



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:17 AM UTC

PDB ID : 6MJ2 / pdb_00006mj2
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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

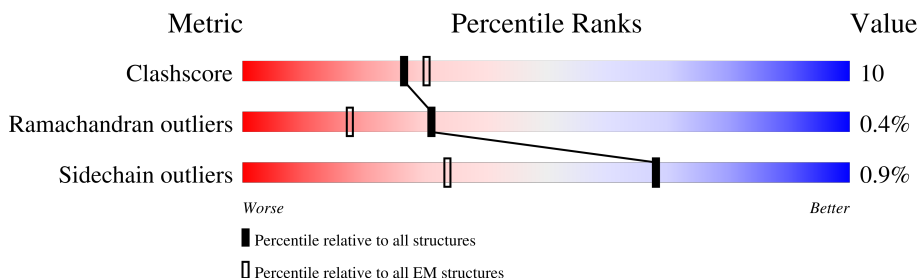
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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	84% 65% 23% • 11%
1	B	1503	89% 65% 22% • 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		

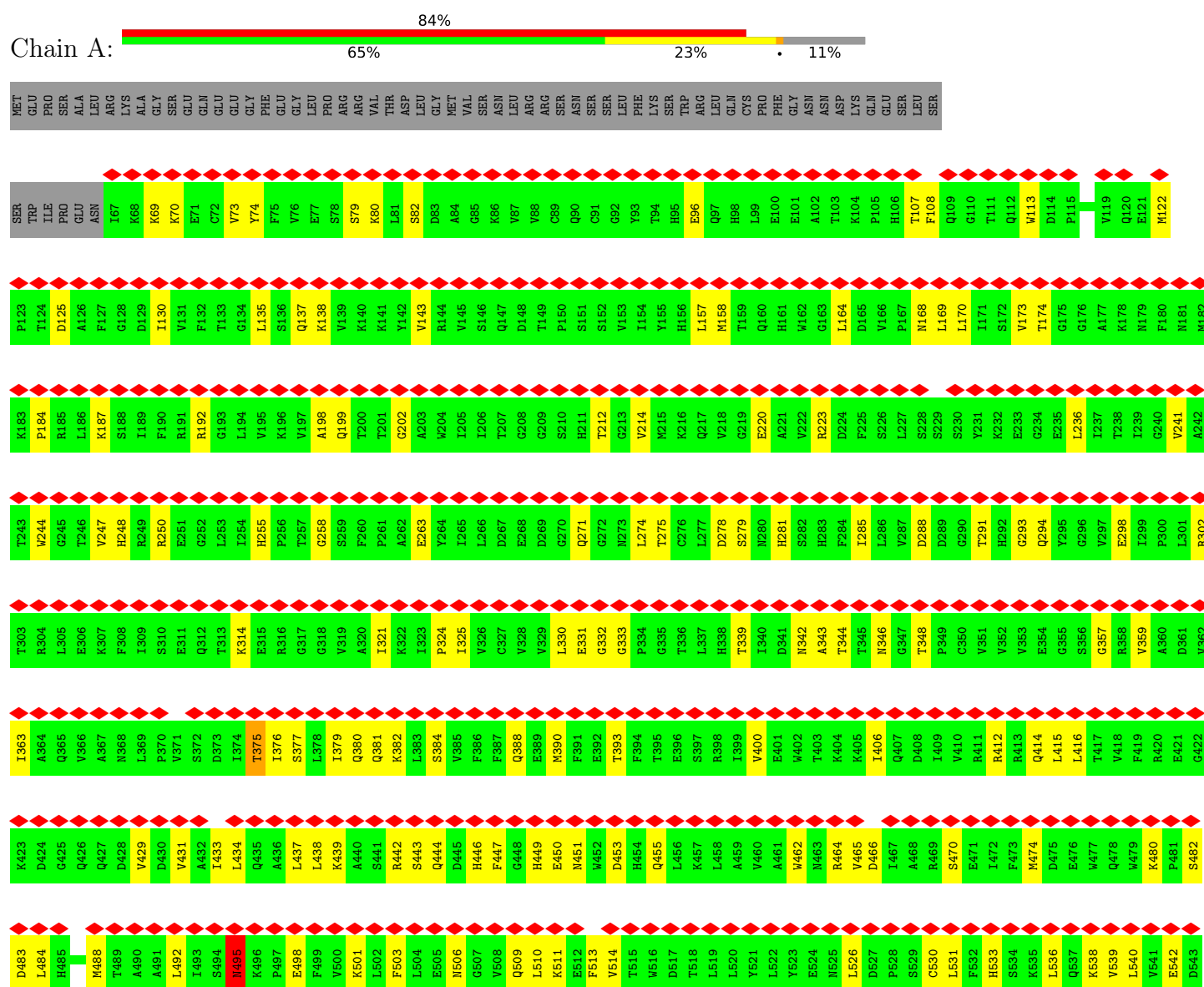
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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	

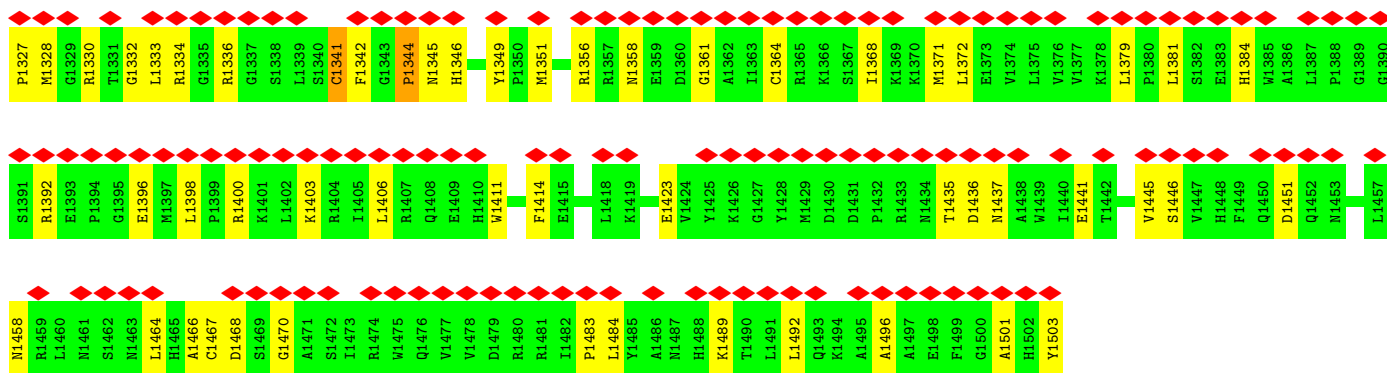
3 Residue-property plots

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.

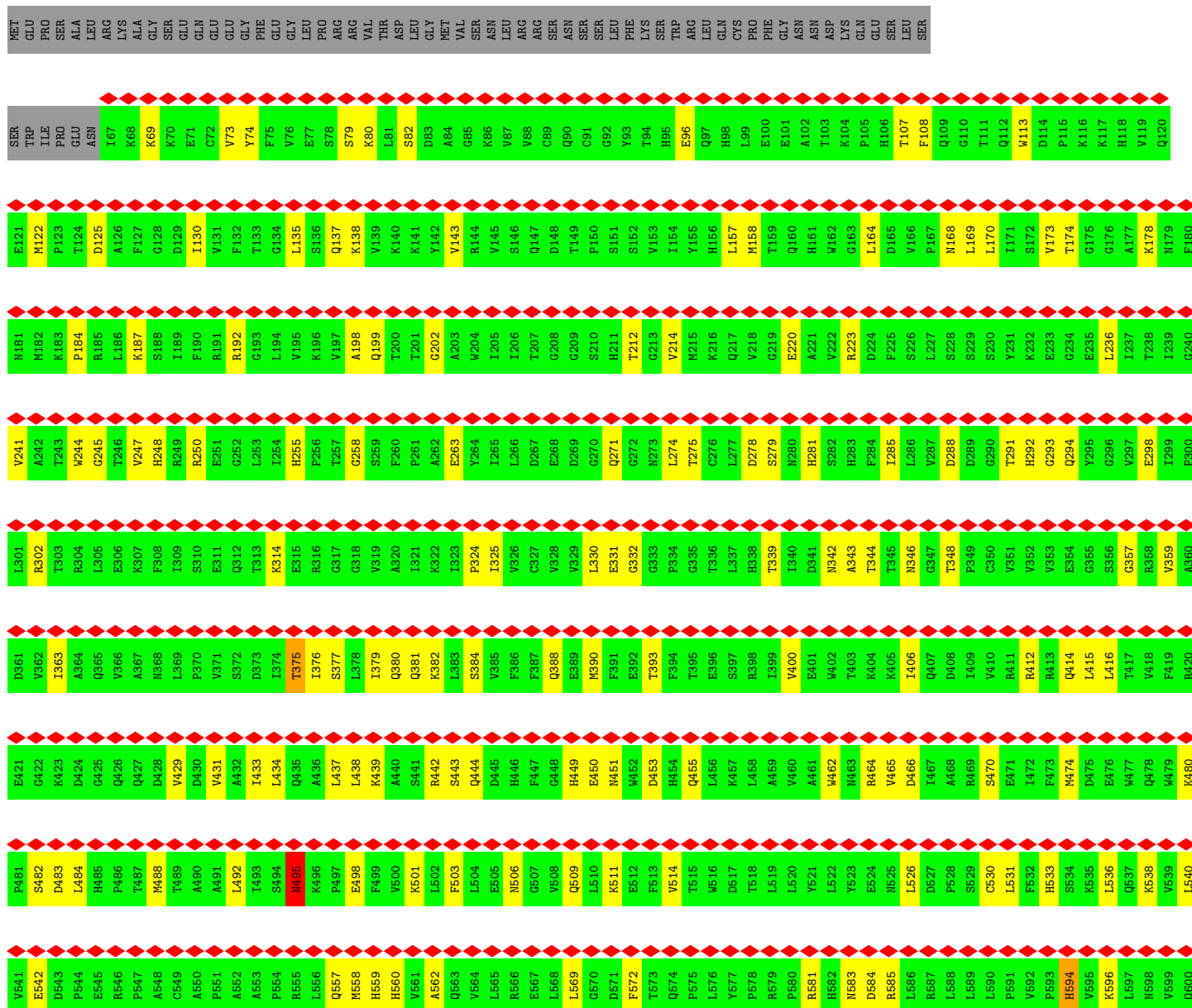
- Molecule 1: Transient receptor potential cation channel subfamily M member 2



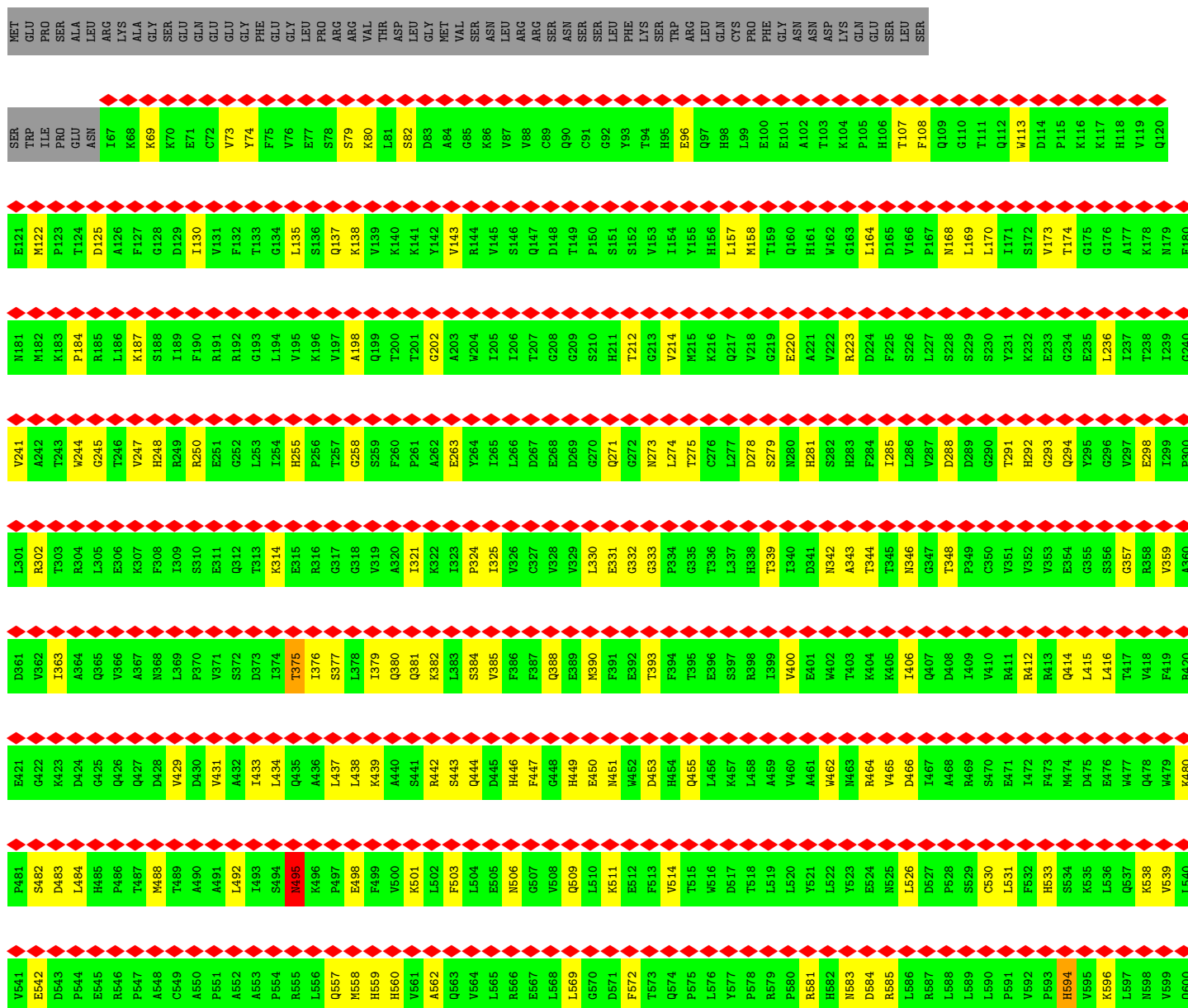




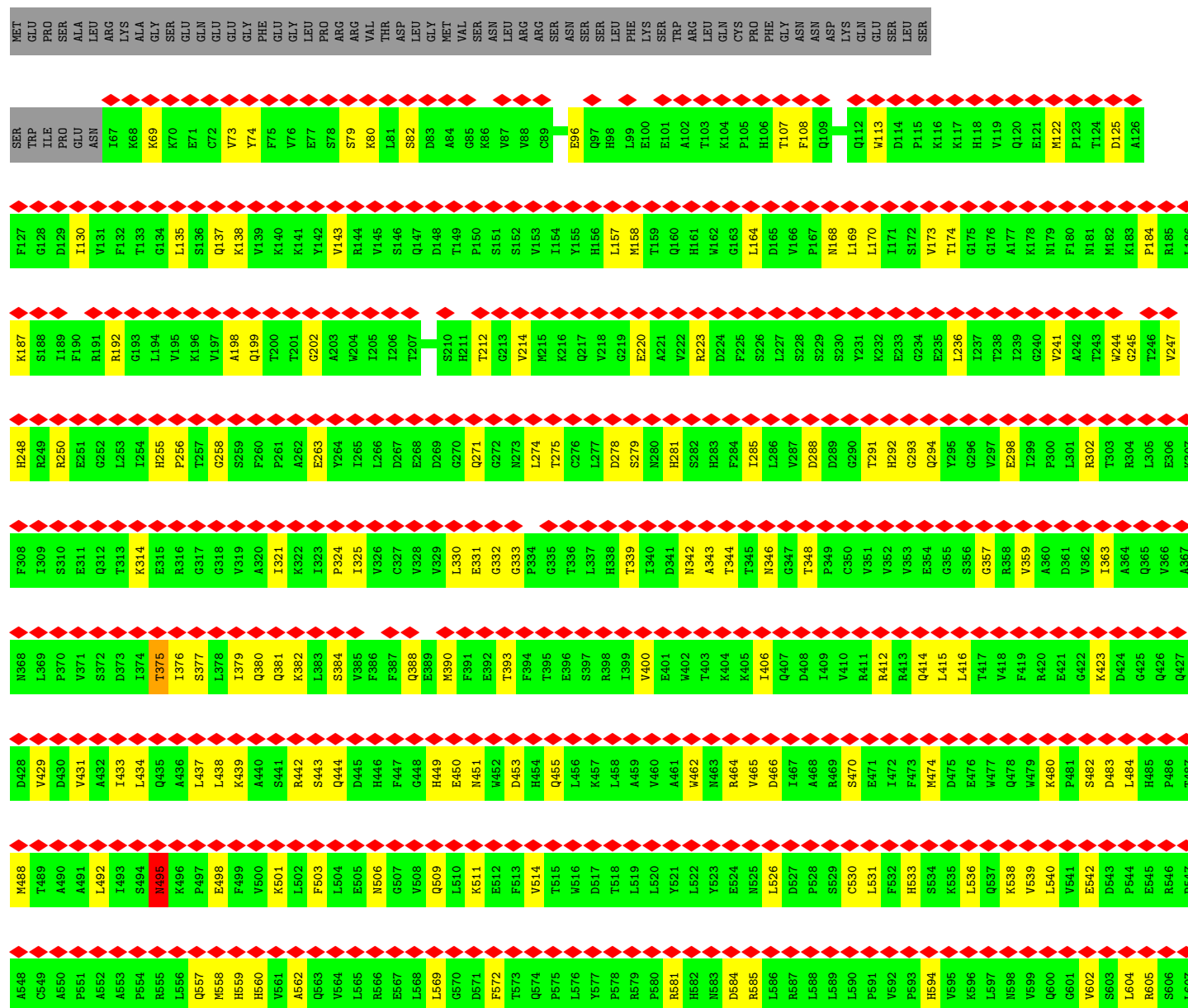
• Molecule 1: Transient receptor potential cation channel subfamily M member 2



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	A1346	T1347	L1348	P1349	M1350	M1351	V1352	L1353	R1354	W1355	R1356	R1357	N1358	E1359	D1360	G1361	I1362	I1363	C1364	R1365	R1366	S1367	R1368	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	P1274	F1275	Y1276	T1277	A1278	E1279	R1280	K1281	D1282	A1283	A1284	A1285	M1286	D1287	P1288	M1289	D1290	D1291	L1292	L1293	E1294	P1295	L1296	S1297	T1298	I1299	Q1300	Y1301	M1302	V1303	V1304	D1305	G1306	L1307	R1308	D1309	R1310	R1311	S1312	F1313	H1314	G1315	P1316	Y1317	T1318	V1319	Q1320
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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	A1119	A1120	L1121	L1122	S1123	W1124	E1125	I1126	Y1127	L1128	K1129	E1130	N1131	Y1132	L1133	Q1134	N1135	R1136	Q1137	F1138	Q1139	Q1140	
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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	W873	G874	Y875	V876	L877	L878	F879	V880	A881	Q882	L883	T884	C885	R886	L887	I888	P889	A890	T891	L892	Y893	P894	G895	R896	W897	I898	L899	S900
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	P822	P823	V824	P825	S826	W827	C828	E829	C830	A831	I832	L833	L834	W835	L836	F837	S838	L839	V840
A721	L722	E723	A724	K725	D726	M727	K728	F729	V730	S731	H732	G733	G734	I735	Q736	F737	L738	L739	T740	K741	V742	W743	G744	W745	G746	L747	S748	V749	D750	N751	G752	L753	W754	R755	V756	T757	L758	C759	M760	L761	A762	F763	P764	L765	L766	L767	T768	G769	S770	L770	I771	S772	F773	E775	K776	L777	R778	Q779	D780
E661	L662	S663	K664	E665	E666	E667	D668	T669	D670	S671	S672	E673	H674	M675	L676	A677	L678	A679	E680	E681	I682	E683	H684	E685	A686	I687	G688	V689	F690	T691	E692	G693	Y694	R695	K696	D697	E698	E699	R700	I641	W642	A643	Q644	S645	Q646	D647	C648	I649	A650	A651	A652	L653	A654	C655	S656	K657	L658	L659	K660



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SER	GLY	PHE	SER	SER	GLU	ALA	ASP	VAL	THR	LEU	ALA	SER	GLN	LYS	ALA	GLU	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							
K1141	Q1142	R1143	P1144	E1145	Q1146	K1147	T1148	E1149	D1150	I1151	S1152	M1153	K1154	V1155	D1156	A1157	M1158	V1159	D1160	L1161	L1162	D1163	L1164	D1165	PRO	LEU	LYS	ARG	SER	GLY	MET	GLU	GLN	ARG	LEU	ALA	SER	LEU	GLU	GLU	GLN	VAL	ALA	GLN	THR	ALA	GLN	LEU	HIS	TRP	ILE	VAL	ARG	THR	LEU	ARG	ALA			
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	
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ASP	VAL	PRO	THR	LEU	ALA	SER	GLN	LYS	ALA	ALA	GLU	GLU	PRO	ASP	ALA	GLU	THR	GLY	GLY	ARG	ARG	LYS	THR	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	K1261	V1262	P1263	W1264	E1265	T1266	E1267				
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R968	G969	A970	Y971	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	W944	GLU	SER	ASP	ALA	THR	GLN	GLN	ARG	PRO	ALA	F1020	P1021	E1022	W1023	L1024	T1025	V1026	L1027			
L908	R909	L910	M911	H912	I913	F914	T915	T916	S917	K918	T919	L920	G921	P922	K923	I924	I925	I926	V927	W928	R929	ASN	M930	N931	K932	D933	V934	F935	F936	F937	L938	F939	PRO	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	Y965	L966	F967	
F948	Y949	D950	P951	D952	E953	C954	G955	L956	M957	K958	K959	A960	A961	L962	Y963	F964	S965	D966	F967	W968	N969	K970	L971	D972	L973	V974	G975	A976	I977	L978	F979	V980	D981	A982	F983	L984	S985	R986	L987	I988	P989	A990	T991	L992	Y993	P994	G995	R996	V997	I998	L999	S900	L901	D902	F903	I904	L905	F906	C907			
A788	R789	A790	F791	T792	T793	A794	P795	V796	V797	V798	F799	H800	L801	N802	I803	L804	S805	Y806	F807	A808	F809	L810	C811	L812	F813	A814	Y815	R816	V817	M818	V819	D820	M821	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			
K728	F729	V730	S731	H732	G733	G734	I735	Q736	A737	F738	L739	T740	K741	V742	W743	W744	G745	Q746	L747	G748	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	T775	K776	T777	L778	Q779	V780	D781	L782	E783	A784	W785	A786	R787			
D668	T669	R670	S671	S672	S673	E674	M675	T676	F677	L678	A679	E680	E681	Y682	E683	H684	R685	A686	I687	G688	V689	F690	T691	E692	C693	Y694	R695	E696	L697	E698	G699	M640	R700	I641	W642	K703	L704	L705	T706	R707	V708	S709	E710	A711	W712	L653	A654	C655	T715	T716	S656	K657	I658	L659	R660	E661	L662	S663	K664	E665	E666	E667

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				
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	M1434	T1435	D1436	N1437	A1438	W1439	I1440	E1441	T1442	V1443	A1444	V1445	S1446	V1447

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.26	0/11050	0.69	10/14990 (0.1%)
1	B	0.25	0/11050	0.69	10/14990 (0.1%)
1	C	0.25	0/11050	0.69	10/14990 (0.1%)
1	D	0.25	0/11050	0.69	10/14990 (0.1%)
All	All	0.25	0/44200	0.69	40/59960 (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 (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	ARG	CD-NE-CZ	6.92	134.09	124.40
1	B	685	ARG	CD-NE-CZ	6.92	134.09	124.40
1	D	685	ARG	CD-NE-CZ	6.92	134.09	124.40
1	C	685	ARG	CD-NE-CZ	6.90	134.06	124.40
1	A	1064	LYS	CA-CB-CG	6.77	127.65	114.10
1	B	1064	LYS	CA-CB-CG	6.76	127.62	114.10
1	C	1064	LYS	CA-CB-CG	6.76	127.62	114.10
1	D	1064	LYS	CA-CB-CG	6.74	127.59	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	495	ASN	CA-C-N	6.69	133.75	121.70
1	D	495	ASN	C-N-CA	6.69	133.75	121.70
1	B	495	ASN	CA-C-N	6.67	133.72	121.70
1	B	495	ASN	C-N-CA	6.67	133.72	121.70
1	C	495	ASN	CA-C-N	6.67	133.71	121.70
1	C	495	ASN	C-N-CA	6.67	133.71	121.70
1	A	495	ASN	CA-C-N	6.67	133.71	121.70
1	A	495	ASN	C-N-CA	6.67	133.71	121.70
1	A	685	ARG	CG-CD-NE	5.86	124.89	112.00
1	B	685	ARG	CG-CD-NE	5.83	124.83	112.00
1	C	685	ARG	CG-CD-NE	5.83	124.82	112.00
1	D	685	ARG	CG-CD-NE	5.83	124.82	112.00
1	C	941	LEU	CB-CA-C	-5.48	102.27	110.88
1	A	941	LEU	CB-CA-C	-5.48	102.28	110.88
1	B	941	LEU	CB-CA-C	-5.48	102.28	110.88
1	D	941	LEU	CB-CA-C	-5.48	102.28	110.88
1	A	594	HIS	CA-C-N	5.11	131.17	121.97
1	A	594	HIS	C-N-CA	5.11	131.17	121.97
1	B	594	HIS	CA-C-N	5.11	131.16	121.97
1	B	594	HIS	C-N-CA	5.11	131.16	121.97
1	C	594	HIS	CA-C-N	5.10	131.14	121.97
1	C	594	HIS	C-N-CA	5.10	131.14	121.97
1	D	594	HIS	CA-C-N	5.10	131.14	121.97
1	D	594	HIS	C-N-CA	5.10	131.14	121.97
1	B	1344	PRO	CA-C-N	5.07	131.21	121.54
1	B	1344	PRO	C-N-CA	5.07	131.21	121.54
1	A	1344	PRO	CA-C-N	5.03	131.15	121.54
1	A	1344	PRO	C-N-CA	5.03	131.15	121.54
1	C	1344	PRO	CA-C-N	5.02	131.13	121.54
1	C	1344	PRO	C-N-CA	5.02	131.13	121.54
1	D	1344	PRO	CA-C-N	5.01	131.11	121.54
1	D	1344	PRO	C-N-CA	5.01	131.11	121.54

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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

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	218	0
1	B	10780	0	10822	216	0
1	C	10780	0	10822	224	0
1	D	10780	0	10822	217	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	867	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 (867) 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:511:LYS:HZ2	1:C:621:PRO:HD2	1.59	0.66
1:C:1356:ARG:NH1	1:C:1371:MET:SD	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:511:LYS:HZ2	1:A:621:PRO:HD2	1.63	0.64
1:B:602:VAL:HG23	1:B:604:LEU:H	1.61	0.64
1:B:511:LYS:HZ2	1:B:621:PRO:HD2	1.62	0.63
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
1:D:511:LYS:HZ2	1:D:621:PRO:HD2	1.64	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:952:LYS:HZ2	1:C:982:ILE:HG23	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
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: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:B:952:LYS:HZ2	1:B:982:ILE:HG23	1.68	0.58
1:D:449:HIS:CE1	1:D:453:ASP:HB2	2.38	0.58
1:D:952:LYS:HZ2	1:D:982:ILE:HG23	1.69	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:A:952:LYS:HZ2	1:A:982:ILE:HG23	1.69	0.57
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: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:C:137:GLN:HE21	1:C:138:LYS:NZ	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:74:TYR:OH	1:D:125:ASP:OD1	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:168:ASN:OD1	1:A:314:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:867:PHE:HE2	1:A:931:MET:HE3	1.74	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:867:PHE:HE2	1:B:931:MET:HE3	1.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:867:PHE:HE2	1:D:931:MET:HE3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:867:PHE:HE2	1:C:931:MET:HE3	1.74	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
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:137:GLN:NE2	1:C:138:LYS:HZ2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:291:THR:HG1	1:D:292:HIS:H	1.59	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
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:A:1364:CYS:HA	1:A:1371:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:291:THR:HG1	1:C:292:HIS:H	1.62	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:C:1364:CYS:HA	1:C:1371:MET:HE3	1.95	0.48
1:A:433:ILE:HG23	1:A:434:LEU:HG	1.96	0.48
1:B:1364:CYS:HA	1:B:1371:MET:HE3	1.95	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:D:1364:CYS:HA	1:D:1371:MET:HE3	1.95	0.47
1:B:363:ILE:HG23	1:B:406:ILE:HG23	1.97	0.47
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:C:645:SER:O	1:C:1129:LYS:NZ	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:416:LEU:O	1:D:439:LYS:NZ	2.45	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:D:946:VAL:O	1:D:975:TYR:OH	2.29	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:A:416:LEU:O	1:A:439:LYS:NZ	2.45	0.46
1:C:1053:GLN:NE2	1:D:1057:GLU:OE2	2.49	0.46
1:C:1403:LYS:HA	1:C:1406:LEU:HB2	1.97	0.46
1:A:1327:PRO:HB2	1:A:1328:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:ARG:HG2	1:A:1146:GLN:H	1.79	0.46
1:B:1327:PRO:HB2	1:B:1328:MET:HE2	1.98	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:1327:PRO:HB2	1:D:1328:MET:HE2	1.98	0.45
1:A:657:LYS:NZ	1:A:723:GLU:OE2	2.50	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:291:THR:HG1	1:B:292:HIS:H	1.65	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: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:619:MET:HE3	1:A:619:MET:HB2	1.83	0.44
1:A:946:VAL:O	1:A:975:TYR:OH	2.29	0.44
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
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:1327:PRO:HB2	1:C:1328:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:LYS:HA	1:B:609:LYS:HD3	1.75	0.43
1:B:657:LYS:NZ	1:B:723:GLU:OE2	2.50	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:657:LYS:NZ	1:C:723:GLU:OE2	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:416:LEU:O	1:C:439:LYS:NZ	2.45	0.43
1:D:619:MET:HE3	1:D:619:MET:HB2	1.83	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:530:CYS:SG	1:A:531:LEU:N	2.91	0.42
1:B:173:VAL:O	1:B:302:ARG:NH2	2.46	0.42
1:B:612:SER:O	1:B:612:SER:OG	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:416:LEU:O	1:B:439:LYS:NZ	2.45	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: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:612:SER:O	1:C:612:SER:OG	2.37	0.42
1:C:619:MET:HE3	1:C:619:MET:HB2	1.83	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
1:C:1489:LYS:O	1:C:1503:TYR:OH	2.35	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:946:VAL:O	1:C:975:TYR:OH	2.29	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
1:C:1307:LEU:O	1:C:1392:ARG:NH2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1349:TYR:HB3	1:A:1351:MET:HE3	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: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: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
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:619:MET:HB2	1:B:619:MET:HE3	1.83	0.40
1:B:939:PHE:O	1:B:943:VAL:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:1349:TYR:HB3	1:C:1351:MET:HE3	2.03	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
1:C:273:ASN:OD1	1:C:273:ASN:N	2.55	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

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	67
1	B	1331/1503 (89%)	1133 (85%)	193 (14%)	5 (0%)	30	67
1	C	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	67
1	D	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	67
All	All	5324/6012 (89%)	4526 (85%)	778 (15%)	20 (0%)	31	67

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
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 ⓘ

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%)	1165 (99%)	11 (1%)	70	78
1	B	1176/1318 (89%)	1165 (99%)	11 (1%)	70	78
1	C	1176/1318 (89%)	1165 (99%)	11 (1%)	70	78
1	D	1176/1318 (89%)	1165 (99%)	11 (1%)	70	78
All	All	4704/5272 (89%)	4660 (99%)	44 (1%)	68	78

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	A	685	ARG
1	A	715	THR
1	A	742	VAL
1	A	749	VAL
1	A	839	LEU
1	A	930	MET
1	A	941	LEU
1	A	1024	LEU
1	A	1064	LYS
1	A	1134	GLN
1	B	73	VAL
1	B	685	ARG
1	B	715	THR
1	B	742	VAL
1	B	749	VAL
1	B	839	LEU
1	B	930	MET
1	B	941	LEU
1	B	1024	LEU
1	B	1064	LYS
1	B	1134	GLN
1	C	73	VAL
1	C	685	ARG

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Mol	Chain	Res	Type
1	C	715	THR
1	C	742	VAL
1	C	749	VAL
1	C	839	LEU
1	C	930	MET
1	C	941	LEU
1	C	1024	LEU
1	C	1064	LYS
1	C	1134	GLN
1	D	73	VAL
1	D	685	ARG
1	D	715	THR
1	D	742	VAL
1	D	749	VAL
1	D	839	LEU
1	D	930	MET
1	D	941	LEU
1	D	1024	LEU
1	D	1064	LYS
1	D	1134	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	381	GLN
1	A	414	GLN
1	A	446	HIS
1	A	449	HIS
1	A	451	ASN
1	A	454	HIS
1	A	506	ASN
1	A	509	GLN
1	A	525	ASN
1	A	557	GLN
1	A	560	HIS
1	A	582	HIS
1	A	583	ASN
1	A	594	HIS
1	A	646	GLN
1	A	800	HIS
1	A	869	ASN

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Mol	Chain	Res	Type
1	A	973	HIS
1	A	1054	GLN
1	A	1056	GLN
1	A	1135	ASN
1	A	1302	ASN
1	A	1448	HIS
1	A	1461	ASN
1	A	1502	HIS
1	B	137	GLN
1	B	381	GLN
1	B	388	GLN
1	B	446	HIS
1	B	449	HIS
1	B	451	ASN
1	B	454	HIS
1	B	506	ASN
1	B	509	GLN
1	B	525	ASN
1	B	557	GLN
1	B	560	HIS
1	B	582	HIS
1	B	594	HIS
1	B	646	GLN
1	B	684	HIS
1	B	736	GLN
1	B	800	HIS
1	B	869	ASN
1	B	973	HIS
1	B	1054	GLN
1	B	1056	GLN
1	B	1106	HIS
1	B	1108	GLN
1	B	1135	ASN
1	B	1302	ASN
1	B	1448	HIS
1	B	1453	ASN
1	B	1461	ASN
1	B	1502	HIS
1	C	137	GLN
1	C	381	GLN
1	C	446	HIS
1	C	449	HIS

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Mol	Chain	Res	Type
1	C	451	ASN
1	C	454	HIS
1	C	506	ASN
1	C	509	GLN
1	C	525	ASN
1	C	557	GLN
1	C	560	HIS
1	C	582	HIS
1	C	594	HIS
1	C	646	GLN
1	C	684	HIS
1	C	736	GLN
1	C	800	HIS
1	C	869	ASN
1	C	973	HIS
1	C	1054	GLN
1	C	1135	ASN
1	C	1302	ASN
1	C	1448	HIS
1	C	1461	ASN
1	C	1502	HIS
1	D	137	GLN
1	D	381	GLN
1	D	446	HIS
1	D	449	HIS
1	D	451	ASN
1	D	454	HIS
1	D	506	ASN
1	D	509	GLN
1	D	525	ASN
1	D	557	GLN
1	D	560	HIS
1	D	582	HIS
1	D	594	HIS
1	D	646	GLN
1	D	736	GLN
1	D	800	HIS
1	D	869	ASN
1	D	973	HIS
1	D	1053	GLN
1	D	1054	GLN
1	D	1135	ASN

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Mol	Chain	Res	Type
1	D	1302	ASN
1	D	1448	HIS
1	D	1461	ASN
1	D	1502	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

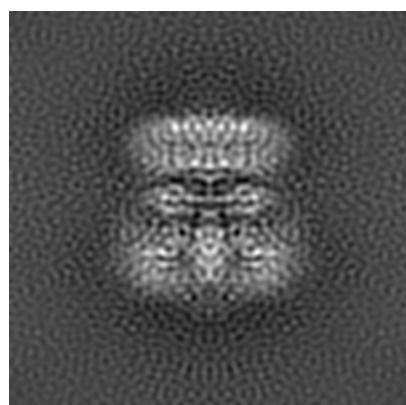
6 Map visualisation [i](#)

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.

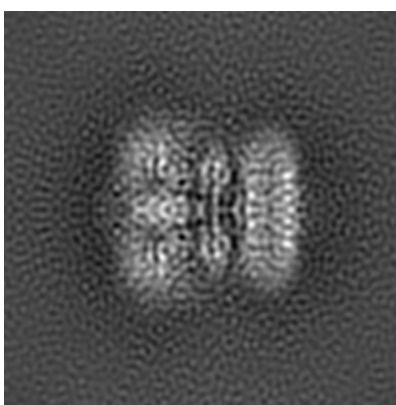
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

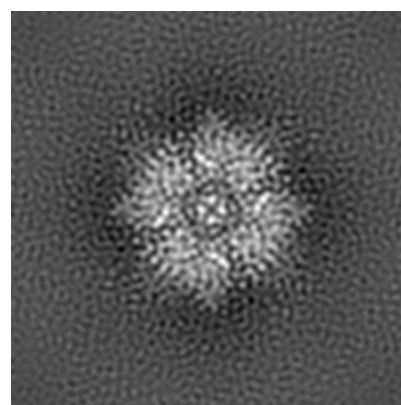
6.1.1 Primary map



X



Y

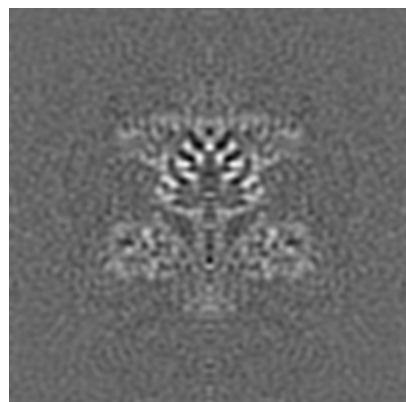


Z

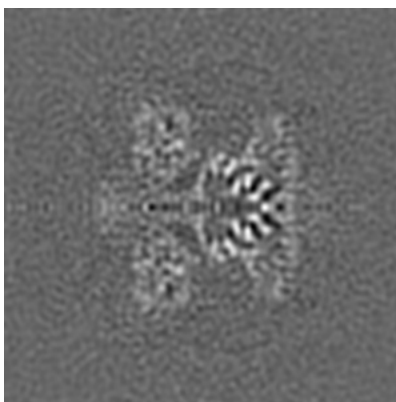
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

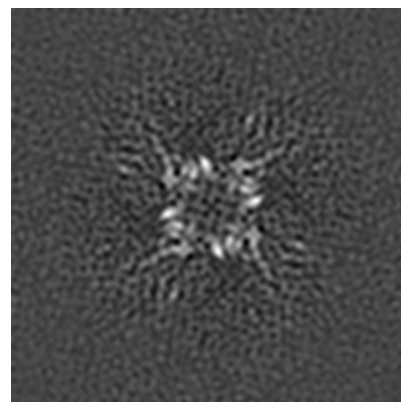
6.2.1 Primary map



X Index: 150



Y Index: 150

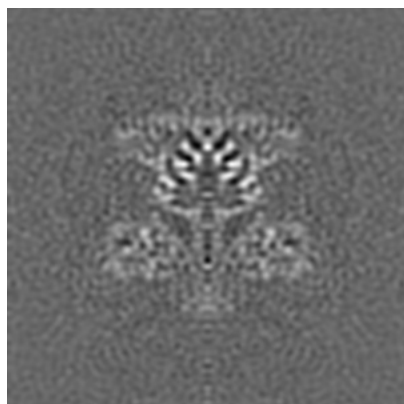


Z Index: 150

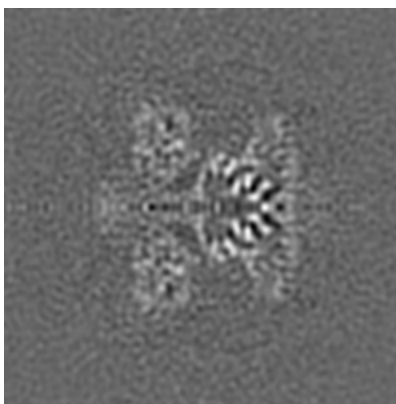
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

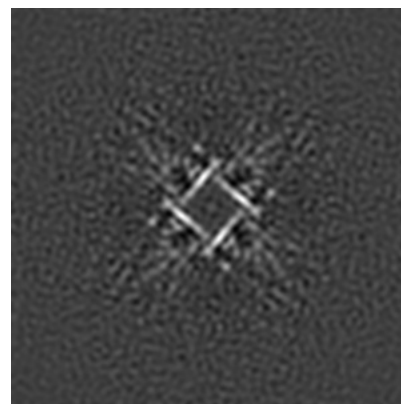
6.3.1 Primary map



X Index: 150



Y Index: 150

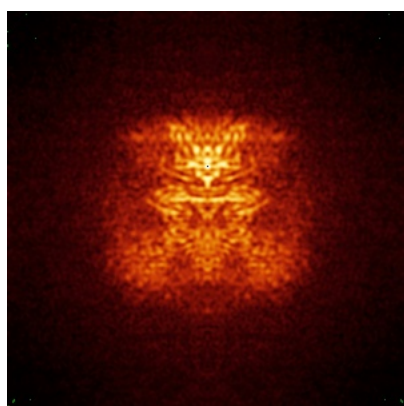


Z Index: 158

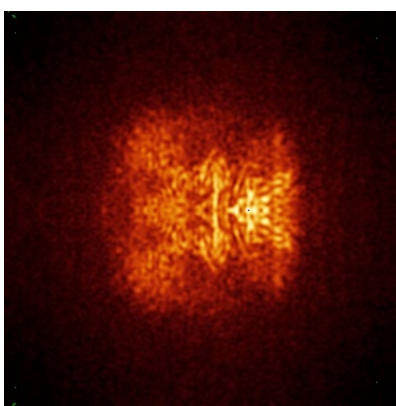
The images above show the largest variance slices of the map in three orthogonal directions.

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

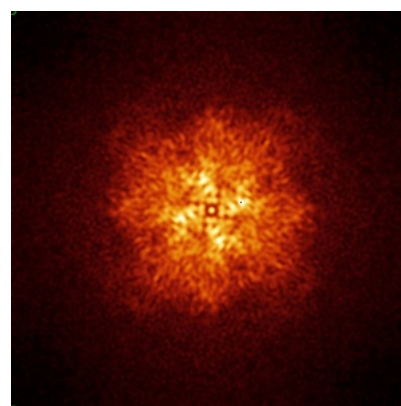
6.4.1 Primary map



X



Y

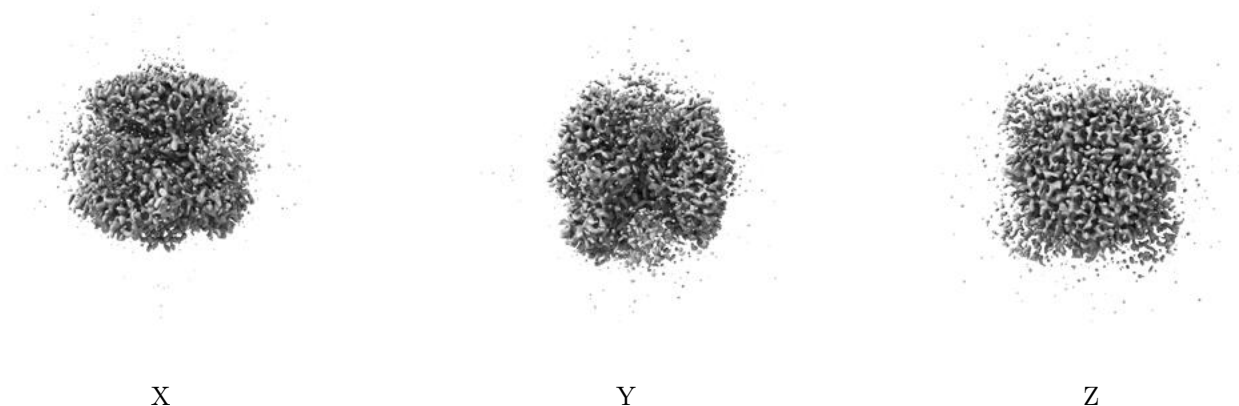


Z

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 2.77. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

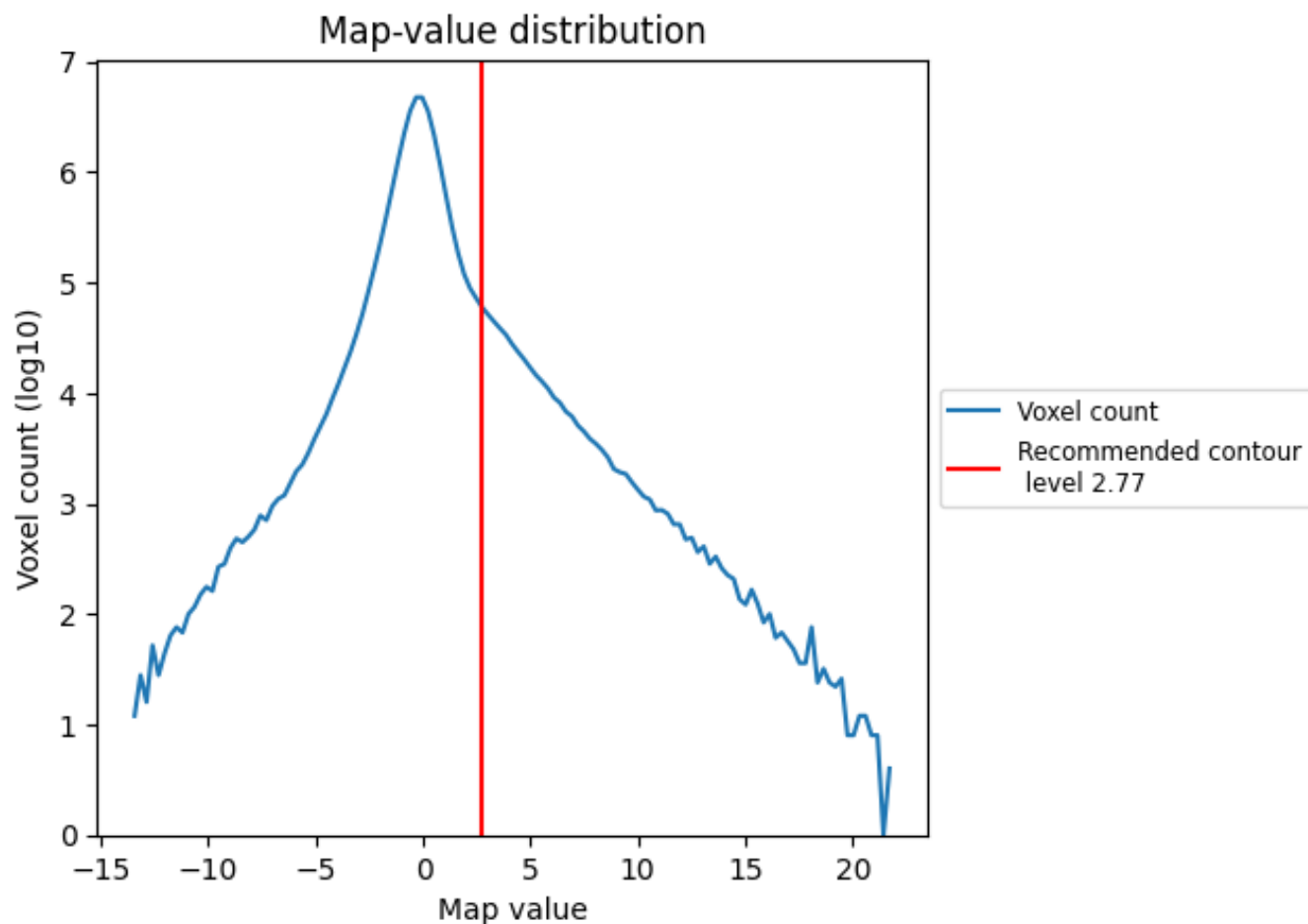
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

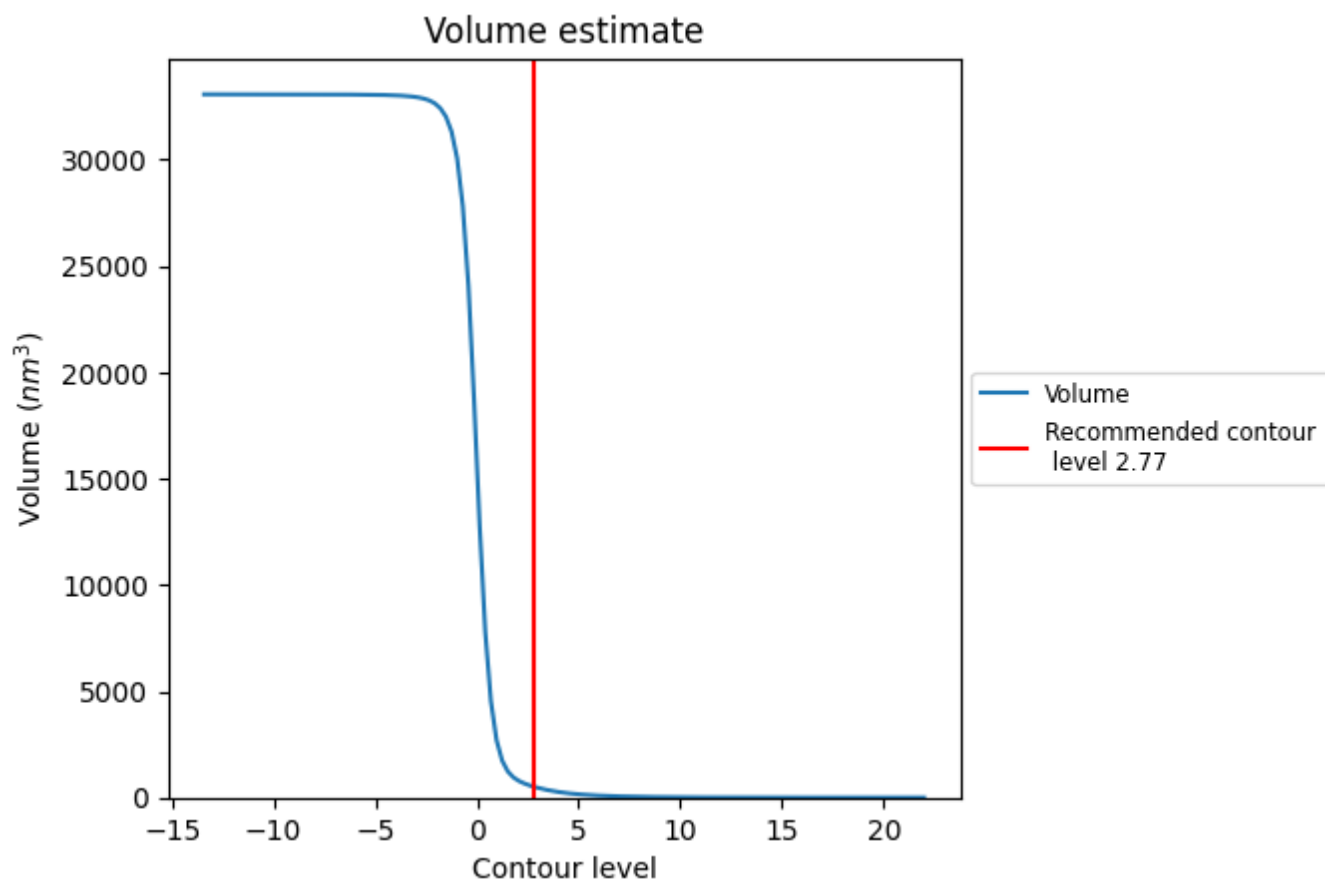
This section contains the results of statistical analysis of the map.

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.

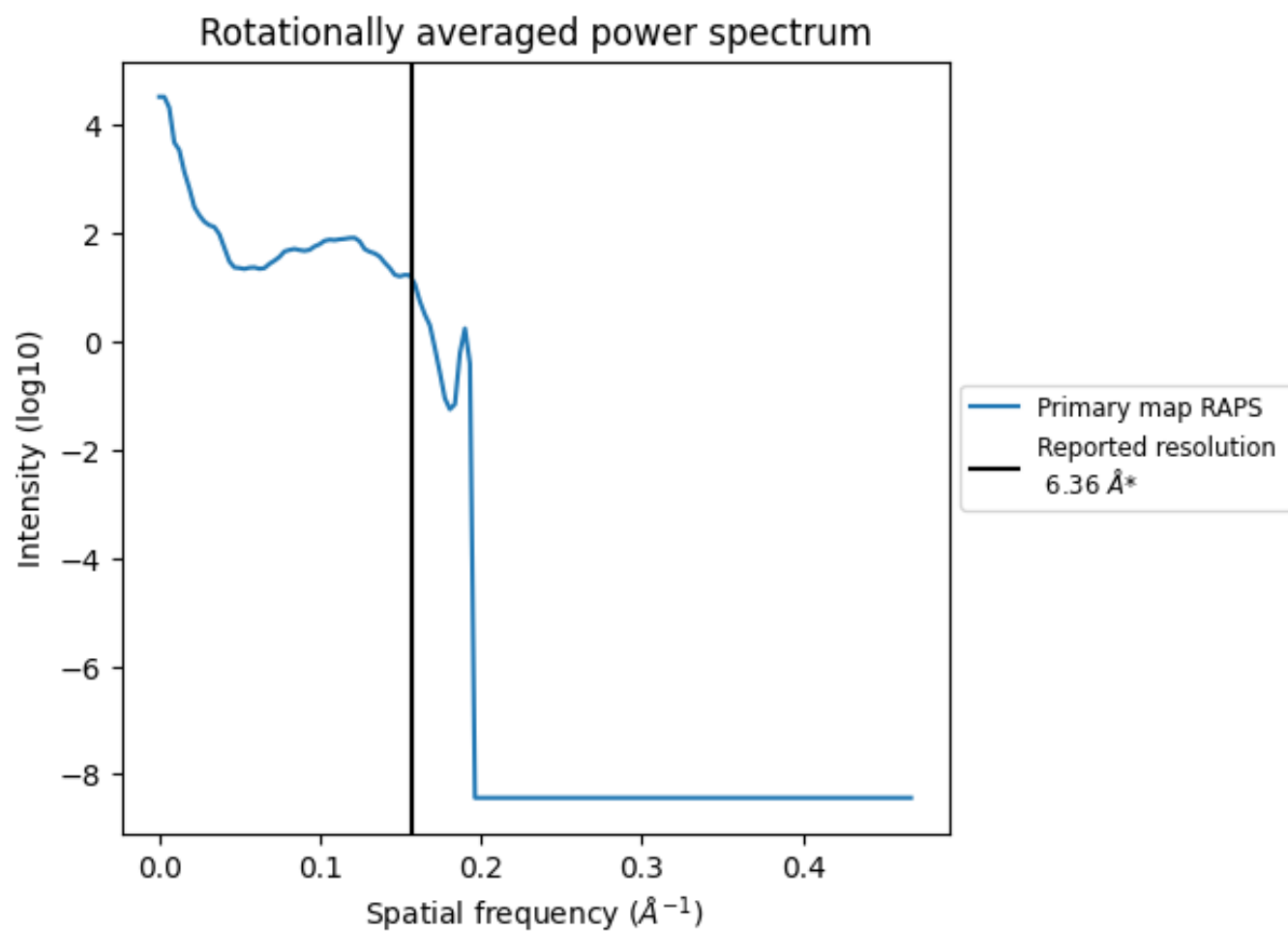
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.157 Å⁻¹

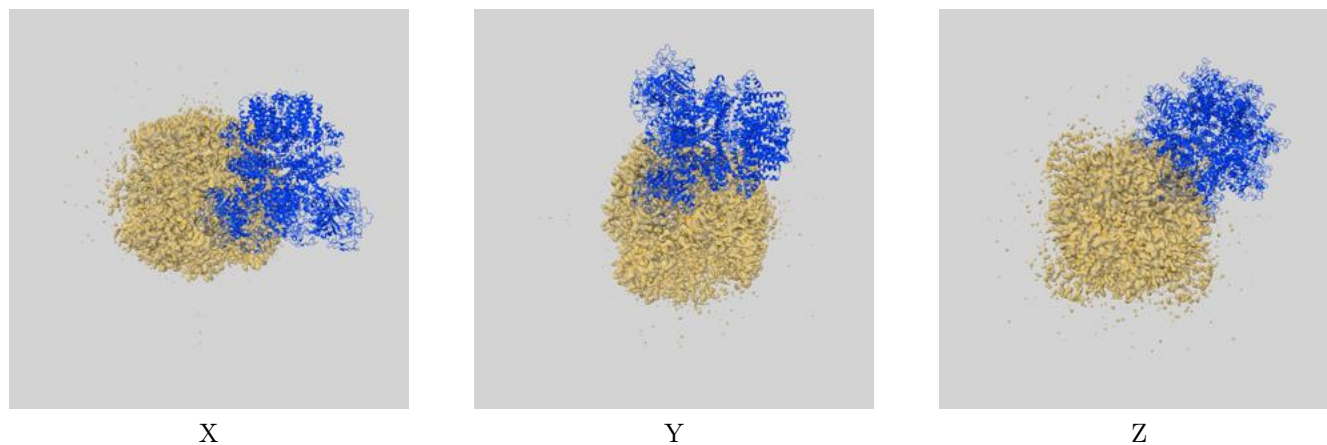
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

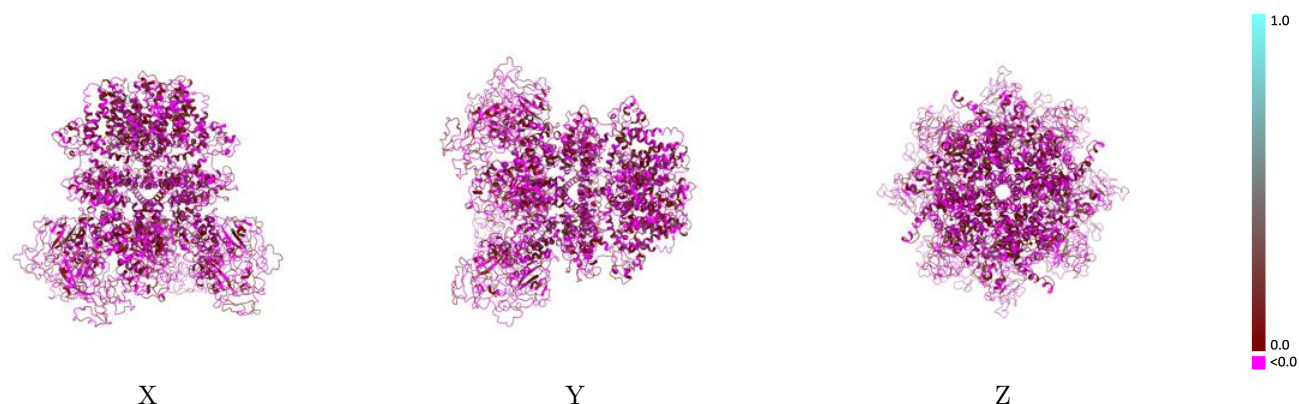
This section contains information regarding the fit between EMDB map EMD-9134 and PDB model 6MJ2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



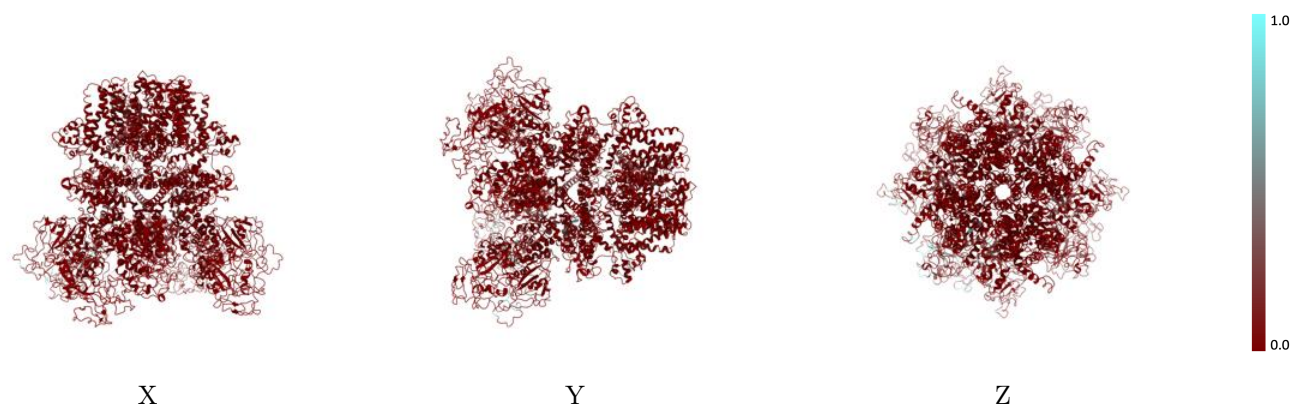
The images above show the 3D surface view of the map at the recommended contour level 2.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



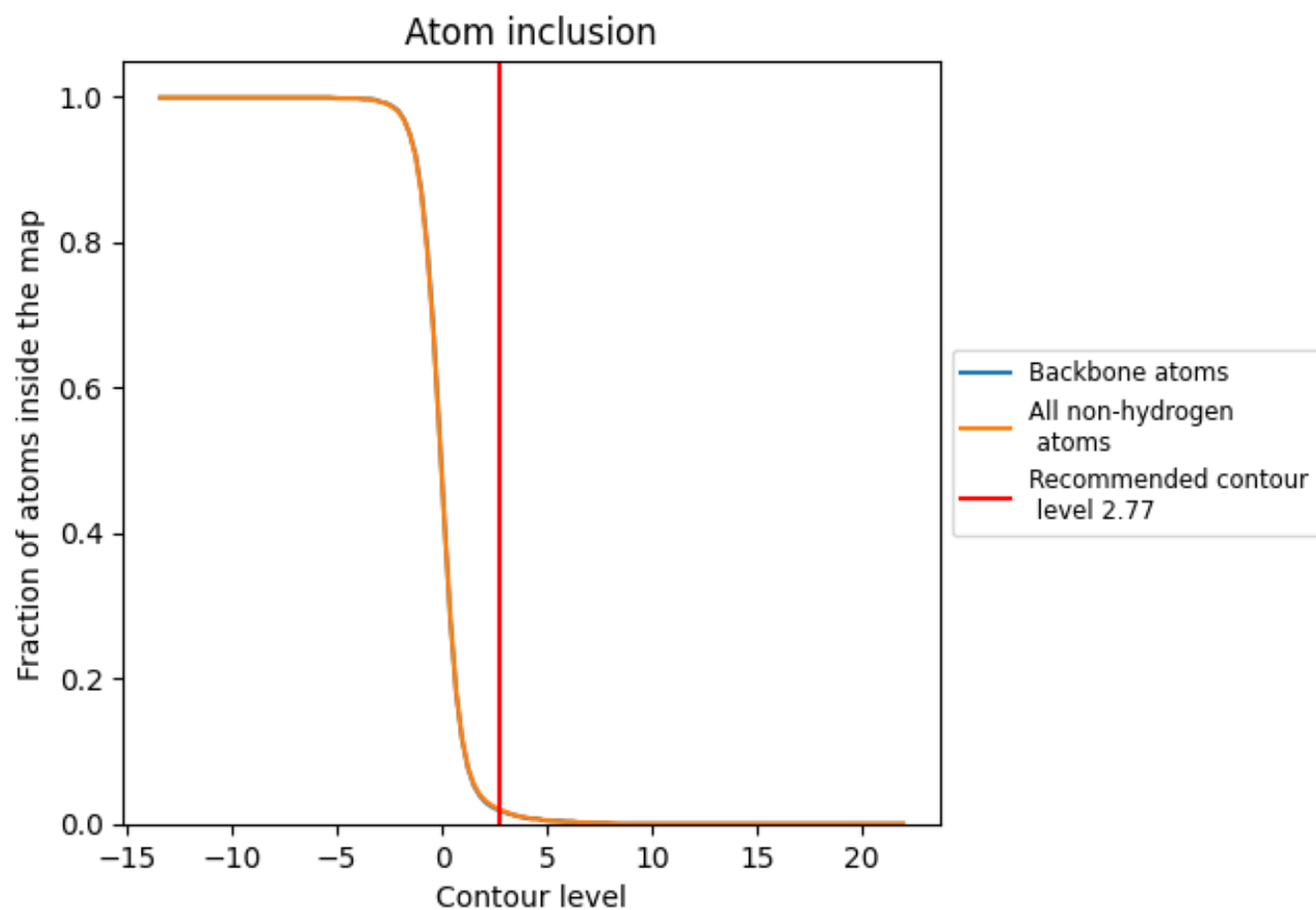
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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	0.0190	-0.0000
A	0.0600	-0.0020
B	0.0000	-0.0020
C	0.0000	0.0030
D	0.0150	-0.0000

