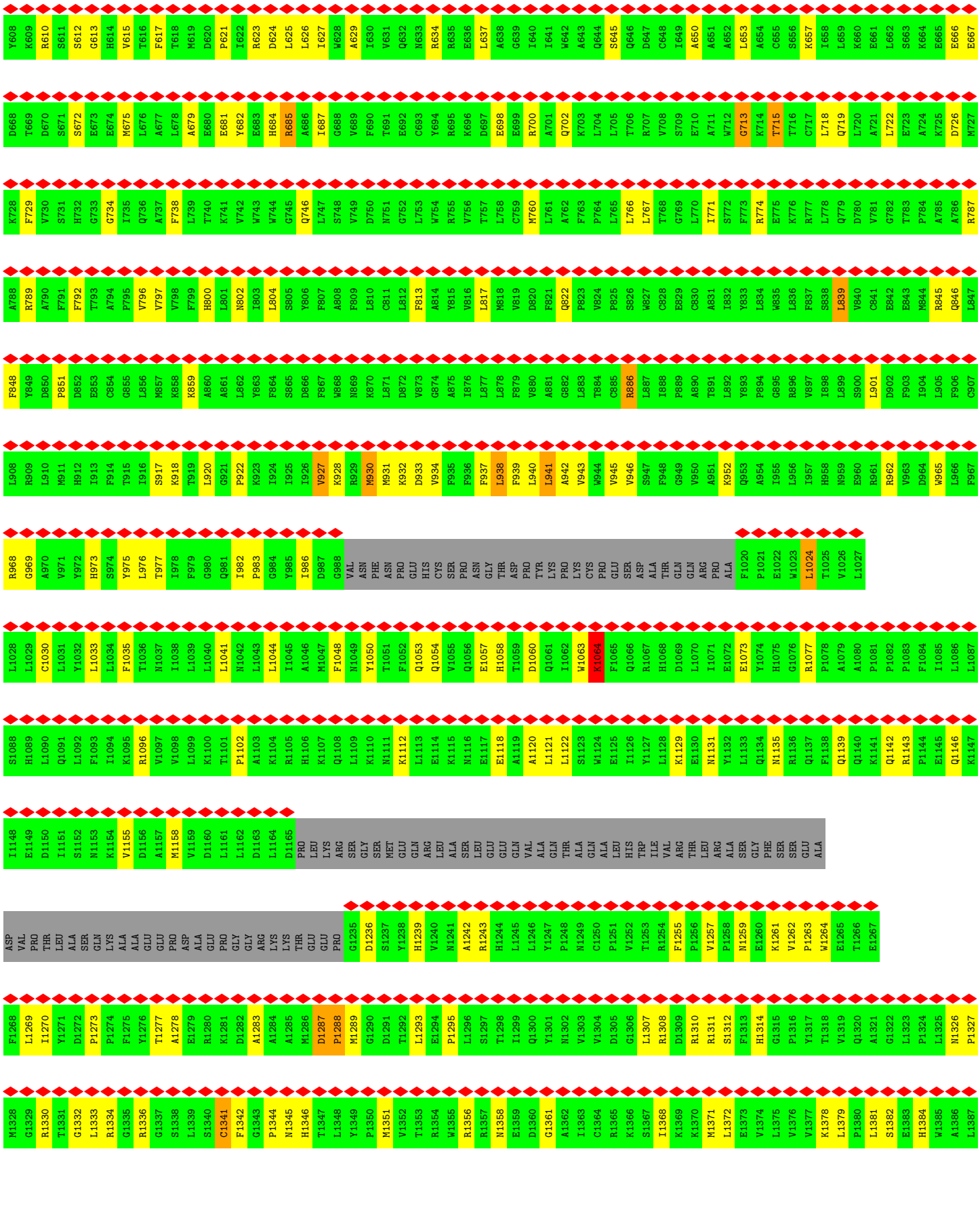








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A788 R789 A790 F791 F792 T793 A794 P795 V796 V797 V798 F799 H800 L801 N802 I803 L804 S805 Y806 F807 A808 F809 L810 C811 L812 F813 A814 Y815 V816 L817 M818 V819 D820 F821 Q822 P823 V824 P825 S826 W827 C828 E829 C830 A831 I832 Y833 L834 W835 L836 F837 S838 L839 V840 C841 E842 E843 M844 R845 Q846 L847
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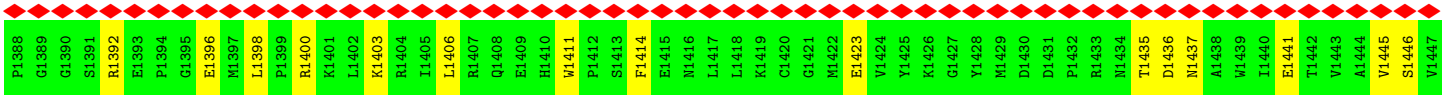
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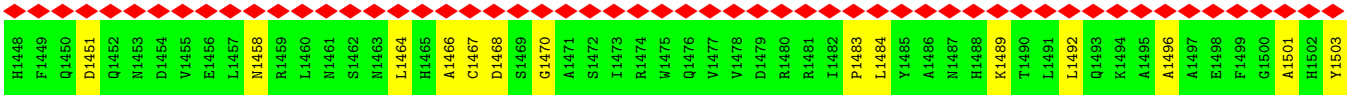
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14199	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 ($e^-/Å^2$)	70.072	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	21.981	Depositor
Minimum map value	-13.418	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.77	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.30	0/11050	0.67	19/14990 (0.1%)
1	B	0.30	0/11050	0.67	19/14990 (0.1%)
1	C	0.30	0/11050	0.67	19/14990 (0.1%)
1	D	0.30	0/11050	0.67	19/14990 (0.1%)
All	All	0.30	0/44200	0.67	76/59960 (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	13
1	B	0	13
1	C	0	13
1	D	0	13
All	All	0	52

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	933	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	D	933	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	C	933	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	933	ASP	CB-CG-OD2	-8.74	110.44	118.30
1	C	933	ASP	CB-CG-OD1	8.54	125.99	118.30
1	A	933	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	933	ASP	CB-CG-OD1	8.49	125.94	118.30
1	D	933	ASP	CB-CG-OD1	8.49	125.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	685	ARG	CD-NE-CZ	7.49	134.09	123.60
1	B	685	ARG	CD-NE-CZ	7.49	134.09	123.60
1	D	685	ARG	CD-NE-CZ	7.49	134.09	123.60
1	C	685	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	1048	PHE	CB-CG-CD2	-7.34	115.66	120.80
1	B	1048	PHE	CB-CG-CD2	-7.34	115.66	120.80
1	D	1048	PHE	CB-CG-CD2	-7.34	115.66	120.80
1	C	1048	PHE	CB-CG-CD2	-7.31	115.68	120.80
1	B	938	LEU	CB-CG-CD1	6.62	122.26	111.00
1	A	938	LEU	CB-CG-CD1	6.60	122.22	111.00
1	D	938	LEU	CB-CG-CD1	6.60	122.22	111.00
1	C	938	LEU	CB-CG-CD1	6.59	122.20	111.00
1	A	1064	LYS	CA-CB-CG	6.48	127.65	113.40
1	B	1064	LYS	CA-CB-CG	6.46	127.62	113.40
1	C	1064	LYS	CA-CB-CG	6.46	127.62	113.40
1	D	1064	LYS	CA-CB-CG	6.45	127.59	113.40
1	A	685	ARG	CG-CD-NE	6.23	124.89	111.80
1	B	685	ARG	CG-CD-NE	6.20	124.83	111.80
1	C	685	ARG	CG-CD-NE	6.20	124.82	111.80
1	D	685	ARG	CG-CD-NE	6.20	124.82	111.80
1	A	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	B	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	C	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	D	767	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	C	938	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	938	LEU	CA-CB-CG	5.99	129.07	115.30
1	D	938	LEU	CA-CB-CG	5.99	129.07	115.30
1	B	938	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	941	LEU	CB-CG-CD1	5.84	120.94	111.00
1	C	941	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	941	LEU	CB-CG-CD1	5.83	120.91	111.00
1	D	941	LEU	CB-CG-CD1	5.82	120.89	111.00
1	B	1048	PHE	CB-CG-CD1	5.73	124.81	120.80
1	C	976	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	A	976	LEU	CB-CG-CD1	-5.71	101.28	111.00
1	D	976	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	B	976	LEU	CB-CG-CD1	-5.69	101.32	111.00
1	A	1048	PHE	CB-CG-CD1	5.65	124.76	120.80
1	D	1048	PHE	CB-CG-CD1	5.65	124.76	120.80
1	C	1048	PHE	CB-CG-CD1	5.63	124.74	120.80
1	A	839	LEU	CB-CG-CD2	5.61	120.53	111.00
1	B	839	LEU	CB-CG-CD2	5.61	120.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	839	LEU	CB-CG-CD2	5.59	120.50	111.00
1	D	839	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	813	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	B	813	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	C	813	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	C	804	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	B	804	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	D	804	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	A	804	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	C	839	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	D	813	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	A	839	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	B	839	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	D	839	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	B	817	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	D	817	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	C	817	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	817	LEU	CB-CG-CD1	-5.23	102.10	111.00
1	B	976	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	976	LEU	CA-CB-CG	5.22	127.30	115.30
1	C	976	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	976	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	945	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	B	945	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	C	945	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	D	945	VAL	CG1-CB-CG2	-5.06	102.81	110.90

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	PHE	Peptide
1	A	1050	TYR	Sidechain
1	A	1287	ASP	Peptide
1	A	1341	CYS	Peptide
1	A	1368	ILE	Peptide
1	A	375	THR	Peptide
1	A	388	GLN	Peptide
1	A	495	ASN	Peptide
1	A	615	VAL	Peptide
1	A	617	PHE	Peptide
1	A	713	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	82	SER	Peptide
1	A	927	VAL	Peptide
1	B	1035	PHE	Peptide
1	B	1050	TYR	Sidechain
1	B	1287	ASP	Peptide
1	B	1341	CYS	Peptide
1	B	1368	ILE	Peptide
1	B	375	THR	Peptide
1	B	388	GLN	Peptide
1	B	495	ASN	Peptide
1	B	615	VAL	Peptide
1	B	617	PHE	Peptide
1	B	713	GLY	Peptide
1	B	82	SER	Peptide
1	B	927	VAL	Peptide
1	C	1035	PHE	Peptide
1	C	1050	TYR	Sidechain
1	C	1287	ASP	Peptide
1	C	1341	CYS	Peptide
1	C	1368	ILE	Peptide
1	C	375	THR	Peptide
1	C	388	GLN	Peptide
1	C	495	ASN	Peptide
1	C	615	VAL	Peptide
1	C	617	PHE	Peptide
1	C	713	GLY	Peptide
1	C	82	SER	Peptide
1	C	927	VAL	Peptide
1	D	1035	PHE	Peptide
1	D	1050	TYR	Sidechain
1	D	1287	ASP	Peptide
1	D	1341	CYS	Peptide
1	D	1368	ILE	Peptide
1	D	375	THR	Peptide
1	D	388	GLN	Peptide
1	D	495	ASN	Peptide
1	D	615	VAL	Peptide
1	D	617	PHE	Peptide
1	D	713	GLY	Peptide
1	D	82	SER	Peptide
1	D	927	VAL	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	212	0
1	B	10780	0	10822	209	0
1	C	10780	0	10822	215	0
1	D	10780	0	10822	215	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	43124	0	43288	843	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 (843) 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:569:LEU:HD13	1:A:572:PHE:HB2	1.76	0.68
1:D:569:LEU:HD13	1:D:572:PHE:HB2	1.77	0.67
1:B:569:LEU:HD13	1:B:572:PHE:HB2	1.76	0.67
1:C:569:LEU:HD13	1:C:572:PHE:HB2	1.76	0.66
1:B:962:ARG:H	1:B:965:TRP:HB2	1.60	0.66
1:D:962:ARG:H	1:D:965:TRP:HB2	1.60	0.66
1:A:962:ARG:H	1:A:965:TRP:HB2	1.60	0.66
1:D:602:VAL:HG23	1:D:604:LEU:H	1.61	0.66
1:C:1356:ARG:NH1	1:C:1371:MET:SD	2.69	0.65
1:C:962:ARG:H	1:C:965:TRP:HB2	1.60	0.65
1:D:1356:ARG:NH1	1:D:1371:MET:SD	2.69	0.65
1:A:602:VAL:HG23	1:A:604:LEU:H	1.61	0.65
1:A:1356:ARG:NH1	1:A:1371:MET:SD	2.69	0.65
1:B:1356:ARG:NH1	1:B:1371:MET:SD	2.69	0.65
1:C:602:VAL:HG23	1:C:604:LEU:H	1.61	0.65
1:C:713:GLY:O	1:C:715:THR:OG1	2.16	0.64
1:B:602:VAL:HG23	1:B:604:LEU:H	1.61	0.64
1:D:713:GLY:O	1:D:715:THR:OG1	2.16	0.63
1:A:746:GLN:HE22	1:A:774:ARG:HH11	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:HB2	1:B:113:TRP:HB2	1.82	0.61
1:A:713:GLY:O	1:A:715:THR:OG1	2.16	0.61
1:D:746:GLN:HE22	1:D:774:ARG:HH11	1.48	0.61
1:A:79:SER:HB2	1:A:113:TRP:HB2	1.82	0.61
1:A:174:THR:HG21	1:A:339:THR:HG21	1.83	0.61
1:A:1288:PRO:HA	1:A:1308:ARG:HH21	1.66	0.61
1:C:79:SER:HB2	1:C:113:TRP:HB2	1.82	0.61
1:B:713:GLY:O	1:B:715:THR:OG1	2.16	0.60
1:D:79:SER:HB2	1:D:113:TRP:HB2	1.82	0.60
1:D:174:THR:HG21	1:D:339:THR:HG21	1.83	0.60
1:D:1288:PRO:HA	1:D:1308:ARG:HH21	1.66	0.60
1:B:581:ARG:HA	1:B:584:ASP:HB2	1.84	0.60
1:C:581:ARG:HA	1:C:584:ASP:HB2	1.84	0.60
1:B:174:THR:HG21	1:B:339:THR:HG21	1.83	0.60
1:B:1288:PRO:HA	1:B:1308:ARG:HH21	1.66	0.60
1:C:174:THR:HG21	1:C:339:THR:HG21	1.83	0.60
1:A:581:ARG:HA	1:A:584:ASP:HB2	1.84	0.59
1:B:480:LYS:HB3	1:B:482:SER:H	1.67	0.59
1:D:480:LYS:HB3	1:D:482:SER:H	1.68	0.59
1:B:746:GLN:HE22	1:B:774:ARG:HH11	1.48	0.59
1:C:746:GLN:HE22	1:C:774:ARG:HH11	1.48	0.59
1:B:624:ASP:HA	1:B:627:ILE:HD12	1.85	0.59
1:C:624:ASP:HA	1:C:627:ILE:HD12	1.85	0.59
1:C:1288:PRO:HA	1:C:1308:ARG:HH21	1.66	0.59
1:A:480:LYS:HB3	1:A:482:SER:H	1.68	0.59
1:B:434:LEU:HD12	1:B:462:TRP:HZ2	1.68	0.59
1:C:845:ARG:HH12	1:C:1077:ARG:HG2	1.68	0.59
1:D:581:ARG:HA	1:D:584:ASP:HB2	1.84	0.59
1:D:434:LEU:HD12	1:D:462:TRP:HZ2	1.67	0.59
1:D:845:ARG:HH12	1:D:1077:ARG:HG2	1.68	0.59
1:A:449:HIS:CE1	1:A:453:ASP:HB2	2.38	0.59
1:C:509:GLN:HE21	1:C:511:LYS:H	1.51	0.59
1:D:511:LYS:HZ2	1:D:621:PRO:HD2	1.66	0.59
1:A:624:ASP:HA	1:A:627:ILE:HD12	1.85	0.59
1:A:845:ARG:HH12	1:A:1077:ARG:HG2	1.68	0.59
1:C:449:HIS:CE1	1:C:453:ASP:HB2	2.38	0.59
1:C:480:LYS:HB3	1:C:482:SER:H	1.68	0.59
1:B:449:HIS:CE1	1:B:453:ASP:HB2	2.38	0.58
1:C:434:LEU:HD12	1:C:462:TRP:HZ2	1.68	0.58
1:D:624:ASP:HA	1:D:627:ILE:HD12	1.85	0.58
1:A:434:LEU:HD12	1:A:462:TRP:HZ2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:ARG:HH12	1:B:1077:ARG:HG2	1.68	0.58
1:B:509:GLN:HE21	1:B:511:LYS:H	1.51	0.58
1:D:509:GLN:HE21	1:D:511:LYS:H	1.51	0.58
1:A:511:LYS:HZ2	1:A:621:PRO:HD2	1.68	0.58
1:C:1139:GLN:HA	1:C:1142:GLN:HB2	1.86	0.58
1:D:1139:GLN:HA	1:D:1142:GLN:HB2	1.86	0.58
1:D:449:HIS:CE1	1:D:453:ASP:HB2	2.38	0.58
1:A:1139:GLN:HA	1:A:1142:GLN:HB2	1.86	0.58
1:B:1139:GLN:HA	1:B:1142:GLN:HB2	1.86	0.58
1:B:125:ASP:O	1:B:255:HIS:N	2.34	0.57
1:A:125:ASP:O	1:A:255:HIS:N	2.34	0.57
1:D:952:LYS:HZ2	1:D:982:ILE:HG23	1.69	0.57
1:C:1063:TRP:HE3	1:C:1064:LYS:HD2	1.69	0.57
1:A:509:GLN:HE21	1:A:511:LYS:H	1.51	0.57
1:D:1458:ASN:ND2	1:D:1464:LEU:O	2.38	0.57
1:C:846:GLN:NE2	1:C:1073:GLU:OE2	2.38	0.57
1:B:952:LYS:HZ2	1:B:982:ILE:HG23	1.70	0.57
1:C:137:GLN:HE21	1:C:138:LYS:NZ	2.02	0.57
1:C:511:LYS:HZ2	1:C:621:PRO:HD2	1.70	0.57
1:A:1063:TRP:HE3	1:A:1064:LYS:HD2	1.70	0.57
1:C:143:VAL:HG21	1:C:157:LEU:HD11	1.87	0.57
1:D:137:GLN:HE21	1:D:138:LYS:NZ	2.02	0.57
1:A:1458:ASN:ND2	1:A:1464:LEU:O	2.38	0.56
1:A:137:GLN:HE21	1:A:138:LYS:NZ	2.02	0.56
1:A:143:VAL:HG21	1:A:157:LEU:HD11	1.87	0.56
1:A:342:ASN:O	1:A:346:ASN:ND2	2.39	0.56
1:A:952:LYS:HZ2	1:A:982:ILE:HG23	1.71	0.56
1:B:137:GLN:HE21	1:B:138:LYS:NZ	2.02	0.56
1:D:846:GLN:NE2	1:D:1073:GLU:OE2	2.38	0.56
1:D:1255:PHE:HD2	1:D:1332:GLY:HA2	1.70	0.56
1:B:143:VAL:HG21	1:B:157:LEU:HD11	1.87	0.56
1:B:846:GLN:NE2	1:B:1073:GLU:OE2	2.38	0.56
1:C:1255:PHE:HD2	1:C:1332:GLY:HA2	1.70	0.56
1:B:342:ASN:O	1:B:346:ASN:ND2	2.39	0.56
1:B:1458:ASN:ND2	1:B:1464:LEU:O	2.38	0.56
1:C:342:ASN:O	1:C:346:ASN:ND2	2.39	0.56
1:A:846:GLN:NE2	1:A:1073:GLU:OE2	2.38	0.56
1:B:74:TYR:OH	1:B:125:ASP:OD1	2.24	0.56
1:C:952:LYS:HZ2	1:C:982:ILE:HG23	1.71	0.56
1:C:1458:ASN:ND2	1:C:1464:LEU:O	2.38	0.56
1:B:1063:TRP:HE3	1:B:1064:LYS:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASN:O	1:D:346:ASN:ND2	2.39	0.56
1:D:700:ARG:HE	1:D:1121:LEU:HD23	1.71	0.56
1:B:380:GLN:HG3	1:B:381:GLN:HE21	1.71	0.55
1:B:1239:HIS:O	1:B:1243:ARG:NE	2.39	0.55
1:D:143:VAL:HG21	1:D:157:LEU:HD11	1.87	0.55
1:D:1063:TRP:HE3	1:D:1064:LYS:HD2	1.69	0.55
1:C:380:GLN:HG3	1:C:381:GLN:HE21	1.71	0.55
1:B:1379:LEU:HD23	1:B:1381:LEU:H	1.70	0.55
1:C:1379:LEU:HD23	1:C:1381:LEU:H	1.70	0.55
1:A:1239:HIS:O	1:A:1243:ARG:NE	2.39	0.55
1:D:1392:ARG:HB2	1:D:1398:LEU:HD23	1.88	0.55
1:A:74:TYR:OH	1:A:125:ASP:OD1	2.24	0.55
1:B:1255:PHE:HD2	1:B:1332:GLY:HA2	1.70	0.55
1:C:700:ARG:HE	1:C:1121:LEU:HD23	1.71	0.55
1:D:1314:HIS:HB3	1:D:1327:PRO:HG2	1.89	0.55
1:A:1379:LEU:HD23	1:A:1381:LEU:H	1.70	0.55
1:D:1379:LEU:HD23	1:D:1381:LEU:H	1.70	0.55
1:A:700:ARG:HE	1:A:1121:LEU:HD23	1.71	0.55
1:B:700:ARG:HE	1:B:1121:LEU:HD23	1.71	0.55
1:C:1314:HIS:HB3	1:C:1327:PRO:HG2	1.89	0.55
1:A:1392:ARG:HB2	1:A:1398:LEU:HD23	1.88	0.55
1:B:1396:GLU:HB3	1:B:1400:ARG:HD2	1.89	0.55
1:C:444:GLN:O	1:C:451:ASN:ND2	2.40	0.55
1:D:241:VAL:HA	1:D:285:ILE:HB	1.89	0.55
1:B:1400:ARG:HA	1:B:1403:LYS:HB2	1.89	0.55
1:C:74:TYR:OH	1:C:125:ASP:OD1	2.24	0.55
1:A:1314:HIS:HB3	1:A:1327:PRO:HG2	1.89	0.54
1:B:511:LYS:HZ2	1:B:621:PRO:HD2	1.71	0.54
1:C:241:VAL:HA	1:C:285:ILE:HB	1.89	0.54
1:D:969:GLY:HA2	1:D:973:HIS:HD2	1.71	0.54
1:C:125:ASP:O	1:C:255:HIS:N	2.34	0.54
1:C:503:PHE:HA	1:C:506:ASN:HD22	1.72	0.54
1:B:503:PHE:HA	1:B:506:ASN:HD22	1.72	0.54
1:C:715:THR:HG22	1:C:719:GLN:HB3	1.89	0.54
1:C:969:GLY:HA2	1:C:973:HIS:HD2	1.71	0.54
1:A:514:VAL:HB	1:A:621:PRO:HB3	1.90	0.54
1:A:1255:PHE:HD2	1:A:1332:GLY:HA2	1.70	0.54
1:B:969:GLY:HA2	1:B:973:HIS:HD2	1.71	0.54
1:B:1060:ASP:OD2	1:B:1064:LYS:NZ	2.41	0.54
1:B:1063:TRP:CE3	1:B:1064:LYS:HD2	2.42	0.54
1:B:1314:HIS:HB3	1:B:1327:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1392:ARG:HB2	1:C:1398:LEU:HD23	1.88	0.54
1:D:380:GLN:HG3	1:D:381:GLN:HE21	1.71	0.54
1:A:241:VAL:HA	1:A:285:ILE:HB	1.89	0.54
1:A:969:GLY:HA2	1:A:973:HIS:HD2	1.71	0.54
1:A:1400:ARG:HA	1:A:1403:LYS:HB2	1.89	0.54
1:D:1239:HIS:O	1:D:1243:ARG:NE	2.39	0.54
1:A:715:THR:HG22	1:A:719:GLN:HB3	1.89	0.54
1:B:241:VAL:HA	1:B:285:ILE:HB	1.89	0.54
1:B:449:HIS:CE1	1:B:483:ASP:HB2	2.43	0.54
1:C:1400:ARG:HA	1:C:1403:LYS:HB2	1.89	0.54
1:D:444:GLN:O	1:D:451:ASN:ND2	2.40	0.54
1:D:514:VAL:HB	1:D:621:PRO:HB3	1.90	0.54
1:A:380:GLN:HG3	1:A:381:GLN:HE21	1.71	0.54
1:D:125:ASP:O	1:D:255:HIS:N	2.34	0.54
1:D:1396:GLU:HB3	1:D:1400:ARG:HD2	1.89	0.54
1:A:444:GLN:O	1:A:451:ASN:ND2	2.40	0.54
1:A:1396:GLU:HB3	1:A:1400:ARG:HD2	1.89	0.54
1:B:168:ASN:OD1	1:B:314:LYS:NZ	2.38	0.54
1:B:444:GLN:O	1:B:451:ASN:ND2	2.40	0.54
1:B:1392:ARG:HB2	1:B:1398:LEU:HD23	1.88	0.54
1:C:244:TRP:HB3	1:C:288:ASP:HA	1.90	0.54
1:C:1396:GLU:HB3	1:C:1400:ARG:HD2	1.89	0.54
1:D:1063:TRP:CE3	1:D:1064:LYS:HD2	2.42	0.54
1:A:503:PHE:HA	1:A:506:ASN:HD22	1.72	0.54
1:D:169:LEU:HD22	1:D:434:LEU:HD13	1.90	0.54
1:D:244:TRP:HB3	1:D:288:ASP:HA	1.90	0.54
1:D:1060:ASP:OD2	1:D:1064:LYS:NZ	2.41	0.54
1:A:414:GLN:HG3	1:A:443:SER:HB3	1.91	0.53
1:B:414:GLN:HG3	1:B:443:SER:HB3	1.91	0.53
1:C:1257:VAL:HG13	1:C:1261:LYS:HG3	1.90	0.53
1:C:1239:HIS:O	1:C:1243:ARG:NE	2.39	0.53
1:D:503:PHE:HA	1:D:506:ASN:HD22	1.72	0.53
1:D:715:THR:HG22	1:D:719:GLN:HB3	1.89	0.53
1:D:1257:VAL:HG13	1:D:1261:LYS:HG3	1.90	0.53
1:A:1060:ASP:OD2	1:A:1064:LYS:NZ	2.41	0.53
1:A:1063:TRP:CE3	1:A:1064:LYS:HD2	2.42	0.53
1:B:130:ILE:HG23	1:B:263:GLU:HA	1.90	0.53
1:C:1060:ASP:OD2	1:C:1064:LYS:NZ	2.41	0.53
1:D:168:ASN:OD1	1:D:314:LYS:NZ	2.38	0.53
1:D:449:HIS:CE1	1:D:483:ASP:HB2	2.43	0.53
1:A:343:ALA:HB1	1:A:348:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:HIS:CE1	1:A:483:ASP:HB2	2.43	0.53
1:A:1257:VAL:HG13	1:A:1261:LYS:HG3	1.90	0.53
1:A:1264:TRP:NE1	1:A:1326:ASN:O	2.42	0.53
1:B:1257:VAL:HG13	1:B:1261:LYS:HG3	1.90	0.53
1:B:1264:TRP:NE1	1:B:1326:ASN:O	2.42	0.53
1:D:414:GLN:HG3	1:D:443:SER:HB3	1.91	0.53
1:D:1400:ARG:HA	1:D:1403:LYS:HB2	1.89	0.53
1:A:379:ILE:HG23	1:A:382:LYS:HD2	1.90	0.53
1:C:169:LEU:HD22	1:C:434:LEU:HD13	1.89	0.53
1:C:449:HIS:CE1	1:C:483:ASP:HB2	2.43	0.53
1:B:169:LEU:HD22	1:B:434:LEU:HD13	1.89	0.53
1:B:1358:ASN:OD1	1:B:1361:GLY:N	2.42	0.53
1:C:414:GLN:HG3	1:C:443:SER:HB3	1.91	0.53
1:C:514:VAL:HB	1:C:621:PRO:HB3	1.90	0.53
1:C:1063:TRP:CE3	1:C:1064:LYS:HD2	2.42	0.53
1:C:1264:TRP:NE1	1:C:1326:ASN:O	2.42	0.53
1:C:400:VAL:HG11	1:C:1269:LEU:HD13	1.90	0.53
1:D:400:VAL:HG11	1:D:1269:LEU:HD13	1.90	0.53
1:A:605:ARG:HE	1:A:613:GLY:HA3	1.74	0.53
1:D:74:TYR:OH	1:D:125:ASP:OD1	2.24	0.53
1:D:1264:TRP:NE1	1:D:1326:ASN:O	2.42	0.53
1:B:715:THR:HG22	1:B:719:GLN:HB3	1.89	0.53
1:C:214:VAL:HG13	1:C:330:LEU:HD12	1.91	0.53
1:C:343:ALA:HB1	1:C:348:THR:HB	1.91	0.53
1:D:379:ILE:HG23	1:D:382:LYS:HD2	1.90	0.53
1:A:244:TRP:HB3	1:A:288:ASP:HA	1.90	0.53
1:B:796:VAL:O	1:B:800:HIS:N	2.37	0.53
1:C:130:ILE:HG23	1:C:263:GLU:HA	1.90	0.53
1:C:379:ILE:HG23	1:C:382:LYS:HD2	1.90	0.53
1:B:379:ILE:HG23	1:B:382:LYS:HD2	1.90	0.52
1:D:214:VAL:HG13	1:D:330:LEU:HD12	1.91	0.52
1:B:244:TRP:HB3	1:B:288:ASP:HA	1.90	0.52
1:C:605:ARG:HE	1:C:613:GLY:HA3	1.74	0.52
1:A:169:LEU:HD22	1:A:434:LEU:HD13	1.89	0.52
1:D:681:GLU:HA	1:D:684:HIS:HB3	1.91	0.52
1:A:324:PRO:HB2	1:A:437:LEU:HD13	1.91	0.52
1:A:400:VAL:HG11	1:A:1269:LEU:HD13	1.90	0.52
1:B:324:PRO:HB2	1:B:437:LEU:HD13	1.91	0.52
1:B:605:ARG:HE	1:B:613:GLY:HA3	1.74	0.52
1:C:324:PRO:HB2	1:C:437:LEU:HD13	1.91	0.52
1:A:681:GLU:HA	1:A:684:HIS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ILE:HG23	1:D:263:GLU:HA	1.91	0.52
1:D:343:ALA:HB1	1:D:348:THR:HB	1.91	0.52
1:D:605:ARG:HE	1:D:613:GLY:HA3	1.74	0.52
1:A:538:LYS:O	1:A:542:GLU:N	2.43	0.52
1:A:1384:HIS:HA	1:A:1483:PRO:HG2	1.92	0.52
1:B:214:VAL:HG13	1:B:330:LEU:HD12	1.91	0.52
1:B:514:VAL:HB	1:B:621:PRO:HB3	1.90	0.52
1:B:538:LYS:O	1:B:542:GLU:N	2.43	0.52
1:A:130:ILE:HG23	1:A:263:GLU:HA	1.90	0.52
1:A:1358:ASN:OD1	1:A:1361:GLY:N	2.42	0.52
1:D:324:PRO:HB2	1:D:437:LEU:HD13	1.91	0.52
1:D:538:LYS:O	1:D:542:GLU:N	2.43	0.52
1:A:244:TRP:HA	1:A:247:VAL:HG23	1.92	0.52
1:B:244:TRP:HA	1:B:247:VAL:HG23	1.92	0.52
1:B:400:VAL:HG11	1:B:1269:LEU:HD13	1.91	0.52
1:A:1131:ASN:O	1:A:1135:ASN:ND2	2.43	0.51
1:A:1341:CYS:HB3	1:A:1344:PRO:HG3	1.92	0.51
1:B:1131:ASN:O	1:B:1135:ASN:ND2	2.43	0.51
1:C:244:TRP:HA	1:C:247:VAL:HG23	1.92	0.51
1:C:1131:ASN:O	1:C:1135:ASN:ND2	2.43	0.51
1:D:244:TRP:HA	1:D:247:VAL:HG23	1.92	0.51
1:D:917:SER:HB3	1:D:920:LEU:HG	1.93	0.51
1:A:1334:ARG:O	1:A:1435:THR:OG1	2.29	0.51
1:B:1341:CYS:HB3	1:B:1344:PRO:HG3	1.93	0.51
1:C:538:LYS:O	1:C:542:GLU:N	2.43	0.51
1:A:917:SER:HB3	1:A:920:LEU:HG	1.93	0.51
1:D:1131:ASN:O	1:D:1135:ASN:ND2	2.43	0.51
1:A:214:VAL:HG13	1:A:330:LEU:HD12	1.91	0.51
1:A:331:GLU:HA	1:A:357:GLY:HA2	1.93	0.51
1:A:726:ASP:HB3	1:A:729:PHE:HB3	1.92	0.51
1:A:212:THR:HB	1:A:275:THR:HG21	1.93	0.51
1:D:1341:CYS:HB3	1:D:1344:PRO:HG3	1.92	0.51
1:A:291:THR:OG1	1:A:294:GLN:OE1	2.29	0.51
1:B:331:GLU:HA	1:B:357:GLY:HA2	1.93	0.51
1:D:331:GLU:HA	1:D:357:GLY:HA2	1.93	0.51
1:B:343:ALA:HB1	1:B:348:THR:HB	1.91	0.51
1:B:726:ASP:HB3	1:B:729:PHE:HB3	1.92	0.51
1:C:291:THR:OG1	1:C:294:GLN:OE1	2.29	0.51
1:C:1155:VAL:HA	1:C:1158:MET:HG2	1.93	0.51
1:A:822:GLN:H	1:A:886:ARG:HH22	1.59	0.51
1:D:1334:ARG:O	1:D:1435:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1384:HIS:HA	1:D:1483:PRO:HG2	1.92	0.51
1:B:291:THR:OG1	1:B:294:GLN:OE1	2.29	0.51
1:B:681:GLU:HA	1:B:684:HIS:HB3	1.91	0.51
1:B:1384:HIS:HA	1:B:1483:PRO:HG2	1.92	0.51
1:C:331:GLU:HA	1:C:357:GLY:HA2	1.93	0.51
1:C:917:SER:HB3	1:C:920:LEU:HG	1.93	0.51
1:C:1384:HIS:HA	1:C:1483:PRO:HG2	1.92	0.51
1:C:1492:LEU:HB3	1:C:1503:TYR:HE2	1.76	0.51
1:D:212:THR:HB	1:D:275:THR:HG21	1.93	0.51
1:D:1155:VAL:HA	1:D:1158:MET:HG2	1.93	0.51
1:A:531:LEU:HD22	1:A:666:GLU:HB3	1.93	0.50
1:A:796:VAL:O	1:A:800:HIS:N	2.37	0.50
1:A:1096:ARG:HH22	1:A:1102:PRO:HG3	1.77	0.50
1:B:1334:ARG:O	1:B:1435:THR:OG1	2.29	0.50
1:A:1239:HIS:HB3	1:A:1242:ALA:HB3	1.93	0.50
1:B:822:GLN:H	1:B:886:ARG:HH22	1.59	0.50
1:C:1341:CYS:HB3	1:C:1344:PRO:HG3	1.92	0.50
1:C:1358:ASN:OD1	1:C:1361:GLY:N	2.42	0.50
1:D:158:MET:HB3	1:D:164:LEU:HD12	1.93	0.50
1:B:917:SER:HB3	1:B:920:LEU:HG	1.93	0.50
1:C:531:LEU:HD22	1:C:666:GLU:HB3	1.94	0.50
1:C:1336:ARG:H	1:C:1435:THR:HG21	1.76	0.50
1:D:1358:ASN:OD1	1:D:1361:GLY:N	2.42	0.50
1:A:414:GLN:HA	1:A:439:LYS:HE2	1.93	0.50
1:B:531:LEU:HD22	1:B:666:GLU:HB3	1.94	0.50
1:C:681:GLU:HA	1:C:684:HIS:HB3	1.92	0.50
1:C:726:ASP:HB3	1:C:729:PHE:HB3	1.92	0.50
1:C:1334:ARG:O	1:C:1435:THR:OG1	2.29	0.50
1:D:291:THR:OG1	1:D:294:GLN:OE1	2.29	0.50
1:D:726:ASP:HB3	1:D:729:PHE:HB3	1.92	0.50
1:D:1096:ARG:HH22	1:D:1102:PRO:HG3	1.77	0.50
1:C:414:GLN:HA	1:C:439:LYS:HE2	1.93	0.50
1:D:822:GLN:H	1:D:886:ARG:HH22	1.59	0.50
1:A:1484:LEU:HD23	1:A:1489:LYS:HB2	1.93	0.50
1:B:158:MET:HB3	1:B:164:LEU:HD12	1.93	0.50
1:B:414:GLN:HA	1:B:439:LYS:HE2	1.93	0.50
1:B:1492:LEU:HB3	1:B:1503:TYR:HE2	1.76	0.50
1:C:1261:LYS:HE3	1:C:1269:LEU:HB2	1.94	0.50
1:B:1239:HIS:HB3	1:B:1242:ALA:HB3	1.93	0.50
1:D:414:GLN:HA	1:D:439:LYS:HE2	1.93	0.50
1:D:531:LEU:HD22	1:D:666:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:GLU:HB2	1:D:672:SER:HB3	1.94	0.50
1:D:1484:LEU:HD23	1:D:1489:LYS:HB2	1.93	0.50
1:D:1492:LEU:HB3	1:D:1503:TYR:HE2	1.76	0.50
1:B:1096:ARG:HH22	1:B:1102:PRO:HG3	1.77	0.50
1:B:1336:ARG:H	1:B:1435:THR:HG21	1.76	0.50
1:B:1155:VAL:HA	1:B:1158:MET:HG2	1.93	0.49
1:C:158:MET:HB3	1:C:164:LEU:HD12	1.93	0.49
1:D:796:VAL:O	1:D:800:HIS:N	2.37	0.49
1:A:158:MET:HB3	1:A:164:LEU:HD12	1.93	0.49
1:C:466:ASP:OD1	1:C:466:ASP:N	2.45	0.49
1:C:822:GLN:H	1:C:886:ARG:HH22	1.59	0.49
1:C:1096:ARG:HH22	1:C:1102:PRO:HG3	1.77	0.49
1:C:1239:HIS:HB3	1:C:1242:ALA:HB3	1.93	0.49
1:B:466:ASP:N	1:B:466:ASP:OD1	2.45	0.49
1:B:684:HIS:HA	1:B:687:ILE:HD12	1.95	0.49
1:D:375:THR:O	1:D:377:SER:N	2.46	0.49
1:A:375:THR:O	1:A:377:SER:N	2.46	0.49
1:C:212:THR:HB	1:C:275:THR:HG21	1.93	0.49
1:A:137:GLN:NE2	1:A:138:LYS:NZ	2.60	0.49
1:A:684:HIS:HA	1:A:687:ILE:HD12	1.95	0.49
1:A:1155:VAL:HA	1:A:1158:MET:HG2	1.93	0.49
1:B:137:GLN:NE2	1:B:138:LYS:NZ	2.60	0.49
1:B:1261:LYS:HE3	1:B:1269:LEU:HB2	1.94	0.49
1:C:375:THR:O	1:C:377:SER:N	2.46	0.49
1:A:667:GLU:HB2	1:A:672:SER:HB3	1.94	0.49
1:B:667:GLU:HB2	1:B:672:SER:HB3	1.94	0.49
1:B:1118:GLU:HB3	1:B:1122:LEU:HD23	1.94	0.49
1:D:137:GLN:NE2	1:D:138:LYS:NZ	2.60	0.49
1:D:684:HIS:HA	1:D:687:ILE:HD12	1.95	0.49
1:D:1261:LYS:HE3	1:D:1269:LEU:HB2	1.93	0.49
1:B:69:LYS:HD2	1:B:258:GLY:HA3	1.95	0.49
1:B:931:MET:HA	1:B:934:VAL:HB	1.95	0.49
1:B:1484:LEU:HD23	1:B:1489:LYS:HB2	1.93	0.49
1:C:684:HIS:HA	1:C:687:ILE:HD12	1.95	0.49
1:D:1118:GLU:HB3	1:D:1122:LEU:HD23	1.94	0.49
1:D:1239:HIS:HB3	1:D:1242:ALA:HB3	1.93	0.49
1:A:931:MET:HA	1:A:934:VAL:HB	1.95	0.49
1:C:137:GLN:NE2	1:C:138:LYS:NZ	2.60	0.49
1:C:1262:VAL:HG23	1:C:1263:PRO:HD3	1.95	0.49
1:A:1261:LYS:HE3	1:A:1269:LEU:HB2	1.93	0.49
1:B:212:THR:HB	1:B:275:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ASP:OD1	1:B:288:ASP:N	2.45	0.49
1:D:1336:ARG:H	1:D:1435:THR:HG21	1.76	0.49
1:A:466:ASP:OD1	1:A:466:ASP:N	2.45	0.48
1:B:344:THR:HB	1:B:415:LEU:HD13	1.95	0.48
1:D:1054:GLN:HB2	1:D:1058:HIS:HB2	1.95	0.48
1:D:1262:VAL:HG23	1:D:1263:PRO:HD3	1.95	0.48
1:A:1492:LEU:HB3	1:A:1503:TYR:HE2	1.76	0.48
1:C:667:GLU:HB2	1:C:672:SER:HB3	1.94	0.48
1:C:931:MET:HA	1:C:934:VAL:HB	1.95	0.48
1:A:69:LYS:HD2	1:A:258:GLY:HA3	1.95	0.48
1:C:1484:LEU:HD23	1:C:1489:LYS:HB2	1.93	0.48
1:D:344:THR:HB	1:D:415:LEU:HD13	1.95	0.48
1:D:466:ASP:N	1:D:466:ASP:OD1	2.45	0.48
1:D:931:MET:HA	1:D:934:VAL:HB	1.95	0.48
1:A:1336:ARG:H	1:A:1435:THR:HG21	1.76	0.48
1:A:484:LEU:O	1:A:488:MET:N	2.40	0.48
1:B:433:ILE:HG23	1:B:434:LEU:HG	1.96	0.48
1:B:484:LEU:O	1:B:488:MET:N	2.40	0.48
1:C:344:THR:HB	1:C:415:LEU:HD13	1.95	0.48
1:C:1054:GLN:HB2	1:C:1058:HIS:HB2	1.96	0.48
1:A:1118:GLU:HB3	1:A:1122:LEU:HD23	1.94	0.48
1:B:1351:MET:HB2	1:B:1446:SER:HA	1.96	0.48
1:C:69:LYS:HD2	1:C:258:GLY:HA3	1.95	0.48
1:A:135:LEU:HD21	1:A:279:SER:HA	1.96	0.48
1:A:168:ASN:OD1	1:A:314:LYS:NZ	2.38	0.48
1:A:344:THR:HB	1:A:415:LEU:HD13	1.95	0.48
1:A:977:THR:HB	1:A:982:ILE:HD13	1.96	0.48
1:A:1054:GLN:HB2	1:A:1058:HIS:HB2	1.96	0.48
1:B:137:GLN:NE2	1:B:138:LYS:HZ2	2.10	0.48
1:C:1118:GLU:HB3	1:C:1122:LEU:HD23	1.94	0.48
1:C:1243:ARG:NH1	1:C:1259:ASN:OD1	2.44	0.48
1:A:1262:VAL:HG23	1:A:1263:PRO:HD3	1.95	0.48
1:A:433:ILE:HG23	1:A:434:LEU:HG	1.96	0.48
1:C:796:VAL:O	1:C:800:HIS:N	2.37	0.48
1:D:137:GLN:NE2	1:D:138:LYS:HZ2	2.12	0.48
1:B:1054:GLN:HB2	1:B:1058:HIS:HB2	1.96	0.47
1:B:1143:ARG:HG2	1:B:1146:GLN:H	1.79	0.47
1:B:1262:VAL:HG23	1:B:1263:PRO:HD3	1.95	0.47
1:B:1310:ARG:NH1	1:B:1342:PHE:O	2.47	0.47
1:B:1403:LYS:HA	1:B:1406:LEU:HB2	1.96	0.47
1:B:363:ILE:HG23	1:B:406:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:THR:HB	1:B:982:ILE:HD13	1.96	0.47
1:D:1351:MET:HB2	1:D:1446:SER:HA	1.96	0.47
1:C:168:ASN:OD1	1:C:314:LYS:NZ	2.38	0.47
1:C:1236:ASP:O	1:C:1243:ARG:NH2	2.46	0.47
1:D:69:LYS:HD2	1:D:258:GLY:HA3	1.95	0.47
1:D:135:LEU:HD21	1:D:279:SER:HA	1.96	0.47
1:A:1403:LYS:HA	1:A:1406:LEU:HB2	1.97	0.47
1:B:375:THR:O	1:B:377:SER:N	2.46	0.47
1:D:1310:ARG:NH1	1:D:1342:PHE:O	2.47	0.47
1:A:558:MET:HB3	1:A:585:ARG:HG2	1.96	0.47
1:A:1310:ARG:NH1	1:A:1342:PHE:O	2.47	0.47
1:A:1351:MET:HB2	1:A:1446:SER:HA	1.96	0.47
1:B:135:LEU:HD21	1:B:279:SER:HA	1.96	0.47
1:B:170:LEU:HB2	1:B:325:ILE:HG13	1.97	0.47
1:C:135:LEU:HD21	1:C:279:SER:HA	1.96	0.47
1:C:433:ILE:HG23	1:C:434:LEU:HG	1.96	0.47
1:C:558:MET:HB3	1:C:585:ARG:HG2	1.96	0.47
1:C:1143:ARG:HG2	1:C:1146:GLN:H	1.79	0.47
1:C:1351:MET:HB2	1:C:1446:SER:HA	1.96	0.47
1:D:170:LEU:HB2	1:D:325:ILE:HG13	1.96	0.47
1:D:433:ILE:HG23	1:D:434:LEU:HG	1.96	0.47
1:A:170:LEU:HB2	1:A:325:ILE:HG13	1.97	0.47
1:B:927:VAL:HA	1:B:930:MET:HB2	1.97	0.47
1:C:977:THR:HB	1:C:982:ILE:HD13	1.96	0.47
1:C:1311:ARG:O	1:C:1346:HIS:ND1	2.48	0.47
1:B:558:MET:HB3	1:B:585:ARG:HG2	1.96	0.47
1:C:802:ASN:OD1	1:C:1077:ARG:NH1	2.48	0.47
1:D:558:MET:HB3	1:D:585:ARG:HG2	1.96	0.47
1:A:623:ARG:HA	1:A:626:LEU:HD12	1.97	0.47
1:A:1053:GLN:NE2	1:B:1057:GLU:OE2	2.48	0.47
1:C:363:ILE:HG23	1:C:406:ILE:HG23	1.97	0.47
1:D:977:THR:HB	1:D:982:ILE:HD13	1.96	0.47
1:A:802:ASN:OD1	1:A:1077:ARG:NH1	2.48	0.46
1:B:623:ARG:HA	1:B:626:LEU:HD12	1.97	0.46
1:B:802:ASN:OD1	1:B:1077:ARG:NH1	2.48	0.46
1:C:1310:ARG:NH1	1:C:1342:PHE:O	2.47	0.46
1:A:1057:GLU:OE2	1:D:1053:GLN:NE2	2.48	0.46
1:B:645:SER:O	1:B:1129:LYS:NZ	2.40	0.46
1:C:623:ARG:HA	1:C:626:LEU:HD12	1.97	0.46
1:D:623:ARG:HA	1:D:626:LEU:HD12	1.97	0.46
1:C:1053:GLN:NE2	1:D:1057:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1403:LYS:HA	1:C:1406:LEU:HB2	1.97	0.46
1:C:170:LEU:HB2	1:C:325:ILE:HG13	1.96	0.46
1:C:634:ARG:HB3	1:C:637:LEU:HD13	1.97	0.46
1:D:734:GLY:O	1:D:738:PHE:N	2.49	0.46
1:D:802:ASN:OD1	1:D:1077:ARG:NH1	2.48	0.46
1:D:1143:ARG:HG2	1:D:1146:GLN:H	1.79	0.46
1:A:332:GLY:HA2	1:A:333:GLY:HA3	1.72	0.46
1:B:917:SER:H	1:B:920:LEU:HD12	1.80	0.46
1:C:917:SER:H	1:C:920:LEU:HD12	1.80	0.46
1:C:927:VAL:HA	1:C:930:MET:HB2	1.97	0.46
1:A:137:GLN:NE2	1:A:138:LYS:HZ2	2.13	0.46
1:A:927:VAL:HA	1:A:930:MET:HB2	1.97	0.46
1:D:173:VAL:O	1:D:302:ARG:NH2	2.46	0.46
1:D:934:VAL:HG12	1:D:938:LEU:HD12	1.98	0.46
1:B:1243:ARG:NH1	1:B:1259:ASN:OD1	2.44	0.46
1:D:484:LEU:O	1:D:488:MET:N	2.40	0.46
1:A:1143:ARG:HG2	1:A:1146:GLN:H	1.79	0.46
1:C:274:LEU:HD21	1:C:293:GLY:HA2	1.98	0.46
1:C:734:GLY:O	1:C:738:PHE:N	2.49	0.46
1:D:363:ILE:HG23	1:D:406:ILE:HG23	1.97	0.46
1:D:1236:ASP:O	1:D:1243:ARG:NH2	2.46	0.46
1:B:634:ARG:HB3	1:B:637:LEU:HD13	1.97	0.46
1:B:934:VAL:HG12	1:B:938:LEU:HD12	1.98	0.46
1:D:1403:LYS:HA	1:D:1406:LEU:HB2	1.96	0.46
1:A:734:GLY:O	1:A:738:PHE:N	2.49	0.45
1:B:557:GLN:HB2	1:B:560:HIS:HD2	1.81	0.45
1:C:1024:LEU:HD21	1:D:901:LEU:HD11	1.98	0.45
1:A:198:ALA:HA	1:A:202:GLY:H	1.81	0.45
1:C:332:GLY:HA3	1:C:359:VAL:HB	1.99	0.45
1:C:939:PHE:HA	1:C:942:ALA:HB3	1.98	0.45
1:D:332:GLY:HA2	1:D:333:GLY:HA3	1.72	0.45
1:A:557:GLN:HB2	1:A:560:HIS:HD2	1.81	0.45
1:A:789:ARG:HA	1:A:792:PHE:HD2	1.82	0.45
1:C:291:THR:HG1	1:C:292:HIS:H	1.65	0.45
1:D:274:LEU:HD21	1:D:293:GLY:HA2	1.98	0.45
1:D:927:VAL:HA	1:D:930:MET:HB2	1.97	0.45
1:D:1330:ARG:HG3	1:D:1436:ASP:HB3	1.98	0.45
1:A:634:ARG:HB3	1:A:637:LEU:HD13	1.97	0.45
1:A:917:SER:H	1:A:920:LEU:HD12	1.80	0.45
1:B:734:GLY:O	1:B:738:PHE:N	2.49	0.45
1:B:1435:THR:HG23	1:B:1437:ASN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:PRO:HA	1:D:187:LYS:HD2	1.99	0.45
1:D:332:GLY:HA3	1:D:359:VAL:HB	1.99	0.45
1:D:917:SER:H	1:D:920:LEU:HD12	1.80	0.45
1:A:332:GLY:HA3	1:A:359:VAL:HB	1.99	0.45
1:A:363:ILE:HG23	1:A:406:ILE:HG23	1.96	0.45
1:A:934:VAL:HG12	1:A:938:LEU:HD12	1.98	0.45
1:A:1236:ASP:O	1:A:1243:ARG:NH2	2.46	0.45
1:A:1435:THR:HG23	1:A:1437:ASN:H	1.82	0.45
1:B:184:PRO:HA	1:B:187:LYS:HD2	1.99	0.45
1:B:332:GLY:HA3	1:B:359:VAL:HB	1.99	0.45
1:C:80:LYS:HD3	1:C:96:GLU:HG3	1.99	0.45
1:C:198:ALA:HA	1:C:202:GLY:H	1.81	0.45
1:C:1435:THR:HG23	1:C:1437:ASN:H	1.82	0.45
1:A:438:LEU:O	1:A:442:ARG:NH1	2.50	0.45
1:A:901:LEU:HD11	1:D:1024:LEU:HD21	1.97	0.45
1:A:939:PHE:HA	1:A:942:ALA:HB3	1.98	0.45
1:B:939:PHE:HA	1:B:942:ALA:HB3	1.98	0.45
1:C:438:LEU:O	1:C:442:ARG:NH1	2.50	0.45
1:D:80:LYS:HD3	1:D:96:GLU:HG3	1.99	0.45
1:D:634:ARG:HB3	1:D:637:LEU:HD13	1.97	0.45
1:B:526:LEU:HB3	1:B:533:HIS:HB2	1.99	0.45
1:B:1311:ARG:O	1:B:1346:HIS:ND1	2.48	0.45
1:C:509:GLN:HG3	1:C:511:LYS:HB2	1.99	0.45
1:D:198:ALA:HA	1:D:202:GLY:H	1.81	0.45
1:D:946:VAL:O	1:D:975:TYR:OH	2.29	0.45
1:A:946:VAL:O	1:A:975:TYR:OH	2.29	0.45
1:C:184:PRO:HA	1:C:187:LYS:HD2	1.99	0.45
1:A:1243:ARG:NH1	1:A:1259:ASN:OD1	2.44	0.45
1:A:1278:ALA:HB2	1:A:1283:ALA:HA	1.99	0.45
1:B:278:ASP:HB3	1:B:281:HIS:CD2	2.52	0.45
1:C:557:GLN:HB2	1:C:560:HIS:HD2	1.81	0.45
1:D:939:PHE:HA	1:D:942:ALA:HB3	1.98	0.45
1:A:1311:ARG:O	1:A:1346:HIS:ND1	2.48	0.44
1:C:789:ARG:HA	1:C:792:PHE:HD2	1.82	0.44
1:C:1293:LEU:HG	1:C:1295:PRO:HD2	2.00	0.44
1:D:698:GLU:O	1:D:702:GLN:N	2.49	0.44
1:A:1345:ASN:HB2	1:A:1441:GLU:H	1.83	0.44
1:C:1330:ARG:HG3	1:C:1436:ASP:HB3	1.98	0.44
1:D:438:LEU:O	1:D:442:ARG:NH1	2.50	0.44
1:A:278:ASP:HB3	1:A:281:HIS:CD2	2.52	0.44
1:B:274:LEU:HD21	1:B:293:GLY:HA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1278:ALA:HB2	1:B:1283:ALA:HA	1.99	0.44
1:B:1372:LEU:HG	1:B:1501:ALA:HB2	1.99	0.44
1:C:1345:ASN:HB2	1:C:1441:GLU:H	1.83	0.44
1:D:536:LEU:O	1:D:540:LEU:N	2.46	0.44
1:D:557:GLN:HB2	1:D:560:HIS:HD2	1.81	0.44
1:D:789:ARG:HA	1:D:792:PHE:HD2	1.82	0.44
1:D:1293:LEU:HG	1:D:1295:PRO:HD2	2.00	0.44
1:D:1435:THR:HG23	1:D:1437:ASN:H	1.82	0.44
1:A:74:TYR:HB2	1:A:122:MET:H	1.83	0.44
1:B:74:TYR:HB2	1:B:122:MET:H	1.83	0.44
1:B:1053:GLN:NE2	1:C:1057:GLU:OE2	2.50	0.44
1:B:1345:ASN:HB2	1:B:1441:GLU:H	1.83	0.44
1:C:698:GLU:O	1:C:702:GLN:N	2.49	0.44
1:C:928:LYS:HD2	1:C:928:LYS:HA	1.83	0.44
1:C:932:LYS:HA	1:C:932:LYS:HD2	1.84	0.44
1:C:934:VAL:HG12	1:C:938:LEU:HD12	1.98	0.44
1:D:278:ASP:HB3	1:D:281:HIS:CD2	2.52	0.44
1:D:1278:ALA:HB2	1:D:1283:ALA:HA	1.99	0.44
1:D:1372:LEU:HG	1:D:1501:ALA:HB2	1.99	0.44
1:A:449:HIS:NE2	1:A:483:ASP:HB2	2.33	0.44
1:A:698:GLU:O	1:A:702:GLN:N	2.49	0.44
1:B:198:ALA:HA	1:B:202:GLY:H	1.81	0.44
1:B:789:ARG:HA	1:B:792:PHE:HD2	1.82	0.44
1:C:449:HIS:NE2	1:C:483:ASP:HB2	2.33	0.44
1:C:1160:ASP:OD1	1:C:1160:ASP:N	2.50	0.44
1:D:509:GLN:HG3	1:D:511:LYS:HB2	1.99	0.44
1:A:184:PRO:HA	1:A:187:LYS:HD2	1.99	0.44
1:A:274:LEU:HD21	1:A:293:GLY:HA2	1.98	0.44
1:B:449:HIS:NE2	1:B:483:ASP:HB2	2.33	0.44
1:B:1330:ARG:HG3	1:B:1436:ASP:HB3	1.98	0.44
1:D:1273:PRO:HD2	1:D:1333:LEU:HB2	2.00	0.44
1:A:450:GLU:HA	1:A:453:ASP:HB3	2.00	0.44
1:B:438:LEU:O	1:B:442:ARG:NH1	2.50	0.44
1:C:1411:TRP:NE1	1:C:1414:PHE:O	2.51	0.44
1:D:449:HIS:NE2	1:D:483:ASP:HB2	2.33	0.44
1:A:1273:PRO:HD2	1:A:1333:LEU:HB2	2.00	0.44
1:B:450:GLU:HA	1:B:453:ASP:HB3	2.00	0.44
1:B:1423:GLU:HA	1:B:1445:VAL:HA	2.00	0.44
1:C:450:GLU:HA	1:C:453:ASP:HB3	2.00	0.44
1:D:450:GLU:HA	1:D:453:ASP:HB3	2.00	0.44
1:D:1243:ARG:NH1	1:D:1259:ASN:OD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1311:ARG:O	1:D:1346:HIS:ND1	2.48	0.44
1:D:1345:ASN:HB2	1:D:1441:GLU:H	1.83	0.44
1:A:363:ILE:HG12	1:A:406:ILE:HG12	2.00	0.44
1:B:509:GLN:HG3	1:B:511:LYS:HB2	1.99	0.44
1:C:220:GLU:HG3	1:C:223:ARG:HH21	1.83	0.44
1:C:278:ASP:HB3	1:C:281:HIS:CD2	2.52	0.44
1:C:332:GLY:HA2	1:C:333:GLY:HA3	1.72	0.44
1:C:609:LYS:HA	1:C:609:LYS:HD3	1.75	0.44
1:C:1273:PRO:HD2	1:C:1333:LEU:HB2	2.00	0.44
1:D:248:HIS:HB2	1:D:271:GLN:HB2	2.00	0.44
1:D:1041:LEU:HG	1:D:1044:LEU:HD22	2.00	0.44
1:A:1160:ASP:OD1	1:A:1160:ASP:N	2.50	0.43
1:B:609:LYS:HA	1:B:609:LYS:HD3	1.75	0.43
1:B:698:GLU:O	1:B:702:GLN:N	2.49	0.43
1:B:1293:LEU:HG	1:B:1295:PRO:HD2	2.00	0.43
1:A:465:VAL:HG21	1:A:498:GLU:HB2	2.01	0.43
1:A:1330:ARG:HG3	1:A:1436:ASP:HB3	1.98	0.43
1:A:1372:LEU:HG	1:A:1501:ALA:HB2	1.99	0.43
1:B:80:LYS:HD3	1:B:96:GLU:HG3	1.99	0.43
1:B:530:CYS:SG	1:B:531:LEU:N	2.91	0.43
1:B:766:LEU:O	1:B:787:ARG:NH2	2.51	0.43
1:B:1273:PRO:HD2	1:B:1333:LEU:HB2	2.00	0.43
1:C:922:PRO:HG3	1:C:1063:TRP:HB2	1.99	0.43
1:C:1278:ALA:HB2	1:C:1283:ALA:HA	1.99	0.43
1:C:1423:GLU:HA	1:C:1445:VAL:HA	2.00	0.43
1:D:922:PRO:HG3	1:D:1063:TRP:HB2	1.99	0.43
1:A:173:VAL:O	1:A:302:ARG:NH2	2.46	0.43
1:A:431:VAL:HG11	1:A:464:ARG:HH11	1.84	0.43
1:A:1411:TRP:NE1	1:A:1414:PHE:O	2.51	0.43
1:B:363:ILE:HG12	1:B:406:ILE:HG12	2.00	0.43
1:C:526:LEU:HB3	1:C:533:HIS:HB2	1.99	0.43
1:C:766:LEU:O	1:C:787:ARG:NH2	2.51	0.43
1:D:526:LEU:HB3	1:D:533:HIS:HB2	1.99	0.43
1:D:766:LEU:O	1:D:787:ARG:NH2	2.51	0.43
1:A:526:LEU:HB3	1:A:533:HIS:HB2	1.99	0.43
1:B:198:ALA:HB3	1:B:236:LEU:HD22	2.01	0.43
1:B:437:LEU:O	1:B:455:GLN:NE2	2.49	0.43
1:B:936:PHE:O	1:B:940:LEU:N	2.40	0.43
1:C:107:THR:HG22	1:C:108:PHE:H	1.84	0.43
1:C:288:ASP:OD1	1:C:288:ASP:N	2.45	0.43
1:C:1372:LEU:HG	1:C:1501:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ASP:OD1	1:D:288:ASP:N	2.45	0.43
1:D:1411:TRP:NE1	1:D:1414:PHE:O	2.51	0.43
1:D:1423:GLU:HA	1:D:1445:VAL:HA	2.00	0.43
1:A:80:LYS:HD3	1:A:96:GLU:HG3	1.99	0.43
1:A:107:THR:HG22	1:A:108:PHE:H	1.84	0.43
1:A:650:ALA:HA	1:A:653:LEU:HD13	2.01	0.43
1:A:1311:ARG:NH1	1:A:1312:SER:O	2.52	0.43
1:A:1423:GLU:HA	1:A:1445:VAL:HA	2.00	0.43
1:B:650:ALA:HA	1:B:653:LEU:HD13	2.01	0.43
1:B:922:PRO:HG3	1:B:1063:TRP:HB2	1.99	0.43
1:B:1041:LEU:HG	1:B:1044:LEU:HD22	2.00	0.43
1:C:530:CYS:SG	1:C:531:LEU:N	2.91	0.43
1:C:1236:ASP:OD1	1:C:1236:ASP:N	2.52	0.43
1:A:509:GLN:HG3	1:A:511:LYS:HB2	1.99	0.43
1:A:629:ALA:HB1	1:A:634:ARG:HB2	2.01	0.43
1:A:672:SER:HA	1:A:675:MET:HG2	2.01	0.43
1:A:932:LYS:HA	1:A:932:LYS:HD2	1.84	0.43
1:A:1293:LEU:HG	1:A:1295:PRO:HD2	2.00	0.43
1:B:1467:CYS:SG	1:B:1468:ASP:N	2.92	0.43
1:C:363:ILE:HG12	1:C:406:ILE:HG12	2.00	0.43
1:D:672:SER:HA	1:D:675:MET:HG2	2.01	0.43
1:A:220:GLU:HG3	1:A:223:ARG:HH21	1.83	0.43
1:A:1024:LEU:HD21	1:B:901:LEU:HD11	2.00	0.43
1:A:1467:CYS:SG	1:A:1468:ASP:N	2.92	0.43
1:B:107:THR:HG22	1:B:108:PHE:H	1.84	0.43
1:C:74:TYR:HB2	1:C:122:MET:H	1.83	0.43
1:C:1311:ARG:NH1	1:C:1312:SER:O	2.52	0.43
1:D:74:TYR:HB2	1:D:122:MET:H	1.83	0.43
1:D:845:ARG:HA	1:D:848:PHE:HD2	1.84	0.43
1:D:1311:ARG:NH1	1:D:1312:SER:O	2.52	0.43
1:A:70:LYS:HE3	1:A:70:LYS:HB2	1.89	0.43
1:B:220:GLU:HG3	1:B:223:ARG:HH21	1.83	0.43
1:C:248:HIS:HB2	1:C:271:GLN:HB2	2.00	0.43
1:D:932:LYS:HA	1:D:932:LYS:HD2	1.84	0.43
1:A:248:HIS:HB2	1:A:271:GLN:HB2	2.00	0.43
1:B:1236:ASP:OD1	1:B:1236:ASP:N	2.52	0.43
1:C:983:PRO:HB2	1:C:986:ILE:HG12	2.01	0.43
1:C:1467:CYS:SG	1:C:1468:ASP:N	2.92	0.43
1:A:766:LEU:O	1:A:787:ARG:NH2	2.51	0.43
1:A:922:PRO:HG3	1:A:1063:TRP:HB2	1.99	0.43
1:A:1287:ASP:O	1:A:1289:MET:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1411:TRP:NE1	1:B:1414:PHE:O	2.51	0.43
1:C:845:ARG:HA	1:C:848:PHE:HD2	1.84	0.43
1:C:1378:LYS:NZ	1:C:1382:SER:O	2.51	0.43
1:D:363:ILE:HG12	1:D:406:ILE:HG12	2.00	0.43
1:D:629:ALA:HB1	1:D:634:ARG:HB2	2.01	0.43
1:D:928:LYS:HA	1:D:928:LYS:HD2	1.83	0.43
1:A:530:CYS:SG	1:A:531:LEU:N	2.91	0.42
1:B:390:MET:HB2	1:B:393:THR:HG22	2.01	0.42
1:B:431:VAL:HG11	1:B:464:ARG:HH11	1.84	0.42
1:B:1378:LYS:NZ	1:B:1382:SER:O	2.51	0.42
1:D:245:GLY:O	1:D:250:ARG:NH2	2.52	0.42
1:D:431:VAL:HG11	1:D:464:ARG:HH11	1.84	0.42
1:D:983:PRO:HB2	1:D:986:ILE:HG12	2.01	0.42
1:A:390:MET:HB2	1:A:393:THR:HG22	2.01	0.42
1:A:612:SER:O	1:A:612:SER:OG	2.37	0.42
1:A:845:ARG:HA	1:A:848:PHE:HD2	1.84	0.42
1:B:245:GLY:O	1:B:250:ARG:NH2	2.52	0.42
1:C:245:GLY:O	1:C:250:ARG:NH2	2.52	0.42
1:C:412:ARG:HE	1:C:415:LEU:HD12	1.84	0.42
1:C:629:ALA:HB1	1:C:634:ARG:HB2	2.01	0.42
1:D:198:ALA:HB3	1:D:236:LEU:HD22	2.00	0.42
1:D:220:GLU:HG3	1:D:223:ARG:HH21	1.83	0.42
1:B:173:VAL:O	1:B:302:ARG:NH2	2.46	0.42
1:B:629:ALA:HB1	1:B:634:ARG:HB2	2.01	0.42
1:B:1024:LEU:HD21	1:C:901:LEU:HD11	2.01	0.42
1:B:1239:HIS:HB2	1:B:1243:ARG:HG3	2.01	0.42
1:C:390:MET:HB2	1:C:393:THR:HG22	2.01	0.42
1:C:1041:LEU:HG	1:C:1044:LEU:HD22	2.00	0.42
1:D:107:THR:HG22	1:D:108:PHE:H	1.84	0.42
1:D:498:GLU:HA	1:D:501:LYS:HB3	2.01	0.42
1:D:530:CYS:SG	1:D:531:LEU:N	2.91	0.42
1:D:650:ALA:HA	1:D:653:LEU:HD13	2.01	0.42
1:D:937:PHE:HA	1:D:940:LEU:HB3	2.01	0.42
1:D:1287:ASP:O	1:D:1289:MET:N	2.52	0.42
1:A:498:GLU:HA	1:A:501:LYS:HB3	2.01	0.42
1:A:1041:LEU:HG	1:A:1044:LEU:HD22	2.00	0.42
1:B:412:ARG:HE	1:B:415:LEU:HD12	1.84	0.42
1:B:965:TRP:HA	1:B:968:ARG:HB3	2.02	0.42
1:B:1236:ASP:O	1:B:1243:ARG:NH2	2.46	0.42
1:B:1451:ASP:OD1	1:B:1451:ASP:N	2.52	0.42
1:C:484:LEU:O	1:C:488:MET:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:MET:HB2	1:D:393:THR:HG22	2.01	0.42
1:D:718:LEU:O	1:D:722:LEU:N	2.48	0.42
1:D:1143:ARG:NH2	1:D:1146:GLN:OE1	2.53	0.42
1:D:1307:LEU:O	1:D:1392:ARG:NH2	2.53	0.42
1:D:1467:CYS:SG	1:D:1468:ASP:N	2.92	0.42
1:D:1496:ALA:HB1	1:D:1501:ALA:HB3	2.02	0.42
1:A:198:ALA:HB3	1:A:236:LEU:HD22	2.01	0.42
1:A:1496:ALA:HB1	1:A:1501:ALA:HB3	2.02	0.42
1:B:248:HIS:HB2	1:B:271:GLN:HB2	2.00	0.42
1:B:679:ALA:HA	1:B:682:TYR:HB2	2.02	0.42
1:B:1311:ARG:NH1	1:B:1312:SER:O	2.52	0.42
1:C:650:ALA:HA	1:C:653:LEU:HD13	2.01	0.42
1:C:679:ALA:HA	1:C:682:TYR:HB2	2.02	0.42
1:C:1143:ARG:NH2	1:C:1146:GLN:OE1	2.53	0.42
1:D:465:VAL:HG21	1:D:498:GLU:HB2	2.01	0.42
1:D:1239:HIS:HB2	1:D:1243:ARG:HG3	2.01	0.42
1:A:817:LEU:O	1:A:896:ARG:NH1	2.52	0.42
1:B:250:ARG:HE	1:B:250:ARG:HB2	1.65	0.42
1:B:1143:ARG:NH2	1:B:1146:GLN:OE1	2.53	0.42
1:C:173:VAL:O	1:C:302:ARG:NH2	2.46	0.42
1:C:672:SER:HA	1:C:675:MET:HG2	2.01	0.42
1:C:934:VAL:HA	1:C:937:PHE:HB3	2.02	0.42
1:D:1489:LYS:O	1:D:1503:TYR:OH	2.35	0.42
1:A:412:ARG:HE	1:A:415:LEU:HD12	1.85	0.42
1:C:559:HIS:HA	1:C:562:ALA:HB3	2.02	0.42
1:D:1451:ASP:N	1:D:1451:ASP:OD1	2.53	0.42
1:A:679:ALA:HA	1:A:682:TYR:HB2	2.02	0.42
1:A:1239:HIS:HB2	1:A:1243:ARG:HG3	2.01	0.42
1:B:1287:ASP:O	1:B:1289:MET:N	2.52	0.42
1:C:465:VAL:HG21	1:C:498:GLU:HB2	2.01	0.42
1:C:817:LEU:O	1:C:896:ARG:NH1	2.52	0.42
1:C:1496:ALA:HB1	1:C:1501:ALA:HB3	2.02	0.42
1:A:437:LEU:O	1:A:455:GLN:NE2	2.49	0.42
1:A:934:VAL:HA	1:A:937:PHE:HB3	2.02	0.42
1:A:937:PHE:HA	1:A:940:LEU:HB3	2.02	0.42
1:C:1239:HIS:HB2	1:C:1243:ARG:HG3	2.00	0.42
1:D:1466:ALA:HB1	1:D:1470:GLY:HA3	2.02	0.42
1:A:514:VAL:HG21	1:A:625:LEU:HD11	2.01	0.42
1:A:1466:ALA:HB1	1:A:1470:GLY:HA3	2.02	0.42
1:B:465:VAL:HG21	1:B:498:GLU:HB2	2.01	0.42
1:B:845:ARG:HA	1:B:848:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:679:ALA:HA	1:D:682:TYR:HB2	2.02	0.42
1:D:939:PHE:O	1:D:943:VAL:N	2.53	0.42
1:B:583:ASN:HD22	1:B:602:VAL:HG12	1.85	0.41
1:B:672:SER:HA	1:B:675:MET:HG2	2.01	0.41
1:B:1307:LEU:O	1:B:1392:ARG:NH2	2.53	0.41
1:B:1326:ASN:OD1	1:B:1326:ASN:N	2.49	0.41
1:B:1496:ALA:HB1	1:B:1501:ALA:HB3	2.02	0.41
1:C:137:GLN:NE2	1:C:138:LYS:HZ2	2.17	0.41
1:C:514:VAL:HG21	1:C:625:LEU:HD11	2.01	0.41
1:C:965:TRP:HA	1:C:968:ARG:HB3	2.01	0.41
1:A:192:ARG:NH2	1:A:199:GLN:OE1	2.54	0.41
1:A:1143:ARG:NH2	1:A:1146:GLN:OE1	2.53	0.41
1:A:1261:LYS:HD2	1:A:1269:LEU:HD12	2.02	0.41
1:C:198:ALA:HB3	1:C:236:LEU:HD22	2.00	0.41
1:C:937:PHE:HA	1:C:940:LEU:HB3	2.02	0.41
1:D:559:HIS:HA	1:D:562:ALA:HB3	2.02	0.41
1:A:583:ASN:HD22	1:A:602:VAL:HG12	1.85	0.41
1:B:983:PRO:HB2	1:B:986:ILE:HG12	2.01	0.41
1:C:1287:ASP:O	1:C:1289:MET:N	2.52	0.41
1:D:255:HIS:HA	1:D:256:PRO:HD3	1.89	0.41
1:D:412:ARG:HE	1:D:415:LEU:HD12	1.85	0.41
1:A:771:ILE:O	1:A:787:ARG:NH2	2.54	0.41
1:A:939:PHE:O	1:A:943:VAL:N	2.53	0.41
1:B:192:ARG:NH2	1:B:199:GLN:OE1	2.54	0.41
1:B:492:LEU:O	1:B:495:ASN:ND2	2.54	0.41
1:B:700:ARG:NH2	1:B:1120:ALA:O	2.53	0.41
1:B:718:LEU:O	1:B:722:LEU:N	2.48	0.41
1:C:431:VAL:HG11	1:C:464:ARG:HH11	1.84	0.41
1:C:1466:ALA:HB1	1:C:1470:GLY:HA3	2.02	0.41
1:D:437:LEU:O	1:D:455:GLN:NE2	2.49	0.41
1:D:492:LEU:O	1:D:495:ASN:ND2	2.54	0.41
1:A:250:ARG:HE	1:A:250:ARG:HB2	1.65	0.41
1:A:965:TRP:HA	1:A:968:ARG:HB3	2.01	0.41
1:B:498:GLU:HA	1:B:501:LYS:HB3	2.01	0.41
1:C:498:GLU:HA	1:C:501:LYS:HB3	2.01	0.41
1:C:1277:THR:HA	1:C:1336:ARG:HA	2.03	0.41
1:D:250:ARG:HE	1:D:250:ARG:HB2	1.65	0.41
1:D:612:SER:O	1:D:612:SER:OG	2.37	0.41
1:B:514:VAL:HG21	1:B:625:LEU:HD11	2.01	0.41
1:B:934:VAL:HA	1:B:937:PHE:HB3	2.02	0.41
1:C:437:LEU:O	1:C:455:GLN:NE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1307:LEU:O	1:C:1392:ARG:NH2	2.53	0.41
1:D:416:LEU:O	1:D:439:LYS:NZ	2.45	0.41
1:D:771:ILE:O	1:D:787:ARG:NH2	2.54	0.41
1:B:771:ILE:O	1:B:787:ARG:NH2	2.54	0.41
1:B:1466:ALA:HB1	1:B:1470:GLY:HA3	2.02	0.41
1:C:594:HIS:CE1	1:C:596:LYS:HG2	2.56	0.41
1:C:1261:LYS:HD2	1:C:1269:LEU:HD12	2.02	0.41
1:D:514:VAL:HG21	1:D:625:LEU:HD11	2.01	0.41
1:D:645:SER:O	1:D:1129:LYS:NZ	2.40	0.41
1:D:700:ARG:NH2	1:D:1120:ALA:O	2.53	0.41
1:A:983:PRO:HB2	1:A:986:ILE:HG12	2.01	0.41
1:B:559:HIS:HA	1:B:562:ALA:HB3	2.02	0.41
1:B:937:PHE:HA	1:B:940:LEU:HB3	2.01	0.41
1:B:1277:THR:HA	1:B:1336:ARG:HA	2.03	0.41
1:C:539:VAL:HA	1:C:542:GLU:HB2	2.03	0.41
1:C:771:ILE:O	1:C:787:ARG:NH2	2.54	0.41
1:D:965:TRP:HA	1:D:968:ARG:HB3	2.01	0.41
1:A:700:ARG:NH2	1:A:1120:ALA:O	2.53	0.41
1:A:707:ARG:HG3	1:A:1113:LEU:HD21	2.03	0.41
1:A:760:MET:HE3	1:A:797:VAL:HA	2.03	0.41
1:A:1451:ASP:OD1	1:A:1451:ASP:N	2.52	0.41
1:B:178:LYS:HD2	1:B:178:LYS:HA	1.89	0.41
1:B:1261:LYS:HD2	1:B:1269:LEU:HD12	2.02	0.41
1:C:385:VAL:H	1:C:385:VAL:HG23	1.60	0.41
1:C:583:ASN:HD22	1:C:602:VAL:HG12	1.86	0.41
1:C:707:ARG:HG3	1:C:1113:LEU:HD21	2.03	0.41
1:C:939:PHE:O	1:C:943:VAL:N	2.53	0.41
1:C:1489:LYS:HB2	1:C:1489:LYS:HE2	1.93	0.41
1:D:137:GLN:HE21	1:D:138:LYS:HZ2	1.67	0.41
1:D:423:LYS:HA	1:D:423:LYS:HD3	1.90	0.41
1:D:470:SER:HA	1:D:474:MET:HG2	2.03	0.41
1:D:569:LEU:HA	1:D:657:LYS:HZ3	1.85	0.41
1:D:934:VAL:HA	1:D:937:PHE:HB3	2.02	0.41
1:A:645:SER:O	1:A:1129:LYS:NZ	2.40	0.41
1:A:1277:THR:HA	1:A:1336:ARG:HA	2.03	0.41
1:B:470:SER:HA	1:B:474:MET:HG2	2.03	0.41
1:B:760:MET:HE1	1:B:797:VAL:HA	2.02	0.41
1:C:492:LEU:O	1:C:495:ASN:ND2	2.54	0.41
1:D:314:LYS:HD3	1:D:321:ILE:HD11	2.03	0.41
1:D:539:VAL:HA	1:D:542:GLU:HB2	2.03	0.41
1:D:851:PRO:HA	1:D:859:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LYS:HD3	1:A:321:ILE:HD11	2.04	0.40
1:A:492:LEU:O	1:A:495:ASN:ND2	2.54	0.40
1:A:559:HIS:HA	1:A:562:ALA:HB3	2.02	0.40
1:B:536:LEU:O	1:B:540:LEU:N	2.46	0.40
1:B:594:HIS:CE1	1:B:596:LYS:HG2	2.56	0.40
1:B:939:PHE:O	1:B:943:VAL:N	2.53	0.40
1:D:1261:LYS:HD2	1:D:1269:LEU:HD12	2.02	0.40
1:D:1277:THR:HA	1:D:1336:ARG:HA	2.03	0.40
1:A:241:VAL:HG12	1:A:298:GLU:HG2	2.04	0.40
1:A:510:LEU:HA	1:A:513:PHE:HB3	2.03	0.40
1:A:536:LEU:O	1:A:540:LEU:N	2.46	0.40
1:A:928:LYS:HD2	1:A:928:LYS:HA	1.83	0.40
1:A:1275:PHE:HE1	1:A:1333:LEU:HB3	1.86	0.40
1:C:137:GLN:HE21	1:C:138:LYS:HZ1	1.67	0.40
1:C:314:LYS:HD3	1:C:321:ILE:HD11	2.04	0.40
1:C:700:ARG:NH2	1:C:1120:ALA:O	2.53	0.40
1:C:1275:PHE:HE1	1:C:1333:LEU:HB3	1.86	0.40
1:C:1344:PRO:O	1:C:1346:HIS:ND1	2.54	0.40
1:D:760:MET:HE3	1:D:797:VAL:HA	2.03	0.40
1:A:594:HIS:CE1	1:A:596:LYS:HG2	2.56	0.40
1:B:241:VAL:HG12	1:B:298:GLU:HG2	2.03	0.40
1:B:1344:PRO:O	1:B:1346:HIS:ND1	2.54	0.40
1:D:192:ARG:NH2	1:D:199:GLN:OE1	2.54	0.40
1:D:241:VAL:HG12	1:D:298:GLU:HG2	2.04	0.40
1:D:1030:CYS:HA	1:D:1033:LEU:HB3	2.03	0.40
1:D:1344:PRO:O	1:D:1346:HIS:ND1	2.54	0.40
1:D:1378:LYS:NZ	1:D:1382:SER:O	2.51	0.40
1:A:446:HIS:HB3	1:A:447:PHE:H	1.73	0.40
1:A:539:VAL:HA	1:A:542:GLU:HB2	2.03	0.40
1:A:1307:LEU:O	1:A:1392:ARG:NH2	2.53	0.40
1:A:1344:PRO:O	1:A:1346:HIS:ND1	2.54	0.40
1:B:1160:ASP:N	1:B:1160:ASP:OD1	2.50	0.40
1:C:241:VAL:HG12	1:C:298:GLU:HG2	2.03	0.40
1:C:377:SER:HA	1:C:380:GLN:HB2	2.03	0.40
1:C:446:HIS:HB3	1:C:447:PHE:H	1.73	0.40
1:C:736:GLN:HA	1:C:739:LEU:HG	2.04	0.40
1:C:1115:LYS:HA	1:C:1115:LYS:HD3	1.98	0.40
1:A:470:SER:HA	1:A:474:MET:HG2	2.03	0.40
1:A:897:VAL:O	1:A:900:SER:OG	2.31	0.40
1:B:377:SER:HA	1:B:380:GLN:HB2	2.04	0.40
1:B:896:ARG:HH11	1:B:896:ARG:HD2	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ASN:OD1	1:C:273:ASN:N	2.55	0.40
1:C:569:LEU:HA	1:C:657:LYS:HZ3	1.87	0.40
1:C:851:PRO:HA	1:C:859:LYS:HE3	2.03	0.40
1:D:1112:LYS:HA	1:D:1112:LYS:HD2	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	34	72
1	B	1331/1503 (89%)	1133 (85%)	193 (14%)	5 (0%)	34	72
1	C	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	34	72
1	D	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	34	72
All	All	5324/6012 (89%)	4526 (85%)	778 (15%)	20 (0%)	38	72

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ILE
1	B	376	ILE
1	C	376	ILE
1	D	376	ILE
1	A	384	SER
1	B	384	SER
1	C	384	SER
1	D	384	SER
1	A	1288	PRO
1	B	1288	PRO
1	C	1288	PRO

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Mol	Chain	Res	Type
1	D	1288	PRO
1	A	429	VAL
1	A	1270	ILE
1	B	429	VAL
1	B	1270	ILE
1	C	429	VAL
1	C	1270	ILE
1	D	429	VAL
1	D	1270	ILE

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 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%)	1163 (99%)	13 (1%)	73	84
1	B	1176/1318 (89%)	1163 (99%)	13 (1%)	73	84
1	C	1176/1318 (89%)	1163 (99%)	13 (1%)	73	84
1	D	1176/1318 (89%)	1163 (99%)	13 (1%)	73	84
All	All	4704/5272 (89%)	4652 (99%)	52 (1%)	74	84

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	LEU
1	A	496	LYS
1	A	566	ARG
1	A	610	ARG
1	A	685	ARG
1	A	715	THR
1	A	839	LEU
1	A	886	ARG
1	A	918	LYS
1	A	930	MET
1	A	941	LEU
1	A	1024	LEU

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Mol	Chain	Res	Type
1	A	1064	LYS
1	B	253	LEU
1	B	496	LYS
1	B	566	ARG
1	B	610	ARG
1	B	685	ARG
1	B	715	THR
1	B	839	LEU
1	B	886	ARG
1	B	918	LYS
1	B	930	MET
1	B	941	LEU
1	B	1024	LEU
1	B	1064	LYS
1	C	253	LEU
1	C	496	LYS
1	C	566	ARG
1	C	610	ARG
1	C	685	ARG
1	C	715	THR
1	C	839	LEU
1	C	886	ARG
1	C	918	LYS
1	C	930	MET
1	C	941	LEU
1	C	1024	LEU
1	C	1064	LYS
1	D	253	LEU
1	D	496	LYS
1	D	566	ARG
1	D	610	ARG
1	D	685	ARG
1	D	715	THR
1	D	839	LEU
1	D	886	ARG
1	D	918	LYS
1	D	930	MET
1	D	941	LEU
1	D	1024	LEU
1	D	1064	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	338	HIS
1	A	381	GLN
1	A	446	HIS
1	A	451	ASN
1	A	454	HIS
1	A	506	ASN
1	A	509	GLN
1	A	525	ASN
1	A	560	HIS
1	A	594	HIS
1	A	646	GLN
1	A	684	HIS
1	A	800	HIS
1	A	973	HIS
1	A	1135	ASN
1	A	1461	ASN
1	A	1502	HIS
1	B	137	GLN
1	B	338	HIS
1	B	381	GLN
1	B	446	HIS
1	B	451	ASN
1	B	454	HIS
1	B	506	ASN
1	B	509	GLN
1	B	525	ASN
1	B	560	HIS
1	B	594	HIS
1	B	646	GLN
1	B	684	HIS
1	B	800	HIS
1	B	973	HIS
1	B	1135	ASN
1	B	1461	ASN
1	B	1502	HIS
1	C	137	GLN
1	C	338	HIS
1	C	381	GLN
1	C	446	HIS
1	C	451	ASN
1	C	454	HIS
1	C	506	ASN

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Mol	Chain	Res	Type
1	C	509	GLN
1	C	525	ASN
1	C	560	HIS
1	C	594	HIS
1	C	646	GLN
1	C	684	HIS
1	C	800	HIS
1	C	973	HIS
1	C	1135	ASN
1	C	1461	ASN
1	C	1502	HIS
1	D	137	GLN
1	D	338	HIS
1	D	381	GLN
1	D	446	HIS
1	D	454	HIS
1	D	506	ASN
1	D	509	GLN
1	D	525	ASN
1	D	560	HIS
1	D	594	HIS
1	D	646	GLN
1	D	684	HIS
1	D	973	HIS
1	D	1135	ASN
1	D	1461	ASN
1	D	1502	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

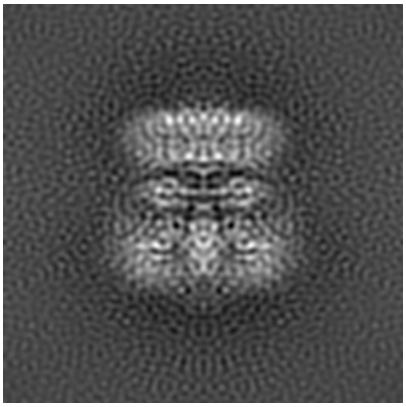
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9134. These allow visual inspection of the internal detail of the map and identification of artifacts.

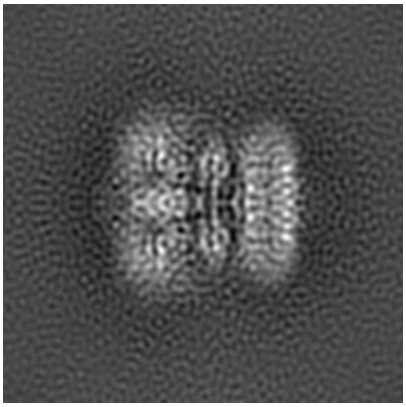
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

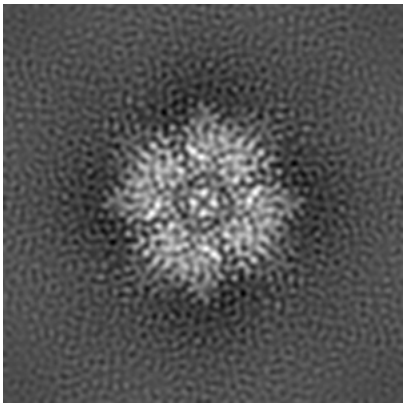
6.1.1 Primary map



X



Y

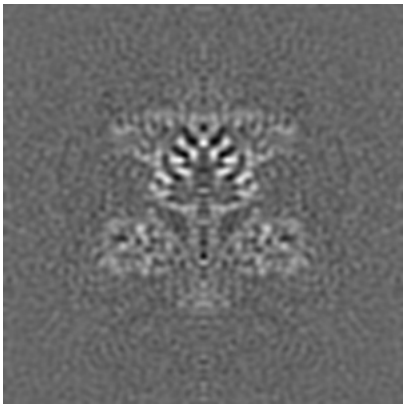


Z

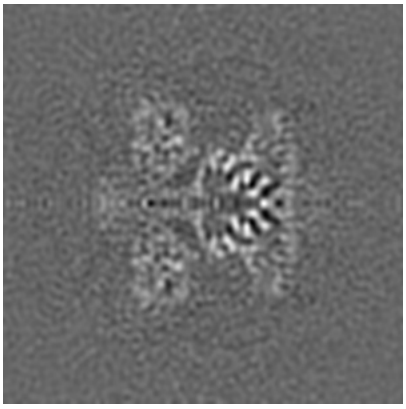
The images above show the map projected in three orthogonal directions.

6.2 Central slices

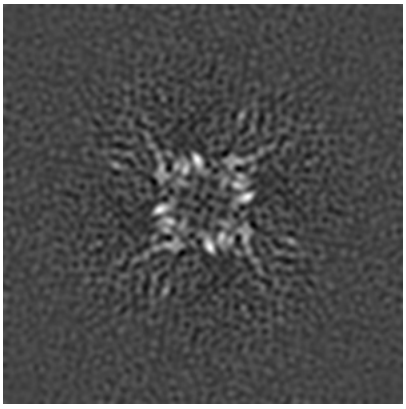
6.2.1 Primary map



X Index: 150



Y Index: 150

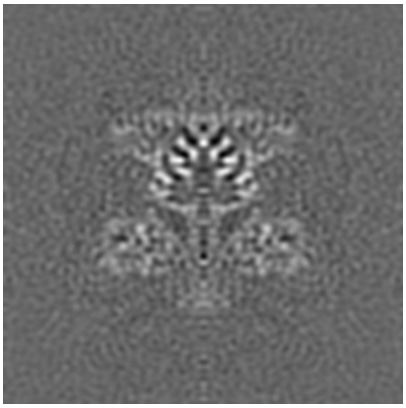


Z Index: 150

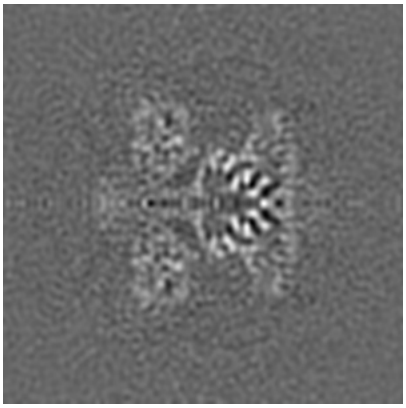
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

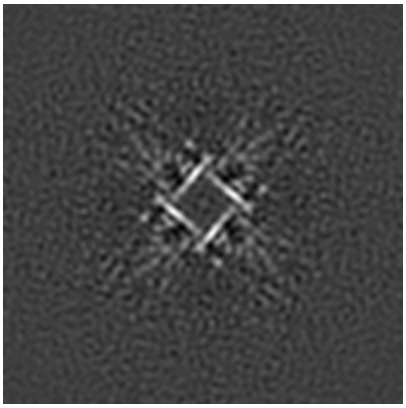
6.3.1 Primary map



X Index: 150



Y Index: 150

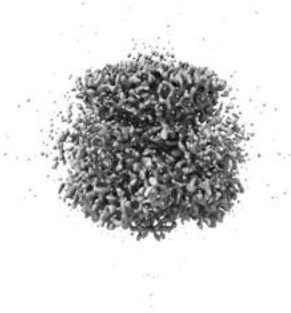


Z Index: 158

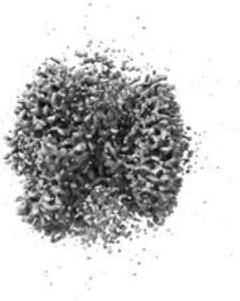
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

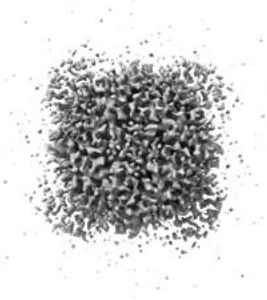
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.77. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

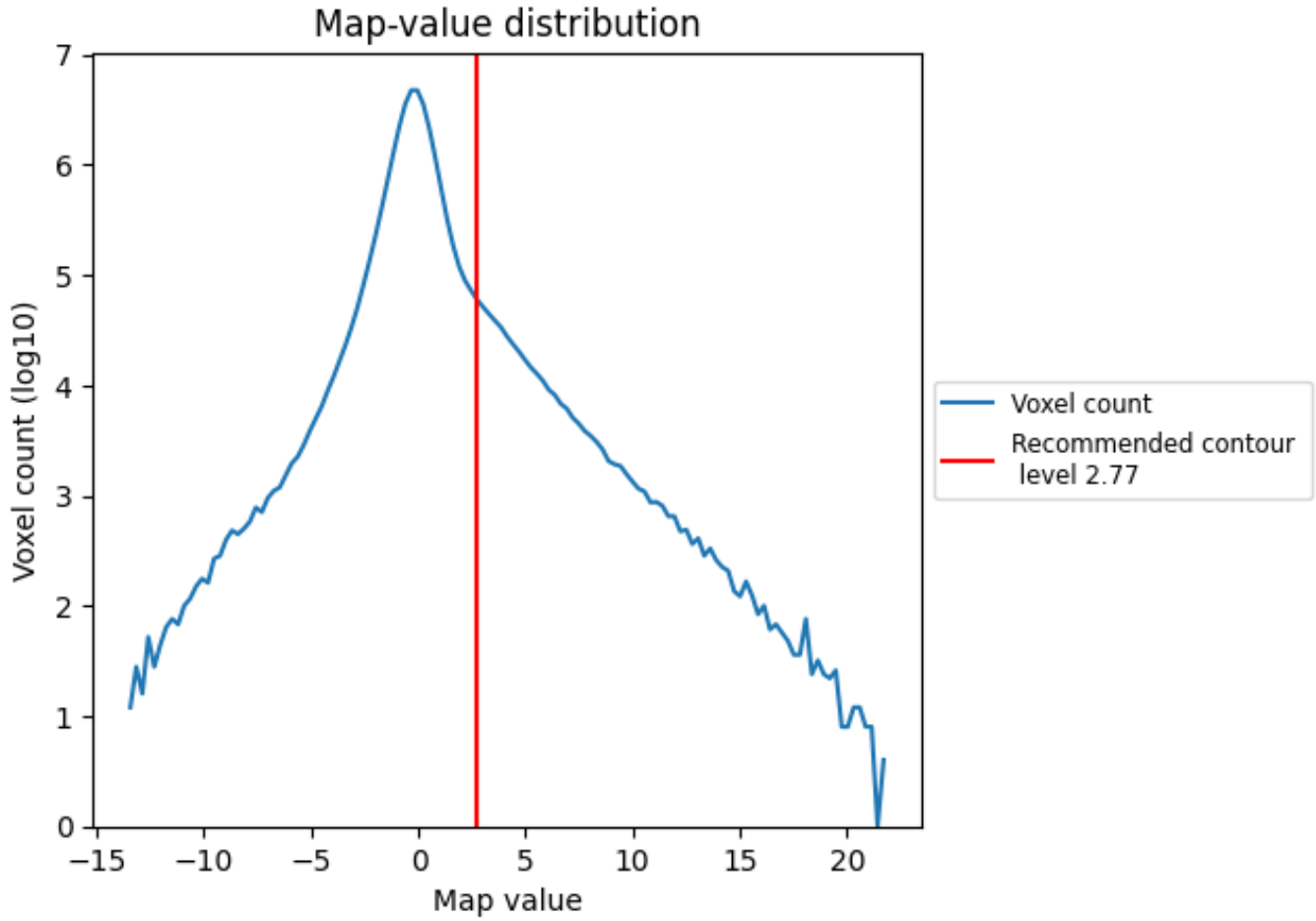
6.5 Mask visualisation (i)

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

7 Map analysis

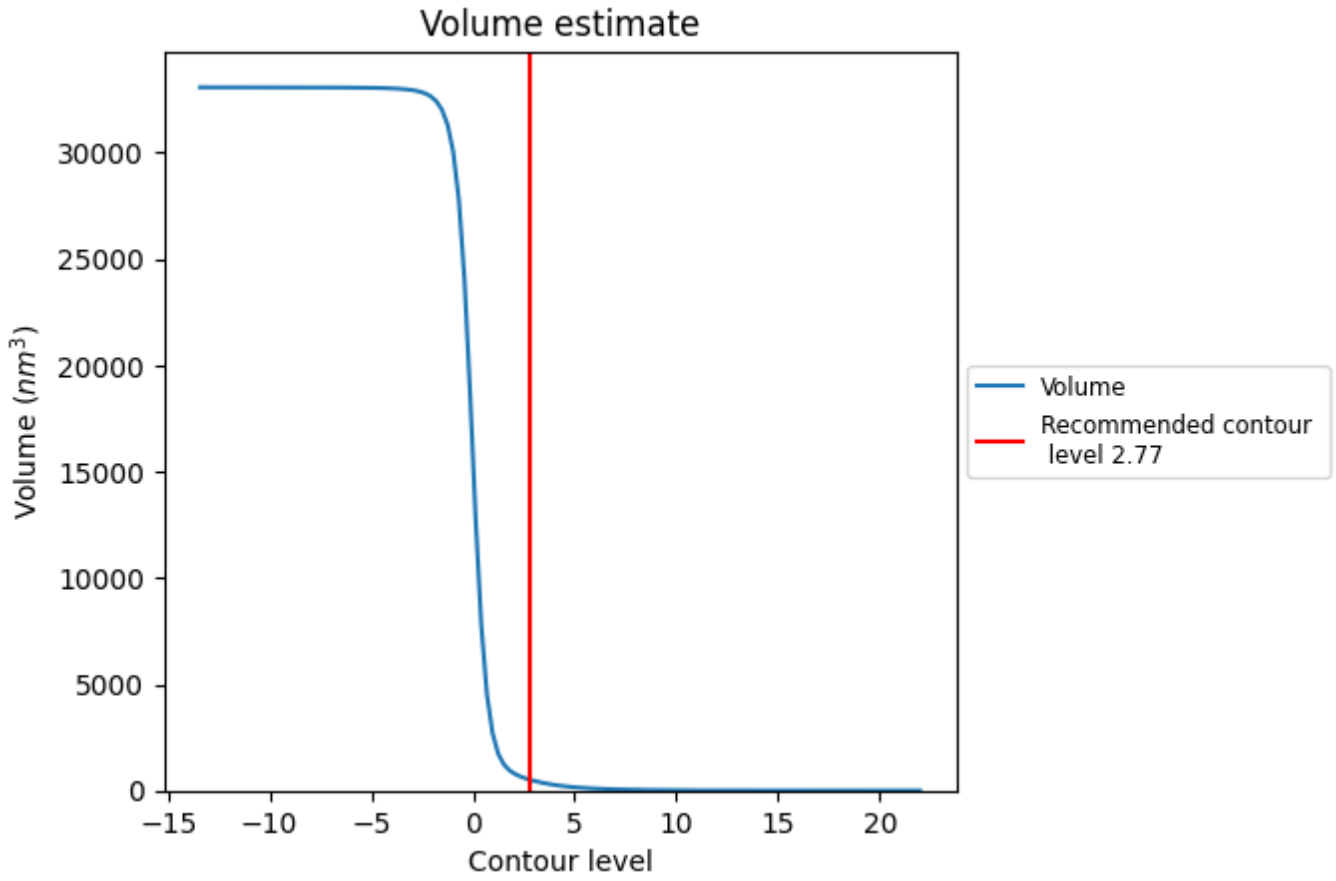
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

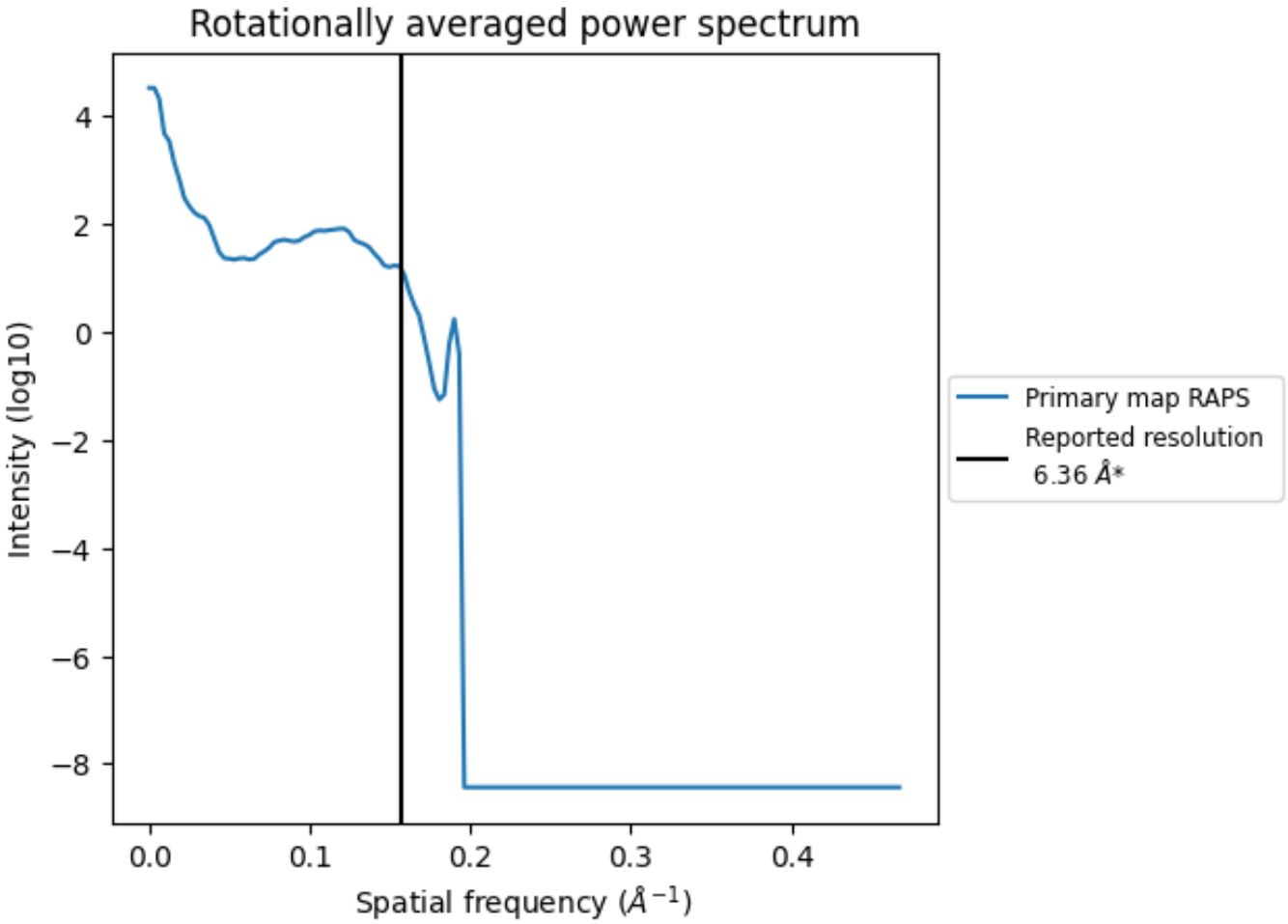
7.2 Volume estimate



The volume at the recommended contour level is 518 nm^3; this corresponds to an approximate mass of 468 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 (i)



*Reported resolution corresponds to spatial frequency of 0.157 Å^{-1}

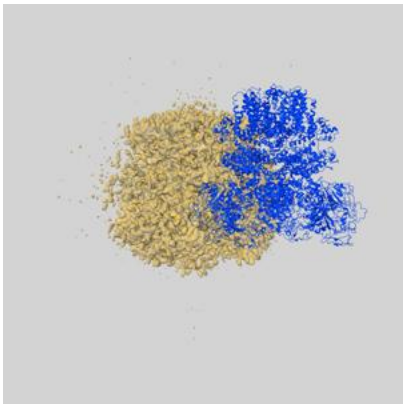
8 Fourier-Shell correlation

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

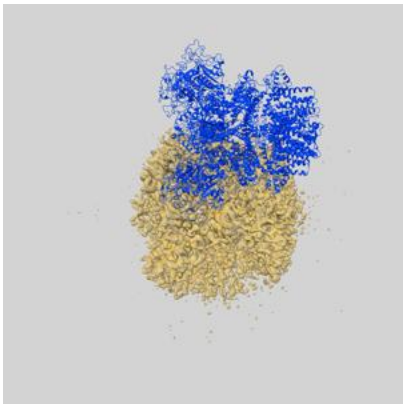
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9134 and PDB model 6MJ2. Per-residue inclusion information can be found in section 3 on page 4.

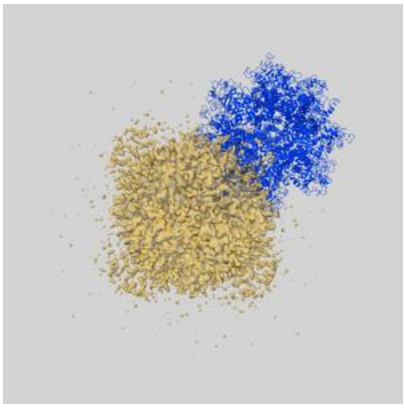
9.1 Map-model overlay



X



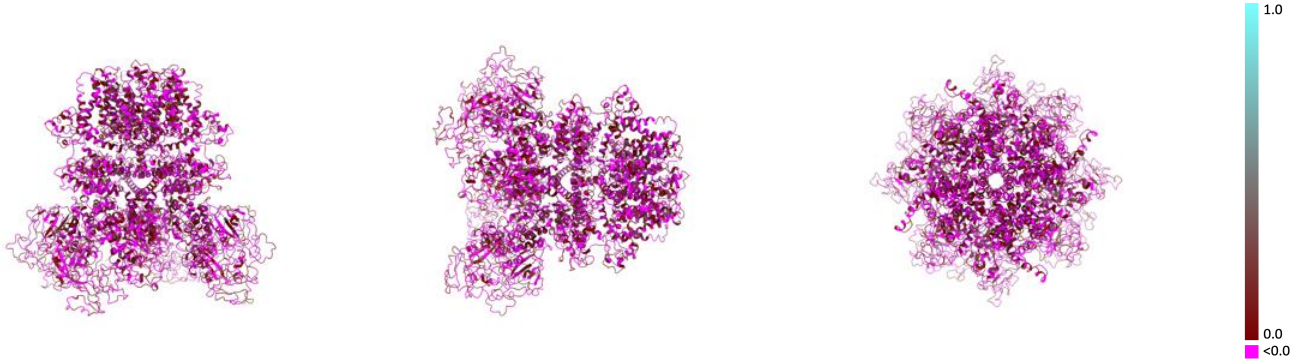
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.77 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.

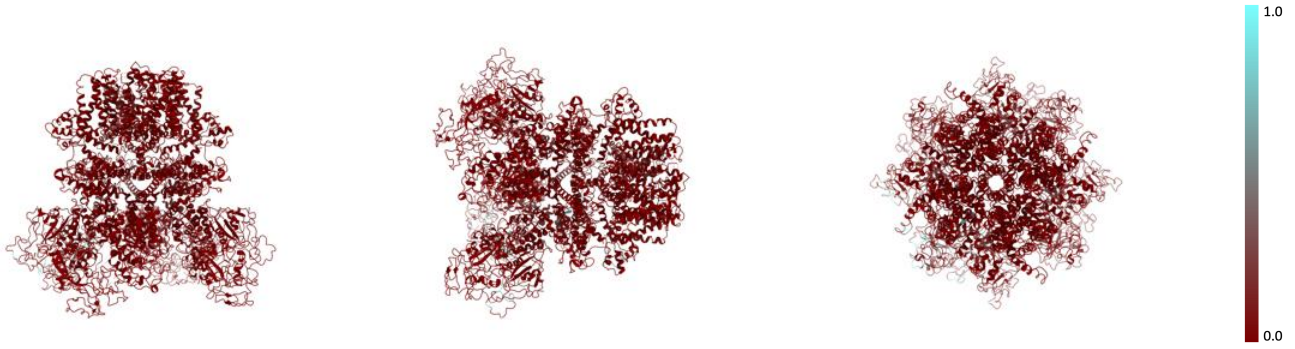
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

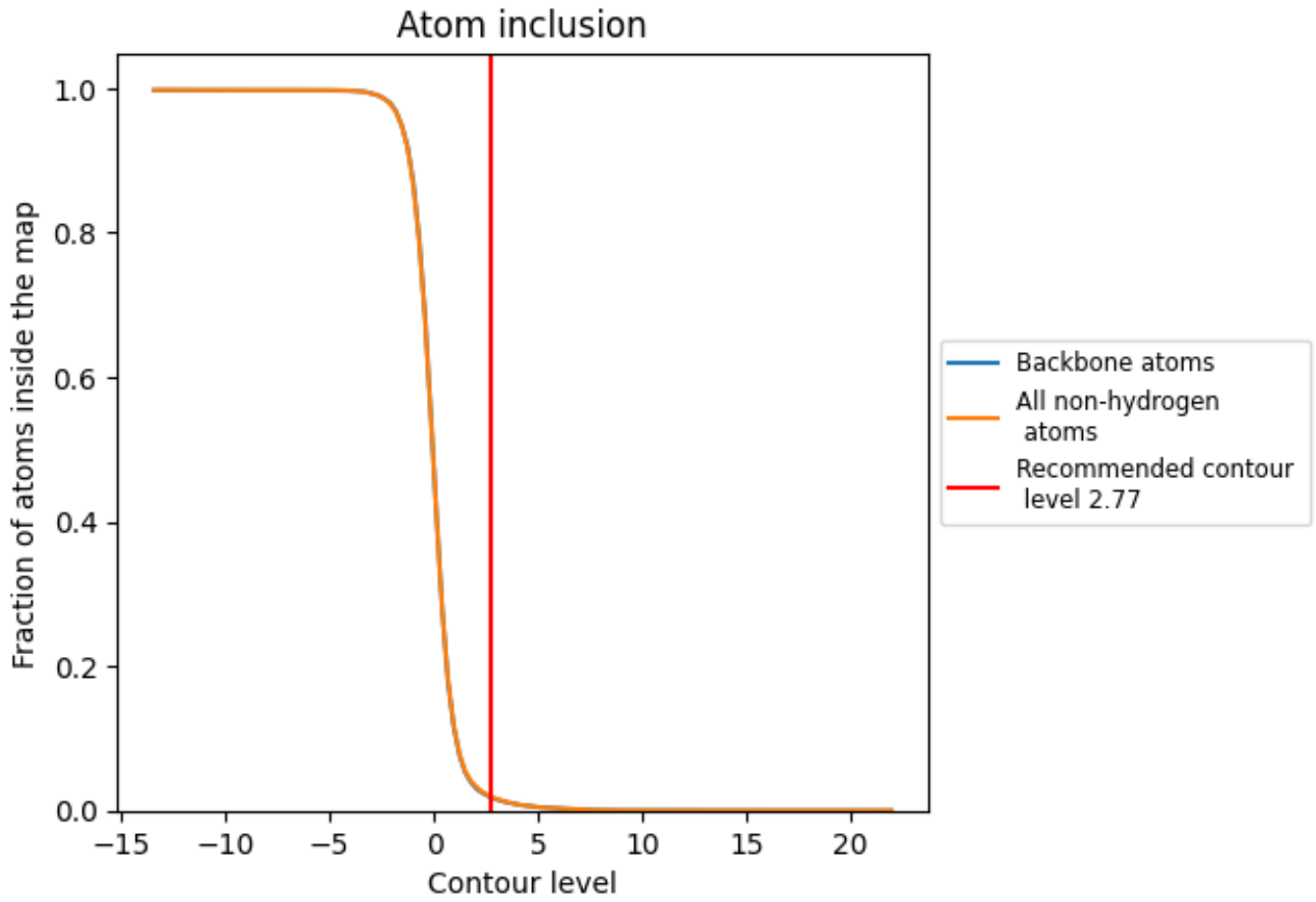
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.77).

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 (2.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0188	-0.0000
A	0.0603	-0.0020
B	0.0003	-0.0020
C	0.0000	0.0030
D	0.0145	-0.0000