



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:31 PM UTC

PDB ID : 8YFG / pdb_00008yfg
EMDB ID : EMD-39223
Title : Human PIEZO1-R2456H_MDFIC
Authors : Zhang, M.F.
Deposited on : 2024-02-24
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

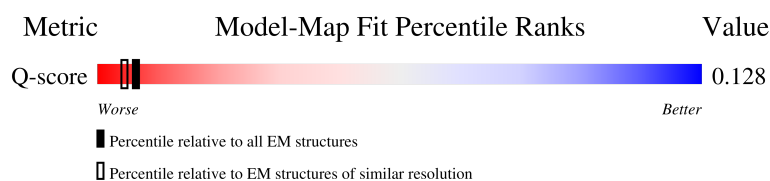
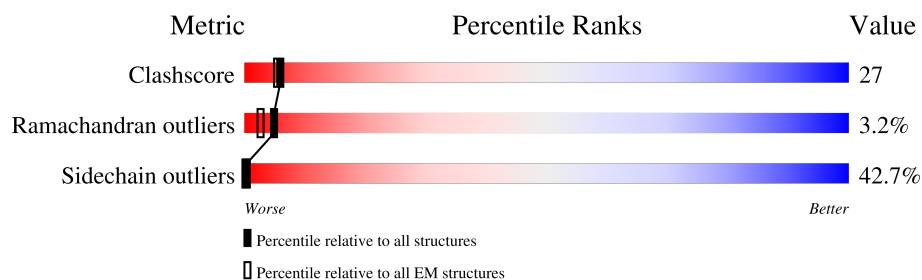
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	2521	
1	B	2521	
1	D	2521	
2	C	246	

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Mol	Chain	Length	Quality of chain
2	E	246	9% • 5% • 91%
2	F	246	8% • 5% • 91%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31599 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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1280	Total	C	N	O	S	0	0
			10394	6871	1728	1734	61		
1	B	1280	Total	C	N	O	S	0	0
			10388	6865	1728	1734	61		
1	D	1280	Total	C	N	O	S	0	0
			10394	6871	1728	1734	61		

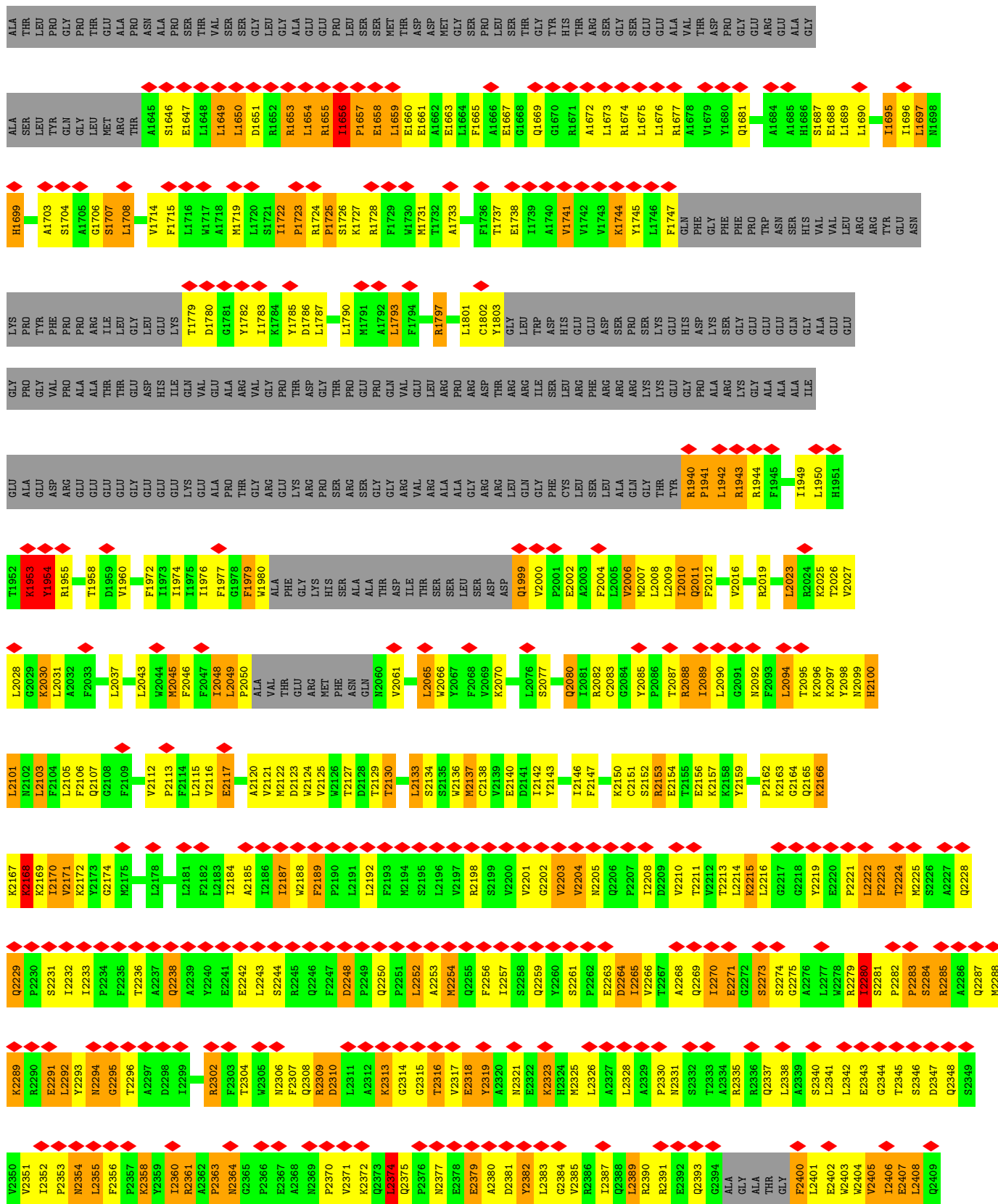
There are 3 discrepancies between the modelled and reference sequences:

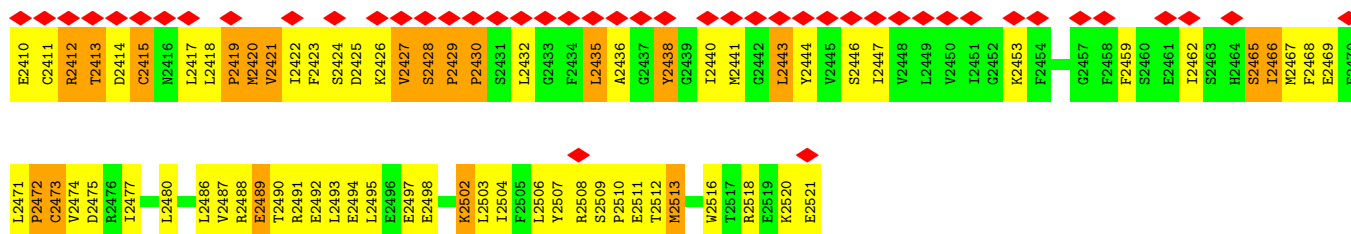
Chain	Residue	Modelled	Actual	Comment	Reference
A	2456	HIS	ARG	variant	UNP Q92508
B	2456	HIS	ARG	variant	UNP Q92508
D	2456	HIS	ARG	variant	UNP Q92508

- Molecule 2 is a protein called MyoD family inhibitor domain-containing protein.

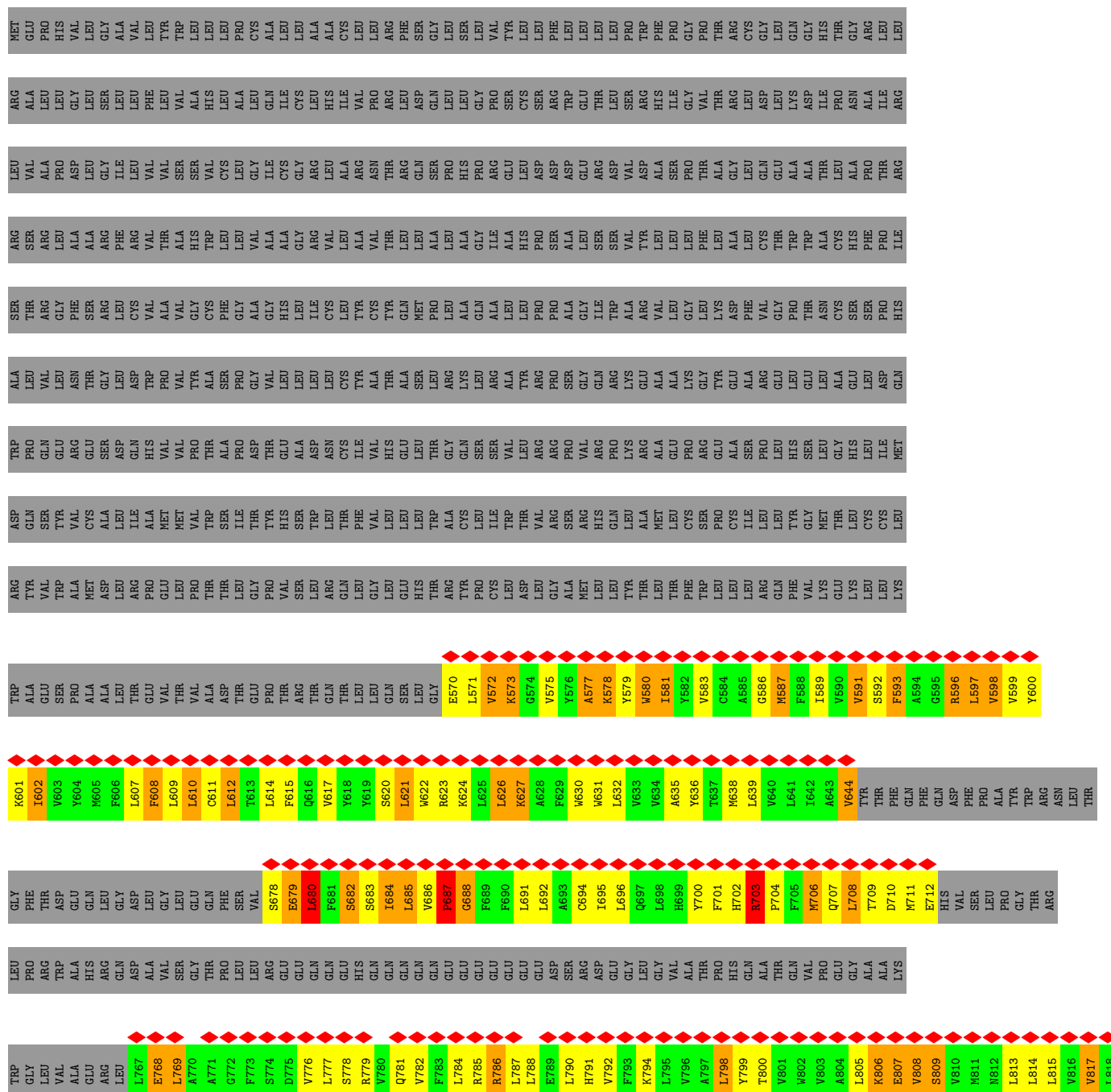
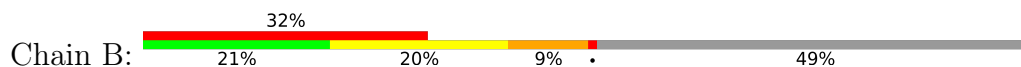
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	21	Total	C	N	O	S	0	0
			141	80	21	33	7		
2	E	21	Total	C	N	O	S	0	0
			141	80	21	33	7		
2	F	21	Total	C	N	O	S	0	0
			141	80	21	33	7		





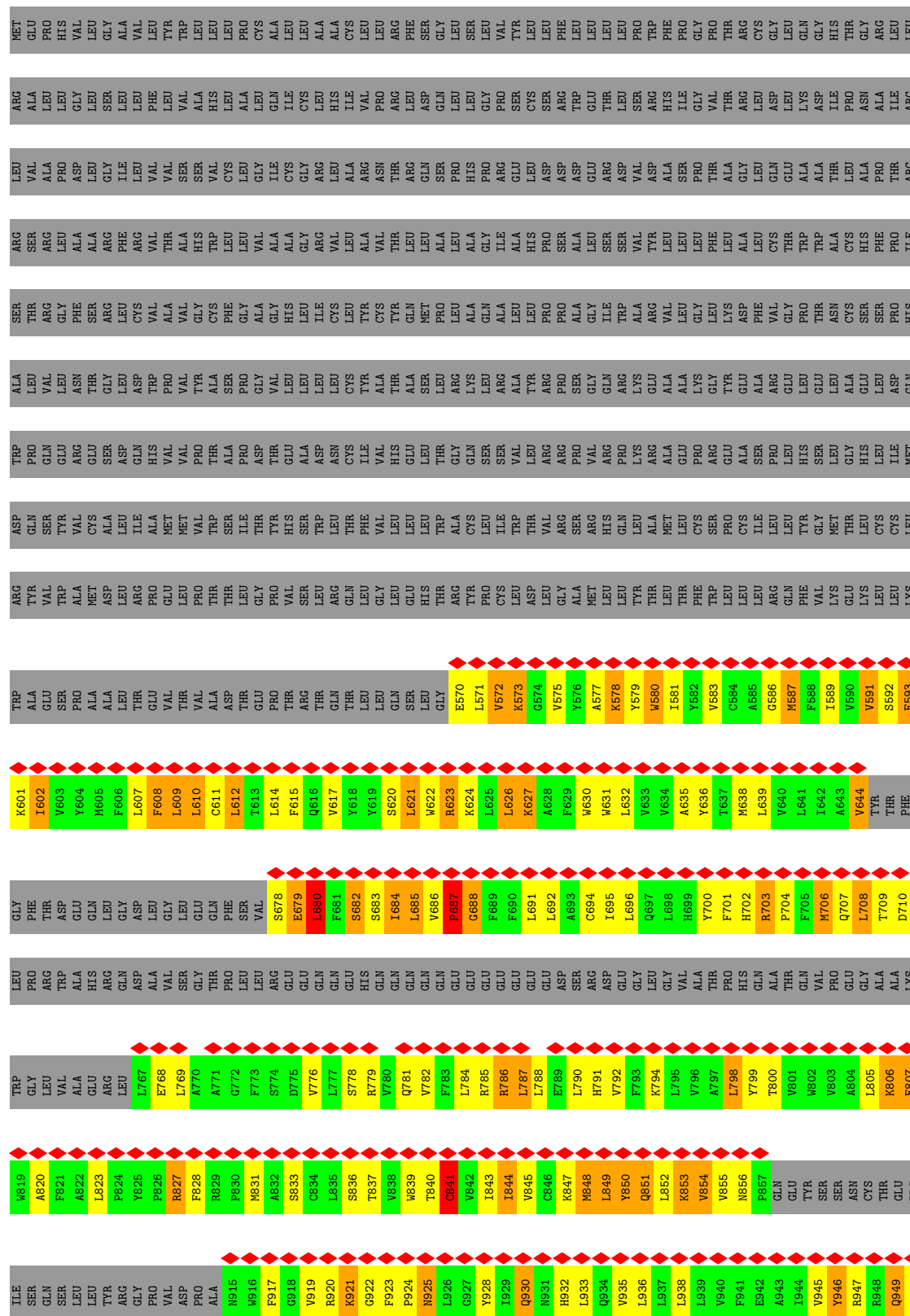


• Molecule 1: Piezo-type mechanosensitive ion channel component 1









LEU	PRO	ALA	GLN	ALA	VAL	PHE	ALA	SER	G970	T971	G972	G973	G974	L975	D976	G977	D978	L979	L980	G981	C982	L983	K984	G985	F986	L987	N988	F989	F990	F991	Y992	K993	F994	G995	L996	E997	C999	F1000	L1001	M1002	A1003	V1004	N1005	V1006	I1007	G1008	Q1009	R1010	M1011	N1012	F1013	L1014	V1015	T1016	L1017	H1018	G1019		
V1021	L1022	V1023	A1024	I1025	L1026	T1027	R1028	R1029	H1030	R1031	Q1032	A1033	I1034	A1035	L1036	L1037	W1038	P1039	N1040	Y1041	C1042	L1043	F1044	L1045	A1046	L1047	F1048	L1049	L1050	Y1051	Q1052	Y1053	L1054	L1055	C1056	L1057	G1058	MET	PRO	PRO	ALA	LEU	CYS	ILE	ASP	TVR	PRO	TRP	ARG	LEU	ALA	VAL	MET	ASN	SER	ALA			
LEU	ILE	LYS	TRP	LEU	TYR	LEU	PRO	ASP	PHE	ARG	ALA	PRO	ASN	S1096	T1097	N1098	L1099	L1100	S1101	D1102	F1103	L1104	L1105	L1106	L1107	C1108	A1109	S1110	Q1111	Q1112	W1113	Q1114	V1115	F1116	S1117	A1118	E1119	R1120	T1121	GLU	GLU	TRP	GLN	ARG	MET	ALA	GLY	VAL	ASN	THR	ASP	ARG	LEU	GLU	PRO	LEU	ARG	GLY	
GLU	PRO	ASN	PRO	VAL	PRO	ASN	PHE	ILE	HIS	CYS	ARG	SER	Y1154	L1155	D1156	M1157	L1158	K1159	V1160	A1161	V1162	F1163	R1164	Y1165	L1166	L1167	W1168	L1169	V1170	L1171	V1172	V1173	V1174	F1175	V1176	T1177	G1178	A1179	T1180	R1181	I1182	S1183	I1184	F1185	G1186	L1187	G1188	Y1189	L1190	L1191	A1192	C1193	F1194	Y1195	L1196	L1197	L1198	F1199	G1200
T1201	A1202	L1203	L1204	Q1205	R1206	D1207	T1208	R1209	A1210	R1211	L1212	V1213	L1214	W1215	D1216	C1217	L1218	I1219	L1220	Y1221	N1222	V1223	T1224	V1225	I1226	I1227	S1228	K1229	N1230	M1231	L1232	S1233	LEU	LEU	ALA	CYS	VAL	PHE	VAL	GLU	GLN	MET	GLN	THR	PHE	CYS	TRP	VAL	ILE	GLN	LEU	PHE	SER	LEU	VAL	CYS	THR	VAL	
LYS	GLY	TYR	ASP	PRO	LYS	GLU	MET	MET	ASP	ARG	ASP	GLN	ASP	CYS	LEU	LEU	PRO	VAL	GLU	A1283	G1284	I1285	I1286	W1287	D1288	S1289	V1290	C1291	F1292	F1293	F1294	L1295	L1296	L1297	Q1298	R1299	R1300	V1301	F1302	L1303	S1304	H1305	Y1306	Y1307	L1308	H1309	V1310	R1311	A1312	D1313	L1314	Q1315	A1316	T1317	A1318	L1319	L1320		
A1321	S1322	R1323	L1327	Y1328	M1332	L1333	I1336	H1339	R1340	E1343	E1344	K1345	S1346	L1347	A1348	Q1349	L1350	K1351	M1354	E1355	R1356	I1357	R1358	A1359	K1360	E1362	K1363	H1364	R1365	Q1366	G1367	R1368	V1369	D1370	ARG	SER	ARG	PRO	GLN	ASP	THR	LEU	GLY	PRO	LYS	ASP	PRO	GLY	LEU	PRO	GLY								
PRO	ASP	SER	VAL	GLY	GLN	SER	SER	PRO	PRO	ARG	GLN	TRP	ARG	PRO	TRP	D1408	H1409	A1410	T1411	V1412	I1413	H1414	S1415	G1416	R1417	Y1418	F1419	E1422	S1423	D1424	S1425	E1426	E1427	GLU	GLU	GLU	ALA	VAL	PRO	GLU	ASP	PRO	ARG	PRO	SER	ALA	ALA	GLN	SER	ALA	GLN	LEU	ALA	TYR	GLN				
ALA	TRP	VAL	THR	ASN	ALA	ALA	VAL	LEU	ARG	ARG	GLN	GLN	GLN	GLN	GLN	ALA	ARG	GLN	GLU	GLN	GLN	GLN	GLN	GLN	PRO	GLY	PRO	GLN	GLU	VAL	PRO	GLU	GLY	PRO	GLU	GLU	ALA	GLU	VAL	ALA	GLY	ARG	SER	HIS	VAL	VAL	ARG	VAL	LEU	SER									
THR	ALA	F1513	L1514	W1515	M1516	L1517	G1518	Q1519	A1520	L1521	E1524	L1529	F1532	T1533	R1534	H1535	H1536	G1537	T1538	M1539	S1540	D1541	V1542	L1543	R1544	A1545	E1546	R1547	Y1548	L1549	L1550	T1551	Q1552	E1553	L1554	L1555	Q1556	G1557	G1558	E1559	V1560	H1561	R1562	G1563	V1564	L1565	D1566	Q1567	L1568	TYR	THR	SER	GLN	ALA	GLU				
ALA	THR	LEU	PRO	PRO	THR	GLU	GLU	ASN	PRO	ALA	PRO	THR	VAL	SER	GLY	LEU	GLY	LEU	GLU	GLU	MET	THR	ASP	ASP	GLY	PRO	LEU	SER	THR	GLY	TYR	HIS	THR	ARG	SER	GLY	GLU	VAL	THR	ASP	PRO	PRO	GLY	GLY	ARG	GLU	ALA	GLY											
ALA	SER	LEU	TYR	GLY	LEU	MET	ARG	A1645	S1646	E1647	L1648	L1649	L1650	D1651	R1652	R1653	L1654	R1655	T1656	P1657	E1658	L1659	E1660	E1662	E1663	L1664	F1665	A1666	E1667	G1668	Q1669	G1670	L1671	L1672	L1673	R1674	L1675	L1676	R1677	A1678	V1679	Y1680	Q1681	A1684	A1685	H1686	S1687	E1688	L1689	L1690	I1695	I1696	L1697	H1698					
H1699	A1703	S1704	A1705	G1706	S1707	L1708	V1709	L1710	V1714	F1715	L1716	W1717	A1718	M1719	L1720	S1721	I1722	P1723	R1724	P1725	S1726	K1727	R1728	F1729	W1730	M1731	T1732	A1733	F1736	T1737	E1738	I1739	A1740	V1741	V1742	V1743	K1744	Y1745	L1746	F1747	GLN	PHE	GLY	PHE	PHE	PRO	TRP	ASN	HIS	VAL	VAL	LEU	ARG	ARG	TYR				

- Molecule 2: MyoD family inhibitor domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.136	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	410.4, 410.4, 410.4	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.57, 0.57, 0.57	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	2/10646 (0.0%)	0.94	59/14437 (0.4%)
1	B	0.56	2/10639 (0.0%)	0.94	58/14428 (0.4%)
1	D	0.57	5/10646 (0.0%)	0.93	57/14437 (0.4%)
2	C	0.79	0/141	1.55	4/188 (2.1%)
2	E	0.52	0/141	0.96	0/188
2	F	0.64	0/141	1.84	4/188 (2.1%)
All	All	0.56	9/32354 (0.0%)	0.95	182/43866 (0.4%)

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	D	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2106	PHE	C-O	6.80	1.32	1.24
1	D	2281	SER	C-O	-6.19	1.19	1.24
1	A	1160	VAL	CA-CB	6.03	1.62	1.54
1	B	1160	VAL	CA-CB	6.03	1.62	1.54
1	D	1160	VAL	CA-CB	6.00	1.62	1.54
1	D	2109	PHE	C-O	5.32	1.30	1.24
1	B	2289	LYS	C-N	-5.09	1.27	1.33
1	D	2289	LYS	C-N	-5.08	1.27	1.33
1	A	2289	LYS	C-N	-5.04	1.27	1.33

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	243	ILE	N-CA-C	-19.14	95.53	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	930	GLN	N-CA-C	11.20	126.52	113.19
1	A	930	GLN	N-CA-C	11.18	126.50	113.19
1	D	930	GLN	N-CA-C	11.16	126.47	113.19
2	C	242	GLY	N-CA-C	-10.56	100.06	112.73
1	D	2374	LEU	N-CA-C	-9.97	100.40	111.07
1	B	2374	LEU	N-CA-C	-9.97	100.41	111.07
1	A	2374	LEU	N-CA-C	-9.95	100.43	111.07
1	A	2415	CYS	N-CA-C	-9.76	101.03	113.72
1	D	2415	CYS	N-CA-C	-9.75	101.04	113.72
1	B	2415	CYS	N-CA-C	-9.74	101.05	113.72
1	B	2438	TYR	N-CA-C	9.74	127.03	114.75
1	A	2438	TYR	N-CA-C	9.71	126.99	114.75
1	D	2438	TYR	N-CA-C	9.71	126.98	114.75
1	A	688	GLY	N-CA-C	-9.55	100.94	112.49
1	D	688	GLY	N-CA-C	-9.54	100.94	112.49
1	B	688	GLY	N-CA-C	-9.54	100.95	112.49
1	A	1785	TYR	N-CA-C	-9.44	101.27	113.17
1	D	1785	TYR	N-CA-C	-9.41	101.31	113.17
1	B	1785	TYR	N-CA-C	-9.40	101.32	113.17
1	D	987	ILE	N-CA-C	-9.31	101.31	110.72
1	B	987	ILE	N-CA-C	-9.29	101.34	110.72
1	A	987	ILE	N-CA-C	-9.27	101.36	110.72
1	B	686	VAL	CA-C-N	-9.08	110.43	119.87
1	B	686	VAL	C-N-CA	-9.08	110.43	119.87
1	A	686	VAL	CA-C-N	-9.06	110.45	119.87
1	A	686	VAL	C-N-CA	-9.06	110.45	119.87
1	D	686	VAL	CA-C-N	-9.06	110.45	119.87
1	D	686	VAL	C-N-CA	-9.06	110.45	119.87
1	A	680	LEU	N-CA-C	-8.86	101.32	110.97
1	B	680	LEU	N-CA-C	-8.84	101.33	110.97
1	D	680	LEU	N-CA-C	-8.83	101.35	110.97
1	B	1197	LEU	N-CA-C	-8.43	102.58	113.12
1	A	1197	LEU	N-CA-C	-8.42	102.59	113.12
1	D	1197	LEU	N-CA-C	-8.41	102.61	113.12
1	B	2281	SER	N-CA-C	8.21	122.65	110.10
1	D	1551	THR	N-CA-C	-7.99	105.51	114.62
1	A	1551	THR	N-CA-C	-7.98	105.52	114.62
1	B	1551	THR	N-CA-C	-7.96	105.54	114.62
2	F	243	ILE	CB-CA-C	7.68	117.85	110.63
1	B	2281	SER	CB-CA-C	-7.06	98.17	108.84
1	B	1115	VAL	N-CA-C	-6.99	106.10	111.62
1	A	1115	VAL	N-CA-C	-6.96	106.12	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1115	VAL	N-CA-C	-6.95	106.13	111.62
2	F	243	ILE	N-CA-CB	6.87	122.14	111.57
1	A	2285	ARG	CA-C-N	-6.80	110.48	120.28
1	A	2285	ARG	C-N-CA	-6.80	110.48	120.28
1	A	2285	ARG	N-CA-C	6.74	118.63	111.28
1	B	1204	LEU	N-CA-C	-6.71	104.11	112.90
1	A	608	PHE	N-CA-C	-6.71	103.78	112.23
2	C	243	ILE	CB-CA-C	6.71	122.29	111.29
1	D	702	HIS	N-CA-C	-6.71	103.78	112.23
1	A	1204	LEU	N-CA-C	-6.70	104.12	112.90
1	B	702	HIS	N-CA-C	-6.70	103.79	112.23
1	D	1204	LEU	N-CA-C	-6.69	104.13	112.90
1	B	608	PHE	N-CA-C	-6.69	103.80	112.23
1	A	702	HIS	N-CA-C	-6.68	103.81	112.23
1	D	608	PHE	N-CA-C	-6.68	103.81	112.23
2	C	245	PHE	N-CA-C	-6.66	95.09	109.81
1	A	612	LEU	N-CA-C	-6.51	104.10	111.07
1	B	612	LEU	N-CA-C	-6.50	104.11	111.07
1	D	612	LEU	N-CA-C	-6.49	104.12	111.07
1	B	2285	ARG	CA-C-N	-6.40	111.06	120.28
1	B	2285	ARG	C-N-CA	-6.40	111.06	120.28
1	B	817	VAL	N-CA-C	-6.30	106.56	113.43
1	A	1317	THR	N-CA-C	-6.29	104.50	111.36
1	A	817	VAL	N-CA-C	-6.29	106.57	113.43
1	D	817	VAL	N-CA-C	-6.28	106.58	113.43
1	A	2204	VAL	N-CA-C	6.27	117.51	109.30
1	B	1317	THR	N-CA-C	-6.26	104.53	111.36
1	D	1317	THR	N-CA-C	-6.26	104.54	111.36
1	B	2204	VAL	N-CA-C	6.25	117.49	109.30
1	D	2204	VAL	N-CA-C	6.25	117.48	109.30
1	A	687	PRO	N-CA-C	6.15	121.60	114.03
1	B	687	PRO	N-CA-C	6.15	121.59	114.03
1	D	687	PRO	N-CA-C	6.13	121.57	114.03
2	C	236	ILE	CB-CA-C	-6.10	104.18	111.81
1	D	2281	SER	N-CA-C	6.09	119.91	109.06
1	A	1706	GLY	N-CA-C	-6.04	102.58	111.03
1	B	1706	GLY	N-CA-C	-6.03	102.58	111.03
1	D	1706	GLY	N-CA-C	-6.02	102.60	111.03
1	D	1703	ALA	N-CA-C	5.98	116.18	108.34
1	A	1703	ALA	N-CA-C	5.98	116.18	108.34
1	B	1703	ALA	N-CA-C	5.97	116.17	108.34
1	D	1304	SER	N-CA-C	-5.97	105.92	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1304	SER	N-CA-C	-5.96	105.92	112.72
1	B	1304	SER	N-CA-C	-5.95	105.94	112.72
1	A	632	LEU	N-CA-C	-5.78	104.90	111.14
1	A	703	ARG	N-CA-C	5.77	120.60	112.75
1	A	2130	THR	N-CA-C	-5.77	106.40	113.50
1	B	703	ARG	N-CA-C	5.77	120.59	112.75
1	B	2130	THR	N-CA-C	-5.76	106.41	113.50
1	D	2130	THR	N-CA-C	-5.76	106.42	113.50
1	B	632	LEU	N-CA-C	-5.74	104.94	111.14
1	D	632	LEU	N-CA-C	-5.73	104.95	111.14
1	D	703	ARG	N-CA-C	5.73	120.55	112.75
1	A	2413	THR	N-CA-C	-5.71	104.52	113.02
1	D	2413	THR	N-CA-C	-5.70	104.53	113.02
1	B	2413	THR	N-CA-C	-5.70	104.53	113.02
1	D	591	VAL	N-CA-C	-5.69	103.81	111.44
1	B	591	VAL	N-CA-C	-5.68	103.83	111.44
1	A	591	VAL	N-CA-C	-5.66	103.85	111.44
1	A	1657	PRO	CA-C-O	-5.66	117.02	121.38
1	D	1013	PHE	N-CA-C	-5.66	106.54	113.50
1	A	1013	PHE	N-CA-C	-5.65	106.55	113.50
1	B	1656	ILE	CA-C-N	-5.65	115.94	121.65
1	B	1656	ILE	C-N-CA	-5.65	115.94	121.65
1	D	1656	ILE	CA-C-N	-5.64	115.95	121.65
1	D	1656	ILE	C-N-CA	-5.64	115.95	121.65
1	B	1013	PHE	N-CA-C	-5.63	106.57	113.50
1	A	1656	ILE	CA-C-N	-5.62	115.97	121.65
1	A	1656	ILE	C-N-CA	-5.62	115.97	121.65
1	B	1657	PRO	CA-C-O	-5.61	117.06	121.38
1	D	1657	PRO	CA-C-O	-5.60	117.07	121.38
1	B	1541	ASP	N-CA-C	-5.59	106.81	113.97
1	D	923	PHE	CA-C-N	-5.59	114.50	120.03
1	D	923	PHE	C-N-CA	-5.59	114.50	120.03
1	D	1541	ASP	N-CA-C	-5.58	106.82	113.97
1	A	1541	ASP	N-CA-C	-5.58	106.82	113.97
1	A	923	PHE	CA-C-N	-5.56	114.52	120.03
1	A	923	PHE	C-N-CA	-5.56	114.52	120.03
1	B	923	PHE	CA-C-N	-5.56	114.52	120.03
1	B	923	PHE	C-N-CA	-5.56	114.52	120.03
1	A	2279	ARG	N-CA-C	5.55	116.37	108.54
1	A	2379	GLU	N-CA-C	-5.51	99.06	110.80
1	B	841	CYS	N-CA-C	-5.50	105.18	111.07
1	B	2379	GLU	N-CA-C	-5.50	99.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	CYS	N-CA-C	-5.50	105.18	111.07
1	D	841	CYS	N-CA-C	-5.50	105.19	111.07
1	D	2379	GLU	N-CA-C	-5.49	99.10	110.80
1	B	577	ALA	N-CA-C	-5.45	106.13	112.89
1	D	577	ALA	N-CA-C	-5.44	106.14	112.89
1	A	577	ALA	N-CA-C	-5.41	106.18	112.89
1	A	2429	PRO	N-CA-C	5.40	117.29	110.70
1	D	2429	PRO	N-CA-C	5.40	117.28	110.70
1	B	2429	PRO	N-CA-C	5.39	117.28	110.70
1	B	1037	LEU	N-CA-C	-5.38	106.76	113.38
1	D	2105	LEU	O-C-N	-5.38	115.40	122.39
1	D	1037	LEU	N-CA-C	-5.38	106.77	113.38
1	A	1037	LEU	N-CA-C	-5.36	106.78	113.38
1	D	1016	THR	N-CA-C	-5.36	105.60	111.82
1	B	1016	THR	N-CA-C	-5.35	105.61	111.82
1	A	1016	THR	N-CA-C	-5.33	105.63	111.82
1	D	2264	ASP	N-CA-C	-5.31	103.42	111.34
1	B	2264	ASP	N-CA-C	-5.30	103.44	111.34
1	A	2264	ASP	N-CA-C	-5.30	103.45	111.34
1	D	1554	LEU	CB-CA-C	-5.29	110.45	116.54
1	B	1554	LEU	CB-CA-C	-5.29	110.45	116.54
1	A	1554	LEU	CB-CA-C	-5.28	110.47	116.54
1	A	2280	ILE	N-CA-C	-5.26	101.12	108.80
1	B	2412	ARG	N-CA-C	-5.25	104.56	111.96
1	D	2412	ARG	N-CA-C	-5.22	104.60	111.96
1	A	2412	ARG	N-CA-C	-5.21	104.62	111.96
1	A	607	LEU	N-CA-C	-5.20	106.78	113.23
1	B	607	LEU	N-CA-C	-5.20	106.78	113.23
1	D	607	LEU	N-CA-C	-5.20	106.78	113.23
1	D	1055	LEU	N-CA-C	-5.17	107.11	113.41
1	A	1055	LEU	N-CA-C	-5.15	107.12	113.41
1	D	2282	PRO	N-CA-C	5.15	116.98	110.70
1	B	1055	LEU	N-CA-C	-5.14	107.14	113.41
1	D	2233	ILE	N-CA-C	5.14	113.09	107.60
1	D	2428	SER	CA-C-N	-5.13	115.10	120.38
1	D	2428	SER	C-N-CA	-5.13	115.10	120.38
1	B	2233	ILE	N-CA-C	5.12	113.08	107.60
1	A	2428	SER	CA-C-N	-5.12	115.11	120.38
1	A	2428	SER	C-N-CA	-5.12	115.11	120.38
1	A	2233	ILE	N-CA-C	5.11	113.07	107.60
1	B	2428	SER	CA-C-N	-5.10	115.13	120.38
1	B	2428	SER	C-N-CA	-5.10	115.13	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	245	PHE	N-CA-C	-5.09	98.56	109.81
1	D	2436	ALA	N-CA-C	-5.08	105.87	111.71
1	D	1953	LYS	N-CA-C	5.08	121.62	110.80
1	A	2436	ALA	N-CA-C	-5.07	105.88	111.71
1	B	2436	ALA	N-CA-C	-5.07	105.88	111.71
1	A	1953	LYS	N-CA-C	5.07	121.59	110.80
1	A	2337	GLN	N-CA-C	-5.07	105.84	111.36
1	B	1953	LYS	N-CA-C	5.06	121.58	110.80
1	B	2337	GLN	N-CA-C	-5.06	105.85	111.36
1	D	2337	GLN	N-CA-C	-5.04	105.86	111.36
1	B	1363	LYS	N-CA-C	-5.01	105.92	112.23
1	A	1363	LYS	N-CA-C	-5.00	105.92	112.23
1	D	1363	LYS	N-CA-C	-5.00	105.92	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2105	LEU	Mainchain

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	10394	0	10576	574	0
1	B	10388	0	10569	595	0
1	D	10394	0	10576	567	0
2	C	141	0	118	17	0
2	E	141	0	118	49	0
2	F	141	0	118	46	0
All	All	31599	0	32075	1693	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 27.

All (1693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2171:VAL:HA	2:F:236:ILE:CD1	1.41	1.48
1:D:2171:VAL:HA	2:E:236:ILE:CD1	1.41	1.47
1:D:1695:ILE:HD11	1:D:1714:VAL:CG2	1.55	1.36
1:B:2171:VAL:HA	2:F:236:ILE:CG1	1.57	1.35
1:A:1695:ILE:HD11	1:A:1714:VAL:CG2	1.55	1.34
1:B:2175:MET:HA	2:F:240:CYS:SG	1.67	1.34
1:D:2175:MET:HA	2:E:240:CYS:SG	1.67	1.34
1:B:1695:ILE:HD11	1:B:1714:VAL:CG2	1.55	1.34
1:D:2171:VAL:HA	2:E:236:ILE:CG1	1.57	1.34
1:B:1695:ILE:CD1	1:B:1714:VAL:HG21	1.59	1.31
1:D:1695:ILE:CD1	1:D:1714:VAL:HG21	1.59	1.31
1:A:1695:ILE:CD1	1:A:1714:VAL:HG21	1.59	1.30
1:D:2443:LEU:HD21	1:D:2447:ILE:CD1	1.63	1.28
1:B:2443:LEU:HD21	1:B:2447:ILE:CD1	1.63	1.28
1:A:2443:LEU:HD21	1:A:2447:ILE:CD1	1.63	1.26
1:B:2443:LEU:CD2	1:B:2443:LEU:C	2.10	1.24
1:B:2323:LYS:NZ	1:B:2323:LYS:CB	2.01	1.24
1:A:2323:LYS:NZ	1:A:2323:LYS:CB	2.01	1.23
1:D:2443:LEU:C	1:D:2443:LEU:CD2	2.10	1.22
1:A:2443:LEU:C	1:A:2443:LEU:CD2	2.10	1.22
1:A:2048:ILE:N	1:A:2048:ILE:HD13	1.56	1.20
1:B:2323:LYS:NZ	1:B:2323:LYS:HB3	1.11	1.18
1:D:2323:LYS:NZ	1:D:2323:LYS:CB	2.01	1.18
1:A:1052:GLN:HB3	1:A:1099:LEU:HD11	1.19	1.17
1:A:2323:LYS:NZ	1:A:2323:LYS:HB3	1.11	1.17
1:A:1057:LEU:HG	1:A:1058:GLY:H	1.09	1.17
1:B:1052:GLN:HB3	1:B:1099:LEU:HD11	1.19	1.17
1:B:2443:LEU:C	1:B:2443:LEU:HD22	1.69	1.17
1:A:1515:TRP:CE3	1:A:1516:MET:HE2	1.80	1.16
1:D:2089:ILE:HD13	1:D:2089:ILE:H	1.01	1.16
1:B:1515:TRP:CE3	1:B:1516:MET:HE2	1.80	1.16
1:D:2323:LYS:NZ	1:D:2323:LYS:HB3	1.11	1.16
1:D:1057:LEU:HG	1:D:1058:GLY:N	1.59	1.16
1:D:1515:TRP:CE3	1:D:1516:MET:HE2	1.80	1.15
1:A:2156:GLU:OE2	1:B:1410:ALA:HB2	1.46	1.15
1:D:1052:GLN:HB3	1:D:1099:LEU:HD11	1.19	1.15
1:D:2443:LEU:C	1:D:2443:LEU:HD22	1.69	1.15
1:D:2048:ILE:N	1:D:2048:ILE:HD13	1.56	1.15
1:B:2156:GLU:OE2	1:D:1410:ALA:HB2	1.46	1.14
1:B:2175:MET:CA	2:F:240:CYS:SG	2.35	1.14
1:B:2443:LEU:HD21	1:B:2447:ILE:HD12	1.16	1.14
1:A:2443:LEU:C	1:A:2443:LEU:HD22	1.69	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2171:VAL:CA	2:F:236:ILE:CD1	2.26	1.14
1:D:2323:LYS:CB	1:D:2323:LYS:HZ3	1.60	1.14
1:A:2048:ILE:H	1:A:2048:ILE:CD1	1.55	1.14
1:D:2443:LEU:HD21	1:D:2447:ILE:HD12	1.16	1.13
1:A:2443:LEU:HD21	1:A:2447:ILE:HD12	1.16	1.13
1:B:2048:ILE:N	1:B:2048:ILE:HD13	1.56	1.13
1:D:2171:VAL:CA	2:E:236:ILE:CD1	2.26	1.13
1:D:2080:GLN:HA	1:D:2080:GLN:HE21	1.09	1.12
1:D:2175:MET:CA	2:E:240:CYS:SG	2.35	1.12
1:A:2089:ILE:HD13	1:A:2089:ILE:H	1.02	1.12
1:D:2045:MET:O	1:D:2048:ILE:HD12	1.50	1.12
1:B:2358:LYS:HG3	1:B:2383:LEU:HD22	1.31	1.12
1:B:1057:LEU:HG	1:B:1058:GLY:H	1.09	1.11
1:B:2045:MET:O	1:B:2048:ILE:HD12	1.50	1.11
1:D:1057:LEU:HG	1:D:1058:GLY:H	1.09	1.11
1:D:2358:LYS:HG3	1:D:2383:LEU:HD22	1.31	1.11
1:A:2358:LYS:HG3	1:A:2383:LEU:HD22	1.31	1.11
1:B:2048:ILE:H	1:B:2048:ILE:CD1	1.56	1.11
1:A:1699:HIS:NE2	1:A:1708:LEU:HD12	1.64	1.11
1:D:2171:VAL:HA	2:E:236:ILE:HG12	1.29	1.11
1:A:2080:GLN:HE21	1:A:2080:GLN:HA	1.09	1.10
1:A:2323:LYS:CB	1:A:2323:LYS:HZ3	1.60	1.10
1:A:2045:MET:O	1:A:2048:ILE:HD12	1.50	1.10
1:D:1699:HIS:NE2	1:D:1708:LEU:HD12	1.65	1.09
1:B:1515:TRP:CE3	1:B:1516:MET:CE	2.36	1.09
1:B:1699:HIS:NE2	1:B:1708:LEU:HD12	1.65	1.09
1:B:635:ALA:O	1:B:639:LEU:HD12	1.53	1.09
1:B:1568:LEU:O	1:B:1653:ARG:HB3	1.53	1.08
1:B:2175:MET:CB	2:F:240:CYS:SG	2.41	1.08
1:A:1057:LEU:HG	1:A:1058:GLY:N	1.59	1.08
1:A:1515:TRP:CE3	1:A:1516:MET:CE	2.36	1.08
1:B:2443:LEU:HD23	1:B:2443:LEU:O	1.53	1.08
1:D:1160:VAL:HA	1:D:1550:LEU:HD21	1.35	1.08
1:D:2171:VAL:HA	2:E:236:ILE:HD11	1.33	1.08
1:A:1160:VAL:HA	1:A:1550:LEU:HD21	1.35	1.08
1:D:1515:TRP:CE3	1:D:1516:MET:CE	2.36	1.08
1:B:2080:GLN:HE21	1:B:2080:GLN:HA	1.09	1.08
1:D:1568:LEU:O	1:D:1653:ARG:HB3	1.53	1.08
1:D:2175:MET:CB	2:E:240:CYS:SG	2.41	1.08
1:D:2252:LEU:O	1:D:2256:PHE:HD1	1.37	1.07
1:B:1057:LEU:HG	1:B:1058:GLY:N	1.59	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2171:VAL:HA	2:F:236:ILE:HG12	1.29	1.07
1:A:1568:LEU:O	1:A:1653:ARG:HB3	1.53	1.07
1:B:2171:VAL:HA	2:F:236:ILE:HD11	1.33	1.07
1:A:2252:LEU:O	1:A:2256:PHE:HD1	1.37	1.07
1:D:635:ALA:O	1:D:639:LEU:HD12	1.53	1.07
1:A:635:ALA:O	1:A:639:LEU:HD12	1.53	1.06
1:B:2252:LEU:O	1:B:2256:PHE:HD1	1.37	1.06
1:D:2443:LEU:O	1:D:2443:LEU:HD23	1.53	1.06
1:A:2443:LEU:O	1:A:2443:LEU:HD23	1.53	1.06
1:B:1733:ALA:O	1:B:1737:THR:HG23	1.56	1.06
1:A:2358:LYS:HZ3	1:A:2383:LEU:HD21	1.12	1.05
1:B:2089:ILE:HD13	1:B:2089:ILE:H	1.02	1.05
1:D:2048:ILE:H	1:D:2048:ILE:CD1	1.55	1.05
1:D:2443:LEU:CD2	1:D:2447:ILE:HD12	1.86	1.05
1:B:2171:VAL:CA	2:F:236:ILE:HD11	1.86	1.05
1:B:2100:HIS:CE1	2:F:238:MET:CB	2.40	1.05
1:B:2323:LYS:CB	1:B:2323:LYS:HZ3	1.66	1.05
1:B:2443:LEU:CD2	1:B:2447:ILE:HD12	1.86	1.05
1:D:1733:ALA:O	1:D:1737:THR:HG23	1.56	1.05
1:D:2171:VAL:CG1	2:E:236:ILE:HG12	1.87	1.05
1:D:2100:HIS:CE1	2:E:238:MET:CB	2.40	1.04
1:A:1733:ALA:O	1:A:1737:THR:HG23	1.56	1.04
1:A:2443:LEU:CD2	1:A:2447:ILE:HD12	1.86	1.04
1:B:1737:THR:O	1:B:1741:VAL:HG23	1.57	1.04
1:A:2094:LEU:HD13	1:A:2106:PHE:HA	1.04	1.03
1:B:2171:VAL:CG1	2:F:236:ILE:HG12	1.87	1.03
1:D:1737:THR:O	1:D:1741:VAL:HG23	1.57	1.03
1:B:2358:LYS:HZ3	1:B:2383:LEU:HD21	1.18	1.03
1:D:2171:VAL:CA	2:E:236:ILE:HD11	1.86	1.03
1:A:1737:THR:O	1:A:1741:VAL:HG23	1.57	1.03
1:A:2171:VAL:HA	2:C:236:ILE:HG12	1.40	1.03
1:B:2261:SER:O	1:B:2264:ASP:HB2	1.58	1.03
1:B:2094:LEU:HD13	1:B:2106:PHE:HA	1.04	1.03
1:B:1160:VAL:HA	1:B:1550:LEU:HD21	1.35	1.02
1:B:2518:ARG:HH22	1:D:1418:TYR:HE2	1.06	1.02
1:A:2358:LYS:HZ3	1:A:2383:LEU:CD2	1.73	1.01
1:B:1515:TRP:CZ3	1:B:1516:MET:HE1	1.95	1.01
1:D:2261:SER:O	1:D:2264:ASP:HB2	1.58	1.01
1:A:1516:MET:HA	1:A:1519:GLN:OE1	1.59	1.01
1:A:2261:SER:O	1:A:2264:ASP:HB2	1.58	1.01
1:B:2094:LEU:CD1	1:B:2106:PHE:HA	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1515:TRP:CZ3	1:D:1516:MET:HE1	1.95	1.01
1:D:1516:MET:HA	1:D:1519:GLN:OE1	1.59	1.00
1:A:2094:LEU:CD1	1:A:2106:PHE:HA	1.90	1.00
1:B:1516:MET:HA	1:B:1519:GLN:OE1	1.59	1.00
1:D:2094:LEU:HD13	1:D:2106:PHE:HA	1.42	1.00
1:A:1515:TRP:CZ3	1:A:1516:MET:HE1	1.95	1.00
1:B:2175:MET:HG2	2:F:240:CYS:SG	2.02	1.00
2:F:243:ILE:HA	2:F:247:SER:HA	1.41	1.00
1:A:2443:LEU:HD22	1:A:2444:TYR:N	1.78	0.99
1:B:587:MET:HE2	1:B:587:MET:N	1.77	0.99
1:D:2175:MET:HG2	2:E:240:CYS:SG	2.02	0.99
1:A:587:MET:N	1:A:587:MET:HE2	1.78	0.98
1:A:2281:SER:HB3	1:B:2275:GLY:HA2	1.45	0.98
1:D:587:MET:HE2	1:D:587:MET:N	1.77	0.98
1:D:1161:ALA:HA	1:D:1165:TYR:CE2	1.98	0.98
1:D:2443:LEU:HD22	1:D:2444:TYR:N	1.78	0.98
1:B:1357:ILE:HG22	1:B:2495:LEU:HD22	1.45	0.98
1:B:2443:LEU:HD22	1:B:2444:TYR:N	1.78	0.98
1:A:1161:ALA:HA	1:A:1165:TYR:CE2	1.98	0.98
1:A:1418:TYR:HE2	1:D:2518:ARG:HH22	1.06	0.98
1:A:2265:ILE:HD11	1:A:2423:PHE:CD2	1.98	0.98
1:D:2265:ILE:HD11	1:D:2423:PHE:CD2	1.98	0.98
1:A:1357:ILE:HG22	1:A:2495:LEU:HD22	1.45	0.98
1:A:2265:ILE:CD1	1:A:2423:PHE:CD2	2.47	0.98
1:D:2265:ILE:CD1	1:D:2423:PHE:CD2	2.47	0.98
1:D:1357:ILE:HG22	1:D:2495:LEU:HD22	1.45	0.97
1:A:2089:ILE:H	1:A:2089:ILE:CD1	1.77	0.97
1:B:1161:ALA:HA	1:B:1165:TYR:CE2	1.98	0.97
1:B:2265:ILE:CD1	1:B:2423:PHE:CD2	2.47	0.97
1:A:1699:HIS:CE1	1:A:1708:LEU:HD12	2.00	0.97
1:B:2265:ILE:HD11	1:B:2423:PHE:CD2	1.98	0.97
1:A:2094:LEU:HB2	1:A:2106:PHE:CD1	2.00	0.97
1:B:2089:ILE:H	1:B:2089:ILE:CD1	1.77	0.97
1:D:2265:ILE:HD13	1:D:2423:PHE:CG	2.00	0.97
1:D:2089:ILE:H	1:D:2089:ILE:CD1	1.77	0.96
1:B:2094:LEU:HB2	1:B:2106:PHE:CD1	2.00	0.96
1:A:2265:ILE:HD13	1:A:2423:PHE:CG	2.00	0.96
1:D:2171:VAL:HG13	2:E:236:ILE:HG12	1.45	0.96
1:A:2323:LYS:HB3	1:A:2323:LYS:HZ2	1.22	0.96
1:B:1699:HIS:CE1	1:B:1708:LEU:HD12	2.00	0.96
1:D:586:GLY:C	1:D:587:MET:HE2	1.90	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2171:VAL:CA	2:E:236:ILE:HG12	1.95	0.96
1:D:1699:HIS:CE1	1:D:1708:LEU:HD12	2.00	0.96
1:D:2323:LYS:HB3	1:D:2323:LYS:HZ2	1.22	0.95
1:A:586:GLY:C	1:A:587:MET:HE2	1.90	0.95
1:B:2171:VAL:HG13	2:F:236:ILE:HG12	1.45	0.95
1:B:2265:ILE:HD13	1:B:2423:PHE:CG	2.00	0.95
1:D:1695:ILE:CD1	1:D:1714:VAL:CG2	2.28	0.95
1:A:2518:ARG:HH22	1:B:1418:TYR:HE2	1.06	0.95
1:B:2171:VAL:CA	2:F:236:ILE:HG12	1.95	0.95
1:A:2358:LYS:O	1:A:2421:VAL:HG23	1.67	0.95
1:B:2175:MET:HA	2:F:240:CYS:HG	1.15	0.94
1:D:1160:VAL:HA	1:D:1550:LEU:CD2	1.98	0.94
1:D:2358:LYS:O	1:D:2421:VAL:HG23	1.67	0.94
1:A:2443:LEU:C	1:A:2443:LEU:HD23	1.90	0.94
1:B:586:GLY:C	1:B:587:MET:HE2	1.90	0.94
1:A:1052:GLN:HB3	1:A:1099:LEU:CD1	1.97	0.93
1:D:2171:VAL:N	2:E:236:ILE:HD11	1.83	0.93
1:B:1695:ILE:CD1	1:B:1714:VAL:CG2	2.28	0.93
1:B:2358:LYS:O	1:B:2421:VAL:HG23	1.67	0.93
1:A:1695:ILE:CD1	1:A:1714:VAL:CG2	2.28	0.93
1:B:1160:VAL:HA	1:B:1550:LEU:CD2	1.98	0.93
1:B:1052:GLN:HB3	1:B:1099:LEU:CD1	1.97	0.93
1:D:1699:HIS:ND1	1:D:1707:SER:HB2	1.83	0.93
1:A:1160:VAL:HA	1:A:1550:LEU:CD2	1.98	0.93
1:D:1052:GLN:HB3	1:D:1099:LEU:CD1	1.97	0.93
1:B:2323:LYS:HB3	1:B:2323:LYS:HZ2	1.17	0.92
1:A:1699:HIS:ND1	1:A:1707:SER:HB2	1.83	0.92
1:B:1699:HIS:ND1	1:B:1707:SER:HB2	1.83	0.92
1:B:2171:VAL:N	2:F:236:ILE:HD11	1.83	0.92
1:B:2358:LYS:NZ	1:B:2383:LEU:CD2	2.33	0.92
1:B:2048:ILE:HD13	1:B:2048:ILE:H	0.76	0.92
1:B:2089:ILE:HD13	1:B:2089:ILE:N	1.84	0.91
1:D:2175:MET:CG	2:E:240:CYS:SG	2.59	0.91
1:A:2089:ILE:HD13	1:A:2089:ILE:N	1.84	0.91
1:B:2175:MET:CG	2:F:240:CYS:SG	2.59	0.91
1:B:2358:LYS:HZ3	1:B:2383:LEU:CD2	1.83	0.91
1:D:2358:LYS:NZ	1:D:2383:LEU:CD2	2.33	0.91
1:A:2358:LYS:NZ	1:A:2383:LEU:CD2	2.33	0.90
1:B:600:TYR:OH	1:B:644:VAL:HG11	1.71	0.90
1:D:2171:VAL:HG13	2:E:236:ILE:CG1	2.01	0.90
1:A:2443:LEU:CD2	1:A:2443:LEU:O	2.16	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2252:LEU:O	1:B:2256:PHE:CD1	2.25	0.90
1:A:1052:GLN:CB	1:A:1099:LEU:HD11	2.02	0.90
1:A:2466:ILE:HG21	1:B:2138:CYS:SG	2.11	0.90
1:A:2048:ILE:HD13	1:A:2048:ILE:H	0.75	0.90
1:D:600:TYR:OH	1:D:644:VAL:HG11	1.71	0.90
1:B:2175:MET:HG3	2:F:236:ILE:HG23	1.54	0.90
1:D:2443:LEU:HD21	1:D:2447:ILE:HD11	1.52	0.90
1:B:1999:GLN:HB2	1:B:2050:PRO:C	1.97	0.90
1:D:2048:ILE:HD13	1:D:2048:ILE:H	0.76	0.90
1:A:1999:GLN:HB2	1:A:2050:PRO:C	1.97	0.90
1:B:2443:LEU:HD21	1:B:2447:ILE:HD11	1.52	0.90
1:A:2138:CYS:SG	1:D:2466:ILE:HG21	2.11	0.89
1:A:2443:LEU:HD21	1:A:2447:ILE:HD11	1.52	0.89
1:B:2171:VAL:HG13	2:F:236:ILE:CG1	2.01	0.89
1:D:2252:LEU:O	1:D:2256:PHE:CD1	2.25	0.89
1:A:600:TYR:OH	1:A:644:VAL:HG11	1.71	0.89
1:A:2252:LEU:O	1:A:2256:PHE:CD1	2.25	0.89
1:B:924:PRO:HG2	1:B:928:TYR:HB2	1.55	0.88
1:A:2443:LEU:CD2	1:A:2447:ILE:CD1	2.47	0.88
1:B:2443:LEU:CD2	1:B:2447:ILE:CD1	2.47	0.88
1:B:1052:GLN:CB	1:B:1099:LEU:HD11	2.01	0.88
1:D:1052:GLN:CB	1:D:1099:LEU:HD11	2.02	0.88
1:D:2358:LYS:HZ2	1:D:2383:LEU:CD2	1.86	0.88
1:A:1357:ILE:HG22	1:A:2495:LEU:CD2	2.04	0.88
1:D:1999:GLN:HB2	1:D:2050:PRO:C	1.97	0.88
1:D:2358:LYS:HZ3	1:D:2383:LEU:HD21	1.38	0.88
1:B:2443:LEU:C	1:B:2443:LEU:HD23	1.90	0.88
1:B:2358:LYS:CG	1:B:2383:LEU:HD22	2.04	0.87
2:E:243:ILE:HA	2:E:247:SER:HA	1.56	0.87
1:A:2265:ILE:CD1	1:A:2423:PHE:CG	2.58	0.87
1:D:2089:ILE:HD13	1:D:2089:ILE:N	1.84	0.87
1:D:1357:ILE:HG22	1:D:2495:LEU:CD2	2.04	0.87
1:B:1357:ILE:HG22	1:B:2495:LEU:CD2	2.04	0.87
1:D:2265:ILE:CD1	1:D:2423:PHE:CG	2.58	0.87
1:D:2443:LEU:CD2	1:D:2447:ILE:CD1	2.47	0.87
1:A:2092:ASN:OD1	1:A:2106:PHE:CE1	2.28	0.86
1:A:2358:LYS:CG	1:A:2383:LEU:HD22	2.04	0.86
1:D:2358:LYS:CG	1:D:2383:LEU:HD22	2.04	0.86
1:D:2443:LEU:C	1:D:2443:LEU:HD23	1.90	0.86
1:B:1357:ILE:CG2	1:B:2495:LEU:HD22	2.06	0.86
1:D:924:PRO:HG2	1:D:928:TYR:HB2	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2175:MET:HG3	2:E:236:ILE:HG23	1.54	0.86
1:B:2265:ILE:CD1	1:B:2423:PHE:CG	2.58	0.86
1:D:2175:MET:HA	2:E:240:CYS:HG	1.35	0.86
1:B:2302:ARG:HB2	1:B:2323:LYS:HZ1	1.40	0.86
1:A:924:PRO:HG2	1:A:928:TYR:HB2	1.55	0.86
1:D:1357:ILE:CG2	1:D:2495:LEU:HD22	2.06	0.86
1:D:2080:GLN:HA	1:D:2080:GLN:NE2	1.91	0.86
1:A:2080:GLN:HA	1:A:2080:GLN:NE2	1.91	0.85
1:B:2092:ASN:OD1	1:B:2106:PHE:CE1	2.28	0.85
1:A:626:LEU:O	1:A:626:LEU:HD22	1.77	0.85
1:B:1413:ILE:HG22	1:B:2497:GLU:HB3	1.59	0.85
1:B:2095:THR:HG1	1:B:2143:TYR:HE2	0.87	0.85
1:A:1357:ILE:CG2	1:A:2495:LEU:HD22	2.06	0.85
1:D:1413:ILE:HG22	1:D:2497:GLU:HB3	1.59	0.85
1:B:2080:GLN:HA	1:B:2080:GLN:NE2	1.91	0.85
1:A:2094:LEU:HD12	1:A:2106:PHE:CD1	2.11	0.84
1:B:2094:LEU:HD12	1:B:2106:PHE:CD1	2.11	0.84
1:A:1413:ILE:HG22	1:A:2497:GLU:HB3	1.59	0.84
1:D:626:LEU:O	1:D:626:LEU:HD22	1.77	0.84
1:D:2443:LEU:CD2	1:D:2443:LEU:O	2.16	0.84
1:D:627:LYS:HE3	1:D:627:LYS:HA	1.60	0.84
1:B:2171:VAL:CA	2:F:236:ILE:CG1	2.48	0.84
1:D:2095:THR:HG1	1:D:2143:TYR:HE2	0.85	0.84
1:A:2302:ARG:HB2	1:A:2323:LYS:HZ1	1.42	0.83
1:A:2468:PHE:CG	1:D:2467:MET:HE1	2.13	0.83
1:B:626:LEU:HD22	1:B:626:LEU:O	1.77	0.83
1:D:2302:ARG:HB2	1:D:2323:LYS:HZ1	1.42	0.83
1:A:2174:GLY:HA3	2:C:236:ILE:HG21	1.61	0.83
1:B:2443:LEU:CD2	1:B:2443:LEU:O	2.16	0.82
1:D:1515:TRP:HE3	1:D:1516:MET:HE2	1.43	0.82
1:B:1515:TRP:HE3	1:B:1516:MET:HE2	1.43	0.82
1:A:1529:LEU:O	1:A:1533:THR:HG23	1.80	0.82
1:A:627:LYS:HE3	1:A:627:LYS:HA	1.60	0.82
1:B:2094:LEU:HB2	1:B:2106:PHE:HD1	1.42	0.82
1:B:627:LYS:HE3	1:B:627:LYS:HA	1.60	0.81
1:D:847:LYS:HD2	1:D:928:TYR:HE2	1.45	0.81
1:A:847:LYS:HD2	1:A:928:TYR:HE2	1.45	0.81
1:A:2094:LEU:HD12	1:A:2106:PHE:HD1	1.44	0.81
1:A:2507:TYR:O	1:D:2467:MET:HB3	1.80	0.81
1:B:2358:LYS:NZ	1:B:2383:LEU:HD21	1.95	0.81
1:D:1529:LEU:O	1:D:1533:THR:HG23	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2213:THR:HG23	1:A:2224:THR:HG23	1.61	0.81
1:B:847:LYS:HD2	1:B:928:TYR:HE2	1.45	0.81
1:B:2094:LEU:HD12	1:B:2106:PHE:HD1	1.44	0.81
2:F:227:CYS:N	2:F:230:SER:HG	1.77	0.81
1:B:1529:LEU:O	1:B:1533:THR:HG23	1.80	0.81
1:D:2302:ARG:HB3	1:D:2323:LYS:HZ2	1.44	0.81
1:A:2095:THR:HG1	1:A:2143:TYR:HE2	0.83	0.81
1:B:2289:LYS:HA	1:B:2292:LEU:CD1	2.11	0.81
2:E:227:CYS:N	2:E:230:SER:HG	1.78	0.81
1:B:2213:THR:HG23	1:B:2224:THR:HG23	1.61	0.81
1:D:2171:VAL:HA	2:E:236:ILE:HD13	1.60	0.81
1:D:2289:LYS:HA	1:D:2292:LEU:CD1	2.11	0.81
1:D:2265:ILE:HD13	1:D:2423:PHE:HA	1.64	0.81
1:A:1733:ALA:HB1	1:A:1793:LEU:HD21	1.63	0.80
1:A:2289:LYS:HA	1:A:2292:LEU:CD1	2.11	0.80
2:C:227:CYS:N	2:C:230:SER:HG	1.78	0.80
1:D:2213:THR:HG23	1:D:2224:THR:HG23	1.61	0.80
1:A:2302:ARG:HB3	1:A:2323:LYS:HZ2	1.44	0.80
1:B:2175:MET:HB3	2:F:240:CYS:SG	2.21	0.80
1:D:1733:ALA:HB1	1:D:1793:LEU:HD21	1.63	0.80
1:A:2094:LEU:HB2	1:A:2106:PHE:HD1	1.42	0.80
1:D:2095:THR:OG1	1:D:2143:TYR:HE2	1.65	0.80
1:B:1733:ALA:HB1	1:B:1793:LEU:HD21	1.63	0.80
1:A:2265:ILE:HD13	1:A:2423:PHE:HA	1.64	0.79
1:A:2467:MET:HB3	1:B:2507:TYR:O	1.80	0.79
1:A:2358:LYS:NZ	1:A:2383:LEU:HD21	1.95	0.79
1:B:2094:LEU:HD13	1:B:2106:PHE:CA	2.00	0.79
1:A:2468:PHE:CD1	1:D:2467:MET:HE1	2.18	0.79
1:B:2265:ILE:HD13	1:B:2423:PHE:HA	1.64	0.79
1:D:2175:MET:HB3	2:E:240:CYS:SG	2.21	0.79
1:B:1409:HIS:HD2	1:B:2497:GLU:OE1	1.66	0.78
1:D:2171:VAL:CA	2:E:236:ILE:CG1	2.48	0.78
1:B:2092:ASN:OD1	1:B:2106:PHE:HE1	1.66	0.78
1:A:1515:TRP:HE3	1:A:1516:MET:HE2	1.43	0.78
1:D:1157:MET:O	1:D:1160:VAL:HG22	1.84	0.78
1:D:2358:LYS:NZ	1:D:2383:LEU:HD21	1.95	0.78
1:B:1943:ARG:HD3	1:B:1944:ARG:NH2	1.99	0.78
1:D:1409:HIS:HD2	1:D:2497:GLU:OE1	1.66	0.78
1:A:1943:ARG:HD3	1:A:1944:ARG:NH2	1.99	0.77
1:A:1157:MET:O	1:A:1160:VAL:HG22	1.84	0.77
1:B:1157:MET:O	1:B:1160:VAL:HG22	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2188:TRP:CZ2	1:A:2192:LEU:HD11	2.19	0.77
1:B:2171:VAL:HA	2:F:236:ILE:HD13	1.60	0.77
1:D:1943:ARG:HD3	1:D:1944:ARG:NH2	1.99	0.77
1:A:2092:ASN:OD1	1:A:2106:PHE:HE1	1.66	0.77
1:D:627:LYS:HE3	1:D:627:LYS:O	1.84	0.77
1:B:2188:TRP:CZ2	1:B:2192:LEU:HD11	2.19	0.77
1:B:2302:ARG:HB3	1:B:2323:LYS:HZ2	1.48	0.77
1:A:1515:TRP:CZ3	1:A:1516:MET:CE	2.65	0.77
1:A:1160:VAL:HG12	1:A:1550:LEU:HD23	1.67	0.77
1:A:2080:GLN:HE21	1:A:2080:GLN:CA	1.92	0.77
1:B:1737:THR:OG1	1:B:1790:LEU:HD13	1.84	0.77
1:B:2095:THR:OG1	1:B:2143:TYR:CE2	2.38	0.77
1:A:627:LYS:HE3	1:A:627:LYS:O	1.84	0.76
1:D:2188:TRP:CZ2	1:D:2192:LEU:HD11	2.19	0.76
1:D:1737:THR:OG1	1:D:1790:LEU:HD13	1.84	0.76
1:A:2383:LEU:HD23	1:A:2420:MET:CE	2.16	0.76
1:B:627:LYS:HE3	1:B:627:LYS:O	1.84	0.76
1:B:2261:SER:O	1:B:2264:ASP:CB	2.34	0.76
1:D:2383:LEU:HD23	1:D:2420:MET:CE	2.16	0.76
1:A:1418:TYR:HE2	1:D:2518:ARG:NH2	1.84	0.76
1:B:1160:VAL:HG12	1:B:1550:LEU:HD23	1.67	0.76
1:A:1737:THR:OG1	1:A:1790:LEU:HD13	1.84	0.76
1:D:2101:LEU:O	1:D:2105:LEU:HG	1.86	0.76
1:A:2261:SER:O	1:A:2264:ASP:CB	2.34	0.75
1:D:2302:ARG:CB	1:D:2323:LYS:NZ	2.50	0.75
1:A:2518:ARG:NH2	1:B:1418:TYR:HE2	1.84	0.75
1:A:2095:THR:OG1	1:A:2143:TYR:CE2	2.38	0.75
1:A:2507:TYR:O	1:D:2467:MET:CB	2.35	0.75
1:D:2095:THR:OG1	1:D:2143:TYR:CE2	2.38	0.75
1:A:2094:LEU:HD13	1:A:2106:PHE:CA	2.00	0.75
1:D:2261:SER:O	1:D:2264:ASP:CB	2.34	0.75
1:A:2302:ARG:CB	1:A:2323:LYS:NZ	2.50	0.75
1:B:2383:LEU:HD23	1:B:2420:MET:CE	2.16	0.75
1:D:1160:VAL:HG12	1:D:1550:LEU:HD23	1.67	0.75
1:A:2467:MET:CB	1:B:2507:TYR:O	2.35	0.74
1:A:2101:LEU:O	1:A:2105:LEU:HG	1.86	0.74
1:A:2095:THR:OG1	1:A:2143:TYR:HE2	1.65	0.74
1:B:2302:ARG:CB	1:B:2323:LYS:NZ	2.50	0.74
1:A:627:LYS:HE3	1:A:627:LYS:CA	2.16	0.74
1:B:627:LYS:HE3	1:B:627:LYS:CA	2.16	0.74
1:B:2518:ARG:NH2	1:D:1418:TYR:HE2	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1699:HIS:NE2	1:A:1708:LEU:CD1	2.48	0.74
1:A:2507:TYR:O	1:D:2467:MET:HA	1.88	0.74
1:B:2101:LEU:O	1:B:2105:LEU:HG	1.86	0.74
1:D:627:LYS:HE3	1:D:627:LYS:CA	2.16	0.74
1:A:785:ARG:HA	1:A:790:LEU:HB2	1.70	0.73
1:A:2467:MET:HA	1:B:2507:TYR:O	1.88	0.73
1:D:1699:HIS:NE2	1:D:1708:LEU:CD1	2.48	0.73
1:B:2302:ARG:HB3	1:B:2323:LYS:NZ	2.04	0.73
1:B:2215:LYS:HB3	1:B:2221:PRO:HB3	1.71	0.73
1:B:2002:GLU:O	1:B:2006:VAL:CG2	2.37	0.73
1:B:2323:LYS:CB	1:B:2323:LYS:HZ2	1.79	0.73
1:D:2358:LYS:HZ2	1:D:2383:LEU:HD22	1.52	0.73
1:D:2002:GLU:O	1:D:2006:VAL:CG2	2.37	0.73
1:D:2288:MET:O	1:D:2292:LEU:HG	1.88	0.73
1:A:1057:LEU:CG	1:A:1058:GLY:H	1.97	0.73
1:A:2302:ARG:HB3	1:A:2323:LYS:NZ	2.04	0.73
1:B:2095:THR:OG1	1:B:2143:TYR:HE2	1.65	0.73
1:A:2215:LYS:HB3	1:A:2221:PRO:HB3	1.71	0.72
1:A:2281:SER:H	1:A:2285:ARG:H	1.36	0.72
1:B:2089:ILE:CD1	1:B:2089:ILE:N	2.48	0.72
1:D:1568:LEU:C	1:D:1653:ARG:HB3	2.15	0.72
1:D:2302:ARG:HB3	1:D:2323:LYS:NZ	2.04	0.72
1:A:2002:GLU:O	1:A:2006:VAL:CG2	2.37	0.72
1:B:1568:LEU:C	1:B:1653:ARG:HB3	2.15	0.72
1:D:2215:LYS:HB3	1:D:2221:PRO:HB3	1.71	0.72
1:B:2288:MET:O	1:B:2292:LEU:HG	1.88	0.72
1:D:2002:GLU:O	1:D:2006:VAL:HG23	1.90	0.72
1:A:2124:TRP:CH2	1:D:2172:LYS:HA	2.25	0.72
1:A:2214:LEU:HB2	1:A:2223:PHE:HB3	1.72	0.72
1:A:2288:MET:O	1:A:2292:LEU:HG	1.88	0.72
1:B:2002:GLU:O	1:B:2006:VAL:HG23	1.90	0.72
1:B:785:ARG:HA	1:B:790:LEU:HB2	1.70	0.72
1:B:847:LYS:CD	1:B:928:TYR:HE2	2.03	0.72
1:B:1057:LEU:CG	1:B:1058:GLY:H	1.97	0.72
1:A:593:PHE:H	1:A:601:LYS:HE3	1.55	0.71
1:A:1161:ALA:HA	1:A:1165:TYR:CD2	2.25	0.71
1:A:1529:LEU:O	1:A:1533:THR:CG2	2.38	0.71
1:B:2302:ARG:CB	1:B:2323:LYS:HZ1	2.02	0.71
1:B:2171:VAL:CG1	2:F:239:GLU:OE2	2.37	0.71
1:D:2171:VAL:CG1	2:E:239:GLU:OE2	2.37	0.71
1:A:2002:GLU:O	1:A:2006:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2383:LEU:HD23	1:B:2420:MET:HE2	1.73	0.71
1:A:2172:LYS:HA	1:B:2124:TRP:CH2	2.25	0.71
1:D:1562:ARG:NE	1:D:1566:ASP:HB3	2.06	0.71
1:A:2253:ALA:HB1	1:A:2374:LEU:HD12	1.73	0.71
1:B:1529:LEU:O	1:B:1533:THR:CG2	2.38	0.71
1:D:587:MET:HE2	1:D:587:MET:CA	2.21	0.71
1:B:2172:LYS:HA	1:D:2124:TRP:CH2	2.25	0.71
1:D:785:ARG:HA	1:D:790:LEU:HB2	1.70	0.71
1:B:587:MET:HE2	1:B:587:MET:CA	2.21	0.71
1:B:593:PHE:H	1:B:601:LYS:HE3	1.55	0.71
1:B:1161:ALA:HA	1:B:1165:TYR:CD2	2.25	0.70
1:D:1529:LEU:O	1:D:1533:THR:CG2	2.38	0.70
1:A:847:LYS:CD	1:A:928:TYR:HE2	2.03	0.70
1:A:2383:LEU:HD23	1:A:2420:MET:HE2	1.73	0.70
1:B:1562:ARG:NE	1:B:1566:ASP:HB3	2.06	0.70
1:A:1568:LEU:C	1:A:1653:ARG:HB3	2.15	0.70
1:D:847:LYS:CD	1:D:928:TYR:HE2	2.03	0.70
1:D:2214:LEU:HB2	1:D:2223:PHE:HB3	1.72	0.70
1:A:1562:ARG:NE	1:A:1566:ASP:HB3	2.06	0.70
1:D:1161:ALA:HA	1:D:1165:TYR:CD2	2.25	0.70
1:B:1699:HIS:NE2	1:B:1708:LEU:CD1	2.48	0.70
1:A:587:MET:HE2	1:A:587:MET:CA	2.21	0.70
1:D:2383:LEU:HD23	1:D:2420:MET:HE2	1.73	0.70
1:D:593:PHE:H	1:D:601:LYS:HE3	1.56	0.70
1:D:2080:GLN:HE21	1:D:2080:GLN:CA	1.92	0.70
1:B:2094:LEU:HB2	1:B:2106:PHE:CB	2.22	0.70
1:A:626:LEU:O	1:A:630:TRP:HB2	1.91	0.69
1:B:626:LEU:O	1:B:630:TRP:HB2	1.91	0.69
1:D:626:LEU:O	1:D:630:TRP:HB2	1.91	0.69
1:D:2046:PHE:C	1:D:2048:ILE:HD13	2.17	0.69
1:A:2146:ILE:HG23	1:A:2474:VAL:HB	1.73	0.69
1:B:2046:PHE:C	1:B:2048:ILE:HD13	2.17	0.69
1:B:2175:MET:SD	2:F:239:GLU:HB3	2.32	0.69
1:D:1057:LEU:CG	1:D:1058:GLY:N	2.45	0.69
1:D:2175:MET:SD	2:E:239:GLU:HB3	2.32	0.69
1:A:2094:LEU:HB2	1:A:2106:PHE:CB	2.22	0.69
1:B:2214:LEU:HB2	1:B:2223:PHE:HB3	1.72	0.69
1:D:1156:ASP:O	1:D:1160:VAL:HG13	1.93	0.69
1:A:2089:ILE:CD1	1:A:2089:ILE:N	2.48	0.69
1:A:2188:TRP:CE2	1:A:2192:LEU:HD11	2.27	0.69
1:D:2253:ALA:HB1	1:D:2374:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:PHE:C	1:A:2048:ILE:HD13	2.17	0.69
1:B:2048:ILE:N	1:B:2048:ILE:CD1	2.32	0.69
1:B:2188:TRP:CE2	1:B:2192:LEU:HD11	2.27	0.69
1:D:2146:ILE:HG23	1:D:2474:VAL:HB	1.73	0.69
1:B:2253:ALA:HB1	1:B:2374:LEU:HD12	1.73	0.69
1:D:1057:LEU:CG	1:D:1058:GLY:H	1.97	0.69
1:A:2323:LYS:CB	1:A:2323:LYS:HZ2	1.85	0.69
1:D:2289:LYS:HA	1:D:2292:LEU:HD11	1.75	0.69
1:A:2289:LYS:HA	1:A:2292:LEU:HD12	1.75	0.69
1:B:2304:THR:HG22	1:B:2323:LYS:HZ3	1.58	0.69
1:D:2188:TRP:CE2	1:D:2192:LEU:HD11	2.27	0.69
1:A:2403:TRP:HE1	1:D:2282:PRO:HD2	1.56	0.68
1:A:2289:LYS:HA	1:A:2292:LEU:HD11	1.75	0.68
1:B:1156:ASP:O	1:B:1160:VAL:HG13	1.93	0.68
1:D:2302:ARG:CB	1:D:2323:LYS:HZ1	2.06	0.68
1:D:2304:THR:HG22	1:D:2323:LYS:NZ	2.09	0.68
1:A:2358:LYS:NZ	1:A:2383:LEU:HD22	2.08	0.68
1:D:847:LYS:HD2	1:D:928:TYR:CE2	2.29	0.68
1:A:1733:ALA:CB	1:A:1793:LEU:HD21	2.24	0.68
1:A:2304:THR:HG22	1:A:2323:LYS:NZ	2.09	0.68
1:B:704:PRO:HA	1:B:708:LEU:HB2	1.76	0.68
1:B:2304:THR:HG22	1:B:2323:LYS:NZ	2.09	0.68
1:D:600:TYR:OH	1:D:644:VAL:CG1	2.41	0.68
1:B:2146:ILE:HG23	1:B:2474:VAL:HB	1.73	0.68
1:B:2289:LYS:HA	1:B:2292:LEU:HD12	1.75	0.68
1:B:2046:PHE:C	1:B:2048:ILE:CD1	2.67	0.68
1:B:2094:LEU:HB2	1:B:2106:PHE:HB2	1.75	0.68
1:D:2323:LYS:CB	1:D:2323:LYS:HZ2	1.84	0.68
1:A:1161:ALA:HA	1:A:1165:TYR:HE2	1.59	0.68
1:B:2010:ILE:HG22	1:B:2011:GLN:N	2.09	0.68
1:B:2358:LYS:NZ	1:B:2383:LEU:HD22	2.08	0.68
2:C:241:CYS:O	2:C:244:CYS:HB2	1.94	0.68
1:D:2289:LYS:HA	1:D:2292:LEU:HD12	1.75	0.67
1:D:2046:PHE:C	1:D:2048:ILE:CD1	2.67	0.67
1:A:2046:PHE:C	1:A:2048:ILE:CD1	2.67	0.67
2:C:227:CYS:N	2:C:230:SER:OG	2.27	0.67
1:A:1156:ASP:O	1:A:1160:VAL:HG13	1.93	0.67
1:B:1161:ALA:HA	1:B:1165:TYR:HE2	1.59	0.67
1:D:704:PRO:HA	1:D:708:LEU:HB2	1.76	0.67
1:A:600:TYR:OH	1:A:644:VAL:CG1	2.41	0.67
1:A:847:LYS:HD2	1:A:928:TYR:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:TYR:OH	1:B:644:VAL:CG1	2.41	0.67
1:D:679:GLU:HA	1:D:682:SER:HB2	1.76	0.67
1:D:1733:ALA:CB	1:D:1793:LEU:HD21	2.24	0.67
1:D:2360:ILE:HA	1:D:2370:PRO:HA	1.77	0.67
1:B:679:GLU:HA	1:B:682:SER:HB2	1.76	0.67
1:B:847:LYS:HG3	1:B:928:TYR:CE2	2.30	0.67
1:D:847:LYS:HG3	1:D:928:TYR:CE2	2.30	0.67
1:A:2403:TRP:NE1	1:D:2282:PRO:HD2	2.10	0.67
1:B:1733:ALA:CB	1:B:1793:LEU:HD21	2.24	0.67
1:B:2360:ILE:HA	1:B:2370:PRO:HA	1.77	0.67
1:A:2094:LEU:CD1	1:A:2106:PHE:HD1	2.07	0.66
1:B:2080:GLN:HE21	1:B:2080:GLN:CA	1.92	0.66
2:F:227:CYS:N	2:F:230:SER:OG	2.27	0.66
1:A:704:PRO:HA	1:A:708:LEU:HB2	1.76	0.66
1:A:2094:LEU:HB2	1:A:2106:PHE:HB2	1.75	0.66
1:A:2360:ILE:HA	1:A:2370:PRO:HA	1.77	0.66
1:A:847:LYS:HG3	1:A:928:TYR:CE2	2.30	0.66
1:B:644:VAL:HB	1:B:687:PRO:HB2	1.78	0.66
1:B:2289:LYS:HA	1:B:2292:LEU:HD11	1.75	0.66
1:D:2010:ILE:HG22	1:D:2011:GLN:N	2.09	0.66
1:B:2257:ILE:CB	1:B:2423:PHE:HE2	2.09	0.66
1:A:2465:SER:C	1:A:2467:MET:H	2.04	0.66
2:E:227:CYS:N	2:E:230:SER:OG	2.27	0.66
1:A:2257:ILE:CB	1:A:2423:PHE:HE2	2.09	0.66
1:D:644:VAL:HB	1:D:687:PRO:HB2	1.78	0.66
1:D:1161:ALA:HA	1:D:1165:TYR:HE2	1.59	0.66
1:D:2358:LYS:NZ	1:D:2383:LEU:HD22	2.08	0.65
1:A:2094:LEU:CB	1:A:2106:PHE:HB2	2.26	0.65
1:B:624:LYS:HD2	1:B:711:MET:H	1.62	0.65
1:B:2094:LEU:CB	1:B:2106:PHE:HB2	2.27	0.65
1:A:1010:ARG:HH21	1:A:1014:LEU:HB3	1.61	0.65
1:A:2281:SER:N	1:A:2285:ARG:H	1.93	0.65
1:D:2280:ILE:HG22	1:D:2284:SER:HB2	1.79	0.65
1:A:679:GLU:HA	1:A:682:SER:HB2	1.76	0.65
1:B:2171:VAL:CB	2:F:236:ILE:HG12	2.27	0.65
1:D:2171:VAL:CB	2:E:236:ILE:HG12	2.27	0.65
1:D:2257:ILE:CB	1:D:2423:PHE:HE2	2.09	0.65
1:D:2465:SER:C	1:D:2467:MET:H	2.04	0.65
1:B:1010:ARG:HH21	1:B:1014:LEU:HB3	1.61	0.65
1:A:2302:ARG:HB2	1:A:2323:LYS:NZ	2.11	0.65
1:D:627:LYS:HE3	1:D:627:LYS:C	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:LYS:HD2	1:B:928:TYR:CE2	2.29	0.65
1:B:1515:TRP:CE3	1:B:1516:MET:HE1	2.16	0.65
1:A:2010:ILE:HG22	1:A:2011:GLN:N	2.10	0.65
1:B:2094:LEU:CD1	1:B:2106:PHE:HD1	2.07	0.65
1:A:2094:LEU:O	1:A:2147:PHE:CE2	2.50	0.65
1:B:627:LYS:HE3	1:B:627:LYS:C	2.21	0.64
1:B:1010:ARG:HD2	1:B:1098:ASN:HB3	1.79	0.64
1:B:2150:LYS:HE3	1:B:2475:ASP:OD1	1.97	0.64
1:D:624:LYS:HD2	1:D:711:MET:H	1.62	0.64
1:B:2094:LEU:O	1:B:2147:PHE:CE2	2.50	0.64
1:B:2358:LYS:HZ2	1:B:2383:LEU:CD2	2.11	0.64
1:A:644:VAL:HB	1:A:687:PRO:HB2	1.78	0.64
1:A:2162:PRO:HA	1:B:1408:ASP:HA	1.78	0.64
1:A:627:LYS:HE3	1:A:627:LYS:C	2.21	0.64
1:B:2117:GLU:HA	1:B:2137:MET:HE3	1.79	0.64
1:B:2280:ILE:HB	1:B:2285:ARG:CB	2.28	0.64
1:A:624:LYS:HD2	1:A:711:MET:H	1.62	0.64
1:A:853:LYS:N	1:A:853:LYS:HE2	2.13	0.64
1:A:1010:ARG:HD2	1:A:1098:ASN:HB3	1.79	0.64
1:B:2257:ILE:CA	1:B:2423:PHE:HE2	2.11	0.64
1:D:1010:ARG:HH21	1:D:1014:LEU:HB3	1.61	0.64
1:D:2094:LEU:O	1:D:2147:PHE:CE2	2.50	0.64
1:B:853:LYS:HE2	1:B:853:LYS:N	2.13	0.64
1:D:2150:LYS:HE3	1:D:2475:ASP:OD1	1.97	0.64
1:D:1515:TRP:CZ3	1:D:1516:MET:CE	2.65	0.64
1:D:2304:THR:HG22	1:D:2323:LYS:HZ3	1.63	0.64
1:B:2281:SER:H	1:B:2285:ARG:H	1.46	0.63
1:D:2257:ILE:CA	1:D:2423:PHE:HE2	2.11	0.63
1:A:2281:SER:HB2	1:B:2403:TRP:CE2	2.33	0.63
1:D:2048:ILE:N	1:D:2048:ILE:CD1	2.32	0.63
1:D:1010:ARG:HD2	1:D:1098:ASN:HB3	1.79	0.63
1:A:2150:LYS:HE3	1:A:2475:ASP:OD1	1.97	0.63
1:D:2089:ILE:CD1	1:D:2089:ILE:N	2.48	0.63
1:D:2117:GLU:HA	1:D:2137:MET:HE3	1.79	0.63
1:A:2094:LEU:CD1	1:A:2106:PHE:CD1	2.82	0.63
1:B:1552:GLN:H	1:B:1552:GLN:CD	2.06	0.63
1:D:1552:GLN:CD	1:D:1552:GLN:H	2.06	0.63
1:A:1737:THR:OG1	1:A:1790:LEU:CD1	2.47	0.63
1:A:1515:TRP:CE3	1:A:1516:MET:HE1	2.16	0.63
1:B:2094:LEU:O	1:B:2147:PHE:CZ	2.52	0.63
1:D:2109:PHE:HB2	1:D:2115:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2117:GLU:HA	1:A:2137:MET:HE3	1.80	0.63
1:B:1054:LEU:HA	1:B:1057:LEU:HD23	1.81	0.63
1:B:1940:ARG:HA	1:B:1943:ARG:CD	2.29	0.63
1:D:2094:LEU:O	1:D:2147:PHE:CZ	2.52	0.62
1:D:2175:MET:SD	2:E:239:GLU:CB	2.87	0.62
1:A:2012:PHE:O	1:A:2016:VAL:HG23	1.99	0.62
1:A:2094:LEU:O	1:A:2147:PHE:CZ	2.52	0.62
1:A:2257:ILE:CA	1:A:2423:PHE:HE2	2.11	0.62
1:D:853:LYS:HE2	1:D:853:LYS:N	2.13	0.62
1:D:1054:LEU:HA	1:D:1057:LEU:HD23	1.81	0.62
1:D:2012:PHE:O	1:D:2016:VAL:HG23	1.99	0.62
1:A:1940:ARG:HA	1:A:1943:ARG:CD	2.29	0.62
1:A:2156:GLU:OE2	1:B:1410:ALA:CB	2.37	0.62
1:A:2280:ILE:HG22	1:A:2284:SER:HB2	1.81	0.62
2:F:240:CYS:O	2:F:243:ILE:HG12	1.99	0.62
1:B:2175:MET:SD	2:F:239:GLU:CB	2.87	0.62
1:B:2253:ALA:HB1	1:B:2374:LEU:CD1	2.30	0.62
1:B:2281:SER:HG	1:D:2403:TRP:CD1	2.16	0.62
1:D:1999:GLN:CB	1:D:2050:PRO:C	2.72	0.62
1:B:1057:LEU:CG	1:B:1058:GLY:N	2.45	0.62
1:D:844:ILE:HB	1:D:848:MET:HE2	1.82	0.62
1:D:1737:THR:OG1	1:D:1790:LEU:CD1	2.47	0.62
1:A:1050:LEU:O	1:A:1054:LEU:HD13	2.00	0.62
1:B:844:ILE:HB	1:B:848:MET:HE2	1.82	0.62
1:B:1737:THR:OG1	1:B:1790:LEU:CD1	2.47	0.62
1:A:1552:GLN:CD	1:A:1552:GLN:H	2.06	0.62
1:B:2012:PHE:O	1:B:2016:VAL:HG23	1.99	0.62
1:B:2289:LYS:O	1:B:2292:LEU:HD12	2.00	0.62
1:D:1940:ARG:HA	1:D:1943:ARG:HD2	1.82	0.62
1:D:2117:GLU:HA	1:D:2137:MET:CE	2.30	0.62
1:A:844:ILE:HB	1:A:848:MET:HE2	1.82	0.61
1:A:2253:ALA:HB1	1:A:2374:LEU:CD1	2.30	0.61
1:B:1357:ILE:CG2	1:B:2495:LEU:CD2	2.73	0.61
1:D:2289:LYS:O	1:D:2292:LEU:HD12	2.00	0.61
1:B:2459:PHE:CE1	2:F:243:ILE:HG13	2.34	0.61
1:D:1050:LEU:O	1:D:1054:LEU:HD13	2.00	0.61
1:D:2371:VAL:HG11	1:D:2374:LEU:HD22	1.82	0.61
1:A:2289:LYS:O	1:A:2292:LEU:HD12	2.00	0.61
1:B:2094:LEU:CD1	1:B:2106:PHE:CD1	2.82	0.61
1:D:1940:ARG:HA	1:D:1943:ARG:CD	2.29	0.61
1:A:1054:LEU:HA	1:A:1057:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:SER:O	1:B:687:PRO:HD2	2.01	0.61
1:A:2304:THR:HG22	1:A:2323:LYS:HZ3	1.63	0.61
1:B:2094:LEU:HB2	1:B:2106:PHE:CG	2.35	0.61
1:D:2253:ALA:HB1	1:D:2374:LEU:CD1	2.30	0.61
1:B:1050:LEU:O	1:B:1054:LEU:HD13	2.00	0.61
1:D:847:LYS:CG	1:D:928:TYR:HE2	2.14	0.61
1:D:1940:ARG:O	1:D:1944:ARG:HG2	2.00	0.61
1:A:1177:THR:HG21	1:A:1291:CYS:HB2	1.83	0.61
1:D:683:SER:O	1:D:687:PRO:HD2	2.01	0.61
1:A:1737:THR:O	1:A:1741:VAL:CG2	2.42	0.61
1:B:1177:THR:HG21	1:B:1291:CYS:HB2	1.83	0.61
1:A:2094:LEU:HB2	1:A:2106:PHE:CG	2.35	0.61
1:B:1940:ARG:O	1:B:1944:ARG:HG2	2.00	0.61
1:A:847:LYS:CG	1:A:928:TYR:HE2	2.14	0.61
1:A:2117:GLU:HA	1:A:2137:MET:CE	2.30	0.61
1:B:1940:ARG:HA	1:B:1943:ARG:HD2	1.82	0.61
1:D:1357:ILE:CG2	1:D:2495:LEU:CD2	2.73	0.61
1:D:2175:MET:CG	2:E:236:ILE:HG23	2.30	0.61
1:D:2361:ARG:HG2	1:D:2371:VAL:HG22	1.82	0.61
1:B:847:LYS:CG	1:B:928:TYR:HE2	2.14	0.60
1:B:2117:GLU:HA	1:B:2137:MET:CE	2.30	0.60
1:A:683:SER:O	1:A:687:PRO:HD2	2.01	0.60
1:A:1940:ARG:O	1:A:1944:ARG:HG2	2.00	0.60
1:A:2371:VAL:HG11	1:A:2374:LEU:HD22	1.82	0.60
1:B:2361:ARG:HG2	1:B:2371:VAL:HG22	1.83	0.60
1:B:2371:VAL:HG11	1:B:2374:LEU:HD22	1.82	0.60
2:C:233:CYS:HA	2:C:236:ILE:HD12	1.82	0.60
1:D:922:GLY:HA2	1:D:928:TYR:CZ	2.36	0.60
1:D:1177:THR:HG21	1:D:1291:CYS:HB2	1.83	0.60
1:A:2467:MET:CA	1:B:2507:TYR:O	2.49	0.60
1:B:791:HIS:HB2	1:B:946:TYR:HE2	1.67	0.60
1:B:922:GLY:HA2	1:B:928:TYR:CZ	2.36	0.60
1:D:791:HIS:HB2	1:D:946:TYR:HE2	1.67	0.60
1:D:2170:ILE:C	2:E:236:ILE:HD11	2.27	0.60
1:A:1943:ARG:HD3	1:A:1944:ARG:HH21	1.67	0.60
1:A:2507:TYR:O	1:D:2467:MET:CA	2.49	0.60
1:D:2095:THR:CB	1:D:2143:TYR:CE2	2.85	0.60
1:A:1695:ILE:HD12	1:A:1714:VAL:CG2	2.29	0.60
1:A:2361:ARG:HG2	1:A:2371:VAL:HG22	1.83	0.60
1:A:2302:ARG:CB	1:A:2323:LYS:HZ1	2.06	0.60
1:B:2175:MET:CG	2:F:236:ILE:HG23	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1999:GLN:CB	1:A:2050:PRO:C	2.72	0.60
1:A:1940:ARG:HA	1:A:1943:ARG:HD2	1.82	0.59
1:B:2010:ILE:CG2	1:B:2011:GLN:N	2.65	0.59
1:D:1943:ARG:HD3	1:D:1944:ARG:HH21	1.67	0.59
1:D:2294:ASN:O	1:D:2295:GLY:C	2.46	0.59
1:A:922:GLY:HA2	1:A:928:TYR:CZ	2.36	0.59
1:B:1160:VAL:HG23	1:B:1165:TYR:OH	2.02	0.59
1:D:1699:HIS:HD1	1:D:1707:SER:HB2	1.65	0.59
1:A:2095:THR:CB	1:A:2143:TYR:CE2	2.85	0.59
1:D:2443:LEU:HD22	1:D:2444:TYR:CA	2.33	0.59
1:A:2403:TRP:CD1	1:D:2281:SER:HB2	2.38	0.59
1:D:1654:LEU:HG	1:D:1655:ARG:NH1	2.18	0.59
1:D:1695:ILE:HD11	1:D:1714:VAL:HG21	0.69	0.59
1:B:2170:ILE:C	2:F:236:ILE:HD11	2.27	0.59
1:A:1160:VAL:HG23	1:A:1165:TYR:OH	2.02	0.59
1:B:1699:HIS:HD1	1:B:1707:SER:HB2	1.65	0.59
1:D:1160:VAL:HG23	1:D:1165:TYR:OH	2.02	0.59
1:A:1357:ILE:CG2	1:A:2495:LEU:CD2	2.73	0.59
1:A:2374:LEU:HD21	1:A:2423:PHE:CZ	2.38	0.59
1:B:2294:ASN:O	1:B:2295:GLY:C	2.45	0.59
1:A:1208:THR:HA	1:A:1302:PHE:CD1	2.38	0.59
1:A:1699:HIS:HD1	1:A:1707:SER:HB2	1.65	0.59
1:A:2010:ILE:CG2	1:A:2011:GLN:N	2.66	0.59
1:A:922:GLY:HA2	1:A:928:TYR:CE2	2.38	0.59
1:B:922:GLY:HA2	1:B:928:TYR:CE2	2.38	0.59
1:A:2048:ILE:N	1:A:2048:ILE:CD1	2.32	0.58
1:B:2443:LEU:HD22	1:B:2444:TYR:CA	2.33	0.58
1:D:1208:THR:HA	1:D:1302:PHE:CD1	2.38	0.58
1:D:2010:ILE:CG2	1:D:2011:GLN:N	2.66	0.58
1:D:2175:MET:CA	2:E:240:CYS:HG	1.99	0.58
1:B:1515:TRP:CZ3	1:B:1516:MET:CE	2.65	0.58
1:B:1695:ILE:HD12	1:B:1714:VAL:CG2	2.29	0.58
1:B:1737:THR:O	1:B:1741:VAL:CG2	2.42	0.58
1:B:2171:VAL:HG13	2:F:236:ILE:HG13	1.84	0.58
1:D:814:LEU:HD11	1:D:840:THR:CB	2.34	0.58
1:A:2294:ASN:O	1:A:2295:GLY:C	2.45	0.58
1:B:2095:THR:CB	1:B:2143:TYR:CE2	2.85	0.58
1:D:1737:THR:O	1:D:1741:VAL:CG2	2.42	0.58
1:A:791:HIS:HB2	1:A:946:TYR:HE2	1.67	0.58
1:A:2443:LEU:HD22	1:A:2444:TYR:CA	2.33	0.58
1:B:636:TYR:HA	1:B:639:LEU:CD1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:LYS:HG3	1:B:928:TYR:HE2	1.68	0.58
1:B:1208:THR:HA	1:B:1302:PHE:CD1	2.38	0.58
1:D:2281:SER:O	1:D:2285:ARG:N	2.37	0.58
1:D:2374:LEU:HD21	1:D:2423:PHE:CZ	2.38	0.58
1:A:636:TYR:HA	1:A:639:LEU:CD1	2.34	0.58
1:B:1654:LEU:HG	1:B:1655:ARG:NH1	2.18	0.58
1:D:621:LEU:HA	1:D:624:LYS:HD3	1.85	0.58
1:D:1360:LYS:C	1:D:1362:GLU:H	2.12	0.58
1:A:1654:LEU:HG	1:A:1655:ARG:NH1	2.18	0.58
1:B:1999:GLN:CB	1:B:2050:PRO:C	2.72	0.58
1:B:2374:LEU:HD21	1:B:2423:PHE:CZ	2.38	0.58
1:A:814:LEU:HD11	1:A:840:THR:CB	2.34	0.58
1:D:2170:ILE:O	2:E:236:ILE:HD13	2.03	0.58
1:A:847:LYS:HG3	1:A:928:TYR:HE2	1.68	0.58
1:B:621:LEU:HA	1:B:624:LYS:HD3	1.85	0.58
1:B:1943:ARG:HD3	1:B:1944:ARG:HH21	1.67	0.58
1:B:2175:MET:CA	2:F:240:CYS:HG	2.00	0.58
1:A:1360:LYS:C	1:A:1362:GLU:H	2.12	0.57
1:A:1744:LYS:HZ3	1:A:1744:LYS:HB2	1.70	0.57
1:D:922:GLY:HA2	1:D:928:TYR:CE2	2.38	0.57
1:D:636:TYR:HA	1:D:639:LEU:CD1	2.34	0.57
1:D:2302:ARG:HB2	1:D:2323:LYS:NZ	2.11	0.57
1:A:621:LEU:HA	1:A:624:LYS:HD3	1.85	0.57
1:A:922:GLY:CA	1:A:928:TYR:CE2	2.87	0.57
1:A:1057:LEU:CG	1:A:1058:GLY:N	2.45	0.57
1:A:2120:ALA:CB	1:A:2137:MET:SD	2.93	0.57
1:B:922:GLY:CA	1:B:928:TYR:CE2	2.87	0.57
1:B:2170:ILE:O	2:F:236:ILE:HD13	2.03	0.57
1:B:814:LEU:HD11	1:B:840:THR:CB	2.34	0.57
1:B:2120:ALA:CB	1:B:2137:MET:SD	2.93	0.57
1:D:1650:LEU:HD11	1:D:1654:LEU:HD12	1.87	0.57
1:D:2120:ALA:CB	1:D:2137:MET:SD	2.93	0.57
1:B:627:LYS:HA	1:B:627:LYS:CE	2.20	0.57
1:A:1695:ILE:CD1	1:A:1714:VAL:HG23	2.32	0.57
1:A:1409:HIS:O	1:A:1413:ILE:HG12	2.05	0.57
1:B:1159:LYS:O	1:B:1163:PHE:HB2	2.05	0.57
1:B:1360:LYS:C	1:B:1362:GLU:H	2.12	0.57
1:B:1413:ILE:CG2	1:B:2497:GLU:HB3	2.34	0.57
1:D:1194:PHE:CD1	1:D:1738:GLU:HG2	2.40	0.57
1:D:1568:LEU:HD13	1:D:1659:LEU:HD23	1.87	0.57
1:B:2156:GLU:OE2	1:D:1410:ALA:CB	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2323:LYS:HB3	1:B:2323:LYS:HZ3	0.74	0.57
1:D:1159:LYS:O	1:D:1163:PHE:HB2	2.05	0.57
1:D:1413:ILE:CG2	1:D:2497:GLU:HB3	2.34	0.57
1:A:2172:LYS:HA	1:B:2124:TRP:CZ3	2.40	0.56
1:A:2467:MET:HE1	1:B:2468:PHE:CG	2.40	0.56
1:B:2265:ILE:HD13	1:B:2423:PHE:CA	2.35	0.56
1:D:1160:VAL:CG1	1:D:1550:LEU:HD23	2.34	0.56
1:B:1568:LEU:HD13	1:B:1659:LEU:HD23	1.87	0.56
1:D:922:GLY:CA	1:D:928:TYR:CE2	2.87	0.56
1:A:1568:LEU:HD13	1:A:1659:LEU:HD23	1.87	0.56
1:B:1733:ALA:HB1	1:B:1793:LEU:CD2	2.35	0.56
1:D:2171:VAL:HG13	2:E:236:ILE:HG13	1.83	0.56
1:A:2124:TRP:CZ3	1:D:2172:LYS:HA	2.40	0.56
1:A:2281:SER:CB	1:B:2275:GLY:HA2	2.30	0.56
1:A:2358:LYS:HG2	1:A:2420:MET:HG3	1.88	0.56
1:B:1194:PHE:CD1	1:B:1738:GLU:HG2	2.40	0.56
1:B:1695:ILE:CD1	1:B:1714:VAL:HG23	2.32	0.56
1:B:2094:LEU:CB	1:B:2106:PHE:HD1	2.18	0.56
1:A:1650:LEU:HD11	1:A:1654:LEU:HD12	1.86	0.56
1:A:1733:ALA:CB	1:A:1793:LEU:CD2	2.84	0.56
1:B:2172:LYS:HA	1:D:2124:TRP:CZ3	2.40	0.56
1:D:2358:LYS:HG2	1:D:2420:MET:HG3	1.88	0.56
1:A:1159:LYS:O	1:A:1163:PHE:HB2	2.05	0.56
1:B:1160:VAL:CG1	1:B:1550:LEU:HD23	2.34	0.56
1:B:1733:ALA:CB	1:B:1793:LEU:CD2	2.84	0.56
1:D:1733:ALA:CB	1:D:1793:LEU:CD2	2.84	0.56
1:D:1744:LYS:HZ3	1:D:1744:LYS:HB2	1.70	0.56
1:A:2275:GLY:HA3	1:D:2280:ILE:C	2.30	0.56
1:B:2049:LEU:HD23	1:B:2049:LEU:H	1.71	0.56
1:B:2219:TYR:HD1	1:D:2271:GLU:OE2	1.89	0.56
1:A:1194:PHE:CD1	1:A:1738:GLU:HG2	2.40	0.56
1:B:2358:LYS:HG2	1:B:2420:MET:HG3	1.88	0.55
1:D:1695:ILE:HD12	1:D:1714:VAL:CG2	2.29	0.55
1:D:2171:VAL:CA	2:E:236:ILE:HD13	2.28	0.55
1:A:2208:ILE:H	1:A:2309:ARG:HA	1.72	0.55
1:A:2265:ILE:HD13	1:A:2423:PHE:CA	2.35	0.55
1:B:2208:ILE:H	1:B:2309:ARG:HA	1.72	0.55
1:D:627:LYS:CA	1:D:627:LYS:CE	2.81	0.55
1:D:2208:ILE:H	1:D:2309:ARG:HA	1.72	0.55
1:D:2383:LEU:HD23	1:D:2420:MET:HE3	1.89	0.55
1:A:2045:MET:O	1:A:2048:ILE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1733:ALA:HB1	1:D:1793:LEU:CD2	2.35	0.55
1:A:778:SER:O	1:A:782:VAL:HG23	2.07	0.55
1:A:2219:TYR:HD1	1:B:2271:GLU:OE2	1.89	0.55
1:A:2281:SER:O	1:A:2285:ARG:N	2.40	0.55
1:D:2222:LEU:HG	1:D:2278:TRP:HA	1.89	0.55
1:D:2257:ILE:HA	1:D:2423:PHE:CE2	2.42	0.55
1:A:1160:VAL:CG1	1:A:1550:LEU:HD23	2.34	0.55
1:A:2271:GLU:OE2	1:D:2219:TYR:HD1	1.89	0.55
1:A:2467:MET:HE1	1:B:2468:PHE:CD1	2.41	0.55
1:B:2147:PHE:CZ	1:B:2151:CYS:SG	3.00	0.55
1:B:2257:ILE:CB	1:B:2423:PHE:CE2	2.89	0.55
1:D:778:SER:O	1:D:782:VAL:HG23	2.07	0.55
1:A:2049:LEU:HD23	1:A:2049:LEU:H	1.71	0.55
1:A:2328:LEU:HD13	1:A:2335:ARG:HG3	1.88	0.55
1:D:2328:LEU:HD13	1:D:2335:ARG:HG3	1.88	0.55
1:A:2147:PHE:CZ	1:A:2151:CYS:SG	3.00	0.54
1:B:1744:LYS:HZ3	1:B:1744:LYS:HB2	1.72	0.54
1:A:1733:ALA:HB1	1:A:1793:LEU:CD2	2.35	0.54
1:A:2136:TRP:CZ3	1:A:2488:ARG:NH1	2.75	0.54
1:B:1979:PHE:CG	1:B:2440:ILE:HG21	2.43	0.54
1:D:2147:PHE:CZ	1:D:2151:CYS:SG	3.00	0.54
1:B:2171:VAL:CA	2:F:236:ILE:HD13	2.28	0.54
1:D:636:TYR:HA	1:D:639:LEU:HD13	1.90	0.54
1:A:776:VAL:O	1:A:779:ARG:HG3	2.08	0.54
1:A:1695:ILE:HD11	1:A:1714:VAL:HG21	0.69	0.54
1:A:2257:ILE:CB	1:A:2423:PHE:CE2	2.89	0.54
1:D:2257:ILE:CB	1:D:2423:PHE:CE2	2.89	0.54
1:A:1413:ILE:CG2	1:A:2497:GLU:HB3	2.34	0.54
1:B:2136:TRP:CZ3	1:B:2488:ARG:NH1	2.75	0.54
1:B:2257:ILE:HA	1:B:2423:PHE:CE2	2.42	0.54
1:A:2049:LEU:H	1:A:2049:LEU:CD2	2.19	0.54
1:A:2257:ILE:HA	1:A:2423:PHE:CE2	2.42	0.54
1:B:2465:SER:O	1:B:2467:MET:N	2.40	0.54
1:D:1979:PHE:CG	1:D:2440:ILE:HG21	2.43	0.54
1:D:2049:LEU:HD23	1:D:2049:LEU:H	1.71	0.54
1:D:2136:TRP:CZ3	1:D:2488:ARG:NH1	2.75	0.54
1:A:1979:PHE:HB2	1:A:2440:ILE:HD13	1.90	0.54
1:A:2383:LEU:HD23	1:A:2420:MET:HE3	1.89	0.54
1:B:2328:LEU:HD13	1:B:2335:ARG:HG3	1.88	0.54
1:D:1010:ARG:HB3	1:D:1015:VAL:HG21	1.90	0.54
1:A:1010:ARG:HB3	1:A:1015:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:SER:C	1:A:2467:MET:N	2.64	0.54
1:A:2465:SER:O	1:A:2467:MET:N	2.41	0.54
1:B:1010:ARG:HB3	1:B:1015:VAL:HG21	1.90	0.54
1:B:2171:VAL:HG12	2:F:239:GLU:OE2	2.08	0.54
1:A:2355:LEU:HA	1:A:2382:TYR:HD2	1.73	0.54
1:D:1715:PHE:HA	1:D:1719:MET:HE2	1.90	0.54
1:D:1979:PHE:HB2	1:D:2440:ILE:HD13	1.90	0.54
1:D:2265:ILE:CD1	1:D:2423:PHE:CE2	2.91	0.54
1:D:2265:ILE:HD13	1:D:2423:PHE:CA	2.35	0.54
1:B:636:TYR:HA	1:B:639:LEU:HD13	1.90	0.53
1:B:1979:PHE:HB2	1:B:2440:ILE:HD13	1.90	0.53
1:B:2162:PRO:HA	1:D:1408:ASP:HA	1.89	0.53
1:B:2174:GLY:HA3	2:F:236:ILE:HG21	1.89	0.53
1:B:2383:LEU:HD23	1:B:2420:MET:HE3	1.89	0.53
1:D:820:ALA:O	1:D:1046:ALA:HB1	2.09	0.53
1:D:2170:ILE:C	2:E:236:ILE:CD1	2.81	0.53
1:A:1715:PHE:HA	1:A:1719:MET:HE2	1.90	0.53
1:A:2257:ILE:CA	1:A:2423:PHE:CE2	2.91	0.53
1:B:776:VAL:O	1:B:779:ARG:HG3	2.08	0.53
1:B:1336:ILE:O	1:B:1340:ARG:HG3	2.09	0.53
1:A:1336:ILE:O	1:A:1340:ARG:HG3	2.09	0.53
1:B:2170:ILE:C	2:F:236:ILE:CD1	2.81	0.53
1:B:2355:LEU:HA	1:B:2382:TYR:HD2	1.73	0.53
1:B:2467:MET:HB2	1:B:2468:PHE:CE2	2.43	0.53
1:D:1568:LEU:HA	1:D:1657:PRO:HD2	1.91	0.53
1:B:778:SER:O	1:B:782:VAL:HG23	2.07	0.53
1:B:1298:GLN:HA	1:B:1301:VAL:HG22	1.91	0.53
1:B:1568:LEU:O	1:B:1653:ARG:CB	2.44	0.53
1:B:2363:PRO:HA	1:B:2425:ASP:HB3	1.91	0.53
2:C:232:ASP:O	2:C:236:ILE:HG13	2.09	0.53
1:D:2465:SER:O	1:D:2467:MET:N	2.41	0.53
1:A:636:TYR:HA	1:A:639:LEU:HD13	1.90	0.53
1:A:1979:PHE:CG	1:A:2440:ILE:HG21	2.43	0.53
1:B:587:MET:HE2	1:B:587:MET:HA	1.91	0.53
1:B:2257:ILE:CA	1:B:2423:PHE:CE2	2.91	0.53
1:B:2296:THR:HA	1:B:2330:PRO:HB3	1.91	0.53
1:D:776:VAL:O	1:D:779:ARG:HG3	2.08	0.53
1:A:1568:LEU:HA	1:A:1657:PRO:HD2	1.91	0.53
1:A:2103:LEU:HG	1:A:2151:CYS:HB3	1.90	0.53
1:B:820:ALA:O	1:B:1046:ALA:HB1	2.09	0.53
1:B:2265:ILE:CD1	1:B:2423:PHE:CE2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2465:SER:C	1:D:2467:MET:N	2.64	0.53
1:A:1160:VAL:CB	1:A:1550:LEU:HD23	2.39	0.53
1:A:1298:GLN:HA	1:A:1301:VAL:HG22	1.91	0.53
1:A:2296:THR:HA	1:A:2330:PRO:HB3	1.91	0.53
1:B:1160:VAL:CB	1:B:1550:LEU:HD23	2.39	0.53
1:B:1715:PHE:HA	1:B:1719:MET:HE2	1.90	0.53
1:B:2302:ARG:HB2	1:B:2323:LYS:NZ	2.11	0.53
1:D:2103:LEU:HG	1:D:2151:CYS:HB3	1.90	0.53
1:A:820:ALA:O	1:A:1046:ALA:HB1	2.09	0.52
1:B:2002:GLU:O	1:B:2006:VAL:HG22	2.09	0.52
1:B:2282:PRO:HD2	1:D:2403:TRP:NE1	2.23	0.52
1:D:1336:ILE:O	1:D:1340:ARG:HG3	2.09	0.52
1:A:2363:PRO:HA	1:A:2425:ASP:HB3	1.91	0.52
1:B:1052:GLN:CB	1:B:1099:LEU:CD1	2.76	0.52
1:D:1160:VAL:CB	1:D:1550:LEU:HD23	2.39	0.52
1:D:2174:GLY:HA3	2:E:236:ILE:HG21	1.89	0.52
1:A:1052:GLN:CB	1:A:1099:LEU:CD1	2.76	0.52
1:B:601:LYS:HD2	1:B:848:MET:HE3	1.91	0.52
1:B:1695:ILE:HD12	1:B:1714:VAL:HG23	1.91	0.52
1:A:1695:ILE:HD12	1:A:1714:VAL:HG23	1.91	0.52
1:B:791:HIS:HB2	1:B:946:TYR:CE2	2.45	0.52
1:D:2049:LEU:HD23	1:D:2049:LEU:N	2.25	0.52
1:A:2094:LEU:CB	1:A:2106:PHE:HD1	2.18	0.52
1:A:2130:THR:HG23	1:A:2493:LEU:HB3	1.92	0.52
1:A:2281:SER:HB2	1:B:2403:TRP:NE1	2.25	0.52
1:A:2281:SER:O	1:A:2282:PRO:C	2.52	0.52
1:B:809:SER:HA	1:B:1057:LEU:HB2	1.92	0.52
1:B:2049:LEU:HD23	1:B:2049:LEU:N	2.25	0.52
1:B:2103:LEU:HG	1:B:2151:CYS:HB3	1.90	0.52
1:D:2257:ILE:CA	1:D:2423:PHE:CE2	2.91	0.52
1:A:601:LYS:HD2	1:A:848:MET:HE3	1.91	0.52
1:D:2355:LEU:HA	1:D:2382:TYR:HD2	1.73	0.52
1:B:1568:LEU:HA	1:B:1657:PRO:HD2	1.91	0.52
1:D:1298:GLN:HA	1:D:1301:VAL:HG22	1.91	0.52
1:A:809:SER:HA	1:A:1057:LEU:HB2	1.92	0.52
1:A:2265:ILE:CD1	1:A:2423:PHE:CE2	2.91	0.52
1:A:2280:ILE:HB	1:A:2285:ARG:CB	2.40	0.52
1:A:2358:LYS:HZ2	1:A:2383:LEU:CD2	2.22	0.52
1:B:841:CYS:O	1:B:845:VAL:HG23	2.10	0.52
1:B:2281:SER:O	1:B:2285:ARG:N	2.43	0.52
2:C:243:ILE:HG22	2:C:247:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:PHE:O	1:A:2048:ILE:CD1	2.58	0.52
1:A:2101:LEU:HD13	1:A:2105:LEU:HD11	1.92	0.52
1:B:2101:LEU:HD13	1:B:2105:LEU:HD11	1.92	0.51
1:D:587:MET:HE2	1:D:587:MET:HA	1.91	0.51
1:D:1695:ILE:HD12	1:D:1714:VAL:HG23	1.91	0.51
1:A:627:LYS:CA	1:A:627:LYS:CE	2.81	0.51
1:A:841:CYS:O	1:A:845:VAL:HG23	2.10	0.51
1:B:1695:ILE:HD11	1:B:1714:VAL:HG21	0.69	0.51
1:D:809:SER:HA	1:D:1057:LEU:HB2	1.92	0.51
1:D:2296:THR:HA	1:D:2330:PRO:HB3	1.91	0.51
1:D:2363:PRO:HA	1:D:2425:ASP:HB3	1.91	0.51
1:D:2393:GLN:HG2	1:D:2400:PHE:HA	1.93	0.51
1:A:2136:TRP:CZ3	1:A:2488:ARG:CZ	2.93	0.51
1:B:1208:THR:HA	1:B:1302:PHE:HD1	1.75	0.51
1:D:1188:GLY:HA3	1:D:1221:TYR:OH	2.10	0.51
1:D:2130:THR:HG23	1:D:2493:LEU:HB3	1.92	0.51
1:D:2165:GLN:O	1:D:2166:LYS:C	2.53	0.51
1:D:2171:VAL:HG12	2:E:239:GLU:OE2	2.08	0.51
1:A:791:HIS:HB2	1:A:946:TYR:CE2	2.45	0.51
1:B:2046:PHE:O	1:B:2048:ILE:CD1	2.58	0.51
1:D:841:CYS:O	1:D:845:VAL:HG23	2.10	0.51
1:D:1052:GLN:CB	1:D:1099:LEU:CD1	2.76	0.51
1:B:1188:GLY:HA3	1:B:1221:TYR:OH	2.10	0.51
1:B:2136:TRP:CZ3	1:B:2488:ARG:CZ	2.93	0.51
1:B:2281:SER:N	1:B:2285:ARG:H	2.06	0.51
1:D:2167:LYS:O	1:D:2168:LYS:HB2	2.11	0.51
1:A:2315:GLY:HA2	1:A:2364:ASN:HB3	1.93	0.51
1:B:2130:THR:HG23	1:B:2493:LEU:HB3	1.92	0.51
1:D:580:TRP:HZ3	1:D:701:PHE:HB2	1.76	0.51
1:D:601:LYS:HD2	1:D:848:MET:HE3	1.91	0.51
1:D:1744:LYS:HB2	1:D:1744:LYS:NZ	2.26	0.51
1:D:2002:GLU:O	1:D:2006:VAL:HG22	2.09	0.51
2:E:240:CYS:O	2:E:243:ILE:HG12	2.09	0.51
1:A:2092:ASN:OD1	1:A:2106:PHE:CD1	2.64	0.51
1:B:580:TRP:HZ3	1:B:701:PHE:HB2	1.76	0.51
1:D:1695:ILE:CD1	1:D:1714:VAL:HG23	2.32	0.51
1:D:2101:LEU:HD13	1:D:2105:LEU:HD11	1.92	0.51
1:D:2314:GLY:HA3	1:D:2427:VAL:HG11	1.92	0.51
1:A:580:TRP:HZ3	1:A:701:PHE:HB2	1.76	0.51
1:B:1744:LYS:HB2	1:B:1744:LYS:NZ	2.26	0.51
1:B:2393:GLN:HG2	1:B:2400:PHE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1568:LEU:O	1:D:1653:ARG:CB	2.44	0.51
1:A:1188:GLY:HA3	1:A:1221:TYR:OH	2.10	0.51
1:A:2049:LEU:HD23	1:A:2049:LEU:N	2.25	0.50
1:A:2393:GLN:HG2	1:A:2400:PHE:HA	1.93	0.50
1:D:2046:PHE:O	1:D:2048:ILE:CD1	2.58	0.50
1:A:2314:GLY:HA3	1:A:2427:VAL:HG11	1.92	0.50
1:B:2092:ASN:OD1	1:B:2106:PHE:CD1	2.64	0.50
1:B:2314:GLY:HA3	1:B:2427:VAL:HG11	1.92	0.50
1:D:2136:TRP:CZ3	1:D:2488:ARG:CZ	2.93	0.50
1:A:2202:GLY:H	1:A:2428:SER:HA	1.77	0.50
1:A:2323:LYS:HB3	1:A:2323:LYS:HZ3	0.68	0.50
1:D:602:ILE:HG23	1:D:845:VAL:HG22	1.93	0.50
1:D:2323:LYS:HB3	1:D:2323:LYS:HZ3	0.68	0.50
1:B:587:MET:CA	1:B:587:MET:CE	2.89	0.50
1:A:1409:HIS:C	1:A:1411:THR:N	2.67	0.50
1:A:1568:LEU:O	1:A:1653:ARG:CB	2.44	0.50
1:B:1360:LYS:C	1:B:1362:GLU:N	2.69	0.50
1:A:1410:ALA:HB2	1:D:2156:GLU:OE2	2.12	0.50
1:A:1744:LYS:HB2	1:A:1744:LYS:NZ	2.26	0.50
1:A:2094:LEU:CB	1:A:2106:PHE:CB	2.89	0.50
1:B:602:ILE:HG23	1:B:845:VAL:HG22	1.93	0.50
1:D:2352:ILE:HB	1:D:2385:VAL:HG13	1.94	0.50
1:B:2165:GLN:O	1:B:2166:LYS:C	2.54	0.50
1:B:2315:GLY:HA2	1:B:2364:ASN:HB3	1.93	0.50
1:A:2046:PHE:O	1:A:2048:ILE:HD13	2.12	0.50
1:A:2391:ARG:HB3	1:A:2402:GLU:HG2	1.94	0.50
1:B:644:VAL:HG12	1:B:683:SER:HB2	1.94	0.50
1:B:2010:ILE:HG22	1:B:2011:GLN:H	1.77	0.50
1:B:2274:SER:CB	1:B:2404:TRP:H	2.25	0.50
1:B:2352:ILE:HB	1:B:2385:VAL:HG13	1.94	0.50
1:B:2391:ARG:HB3	1:B:2402:GLU:HG2	1.94	0.50
1:D:791:HIS:HB2	1:D:946:TYR:CE2	2.45	0.50
1:D:1688:GLU:OE1	1:D:1725:PRO:CD	2.60	0.50
1:A:949:GLN:HA	1:A:952:TYR:HB2	1.94	0.50
1:A:1688:GLU:OE1	1:A:1725:PRO:CD	2.60	0.50
1:B:627:LYS:CA	1:B:627:LYS:CE	2.81	0.50
1:B:635:ALA:C	1:B:639:LEU:HD12	2.33	0.50
1:B:949:GLN:HA	1:B:952:TYR:HB2	1.94	0.50
1:B:2167:LYS:O	1:B:2168:LYS:HB2	2.11	0.50
1:D:2202:GLY:H	1:D:2428:SER:HA	1.77	0.50
1:A:1208:THR:HA	1:A:1302:PHE:HD1	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:LYS:C	1:A:1362:GLU:N	2.69	0.49
1:D:1704:SER:HA	1:D:2046:PHE:HE1	1.77	0.49
1:A:2352:ILE:HB	1:A:2385:VAL:HG13	1.94	0.49
1:A:2468:PHE:CE1	1:A:2510:PRO:HG3	2.47	0.49
1:B:922:GLY:HA3	1:B:928:TYR:CE2	2.47	0.49
1:D:2010:ILE:HG22	1:D:2011:GLN:H	1.77	0.49
1:D:2341:LEU:HD13	1:D:2389:LEU:HB3	1.94	0.49
1:D:949:GLN:HA	1:D:952:TYR:HB2	1.94	0.49
1:A:1409:HIS:N	1:A:1412:VAL:HG12	2.27	0.49
1:A:1979:PHE:CD1	1:A:2440:ILE:HG21	2.47	0.49
1:B:2281:SER:O	1:B:2282:PRO:C	2.52	0.49
1:D:1562:ARG:HD2	1:D:1566:ASP:HB2	1.94	0.49
1:D:922:GLY:HA3	1:D:928:TYR:CE2	2.47	0.49
1:A:2002:GLU:O	1:A:2006:VAL:HG22	2.09	0.49
1:B:2171:VAL:HG11	2:F:239:GLU:OE2	2.12	0.49
1:A:1704:SER:HA	1:A:2046:PHE:HE1	1.77	0.49
1:B:1688:GLU:OE1	1:B:1725:PRO:CD	2.60	0.49
1:B:2202:GLY:H	1:B:2428:SER:HA	1.77	0.49
1:B:2293:TYR:HB2	1:B:2294:ASN:OD1	2.13	0.49
1:B:2341:LEU:HD13	1:B:2389:LEU:HB3	1.94	0.49
1:D:1028:ARG:HB3	1:D:1034:ILE:HG12	1.95	0.49
1:D:2280:ILE:HB	1:D:2285:ARG:CB	2.42	0.49
1:D:2315:GLY:HA2	1:D:2364:ASN:HB3	1.93	0.49
1:A:2095:THR:HA	1:A:2147:PHE:CD1	2.48	0.49
1:D:2095:THR:HA	1:D:2147:PHE:CD1	2.48	0.49
1:D:2459:PHE:CE1	2:E:243:ILE:HG13	2.48	0.49
1:A:602:ILE:HG23	1:A:845:VAL:HG22	1.93	0.49
1:B:1979:PHE:CD1	1:B:2440:ILE:HG21	2.47	0.49
1:B:1160:VAL:HA	1:B:1550:LEU:HD23	1.91	0.49
1:B:2049:LEU:H	1:B:2049:LEU:CD2	2.20	0.49
1:D:1979:PHE:CD1	1:D:2440:ILE:HG21	2.47	0.49
1:A:1206:ARG:O	1:A:1210:ALA:HB3	2.13	0.48
1:B:2010:ILE:HD12	1:B:2010:ILE:HA	1.63	0.48
1:B:2289:LYS:CA	1:B:2292:LEU:HD12	2.42	0.48
1:D:2046:PHE:O	1:D:2048:ILE:HD13	2.12	0.48
1:D:2292:LEU:HD22	1:D:2338:LEU:HB3	1.95	0.48
1:D:2391:ARG:HB3	1:D:2402:GLU:HG2	1.94	0.48
1:A:1409:HIS:O	1:A:1410:ALA:C	2.57	0.48
1:B:950:GLU:HB3	1:B:954:ARG:HH21	1.78	0.48
1:D:644:VAL:HG12	1:D:683:SER:HB2	1.94	0.48
1:A:644:VAL:HG12	1:A:683:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:GLY:HA3	1:A:928:TYR:CE2	2.47	0.48
1:A:1208:THR:HB	1:A:1311:ARG:HE	1.78	0.48
1:A:1562:ARG:HD2	1:A:1566:ASP:HB2	1.94	0.48
1:A:2010:ILE:O	1:A:2011:GLN:C	2.57	0.48
1:A:2120:ALA:HB3	1:A:2137:MET:SD	2.53	0.48
1:A:2292:LEU:HD22	1:A:2338:LEU:HB3	1.95	0.48
1:A:2459:PHE:CE1	2:C:243:ILE:HG13	2.49	0.48
1:B:1028:ARG:HB3	1:B:1034:ILE:HG12	1.95	0.48
1:B:1206:ARG:O	1:B:1210:ALA:HB3	2.13	0.48
1:B:1704:SER:HA	1:B:2046:PHE:HE1	1.77	0.48
1:D:806:LYS:HA	1:D:806:LYS:HD3	1.64	0.48
1:D:1206:ARG:O	1:D:1210:ALA:HB3	2.13	0.48
1:D:2435:LEU:HB3	1:D:2438:TYR:H	1.78	0.48
1:A:2275:GLY:CA	1:D:2281:SER:HB3	2.43	0.48
1:A:2289:LYS:CA	1:A:2292:LEU:HD12	2.42	0.48
1:A:2468:PHE:HE1	1:A:2510:PRO:CG	2.26	0.48
1:B:578:LYS:HE3	1:B:578:LYS:HB2	1.58	0.48
1:B:2046:PHE:O	1:B:2048:ILE:HD13	2.12	0.48
1:D:1160:VAL:HG12	1:D:1550:LEU:CD2	2.41	0.48
1:D:1208:THR:HB	1:D:1311:ARG:HE	1.78	0.48
1:D:2175:MET:SD	2:E:239:GLU:HB2	2.53	0.48
1:D:2252:LEU:H	1:D:2252:LEU:HG	1.39	0.48
1:A:950:GLU:HB3	1:A:954:ARG:HH21	1.78	0.48
1:A:1313:ASP:HA	1:A:1547:ARG:HH21	1.78	0.48
1:B:2095:THR:HA	1:B:2147:PHE:CD1	2.48	0.48
1:D:1208:THR:HA	1:D:1302:PHE:HD1	1.75	0.48
1:A:785:ARG:HG2	1:A:790:LEU:HG	1.95	0.48
1:A:2341:LEU:HD13	1:A:2389:LEU:HB3	1.94	0.48
1:B:1208:THR:HB	1:B:1311:ARG:HE	1.78	0.48
1:B:2120:ALA:HB3	1:B:2137:MET:SD	2.53	0.48
1:B:2467:MET:HB3	1:D:2507:TYR:O	2.14	0.48
1:D:2120:ALA:HB3	1:D:2137:MET:SD	2.53	0.48
1:D:2282:PRO:HB2	1:D:2283:PRO:HD3	1.95	0.48
1:D:2293:TYR:HB2	1:D:2294:ASN:OD1	2.13	0.48
1:A:2265:ILE:HD13	1:A:2423:PHE:CB	2.44	0.48
1:A:2275:GLY:HA2	1:D:2281:SER:HB3	1.96	0.48
1:A:2165:GLN:O	1:A:2166:LYS:C	2.56	0.48
1:B:984:LYS:HD2	1:B:984:LYS:HA	1.47	0.48
1:B:1562:ARG:HD2	1:B:1566:ASP:HB2	1.94	0.48
1:B:2467:MET:HB2	1:B:2468:PHE:CZ	2.49	0.48
1:D:978:ASP:HA	1:D:1155:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1313:ASP:HA	1:D:1547:ARG:HH21	1.78	0.48
1:D:1554:LEU:HB3	1:D:1555:LEU:H	1.51	0.48
1:D:2274:SER:CB	1:D:2404:TRP:H	2.25	0.48
1:B:827:ARG:H	1:B:827:ARG:HG2	1.45	0.48
1:B:1313:ASP:HA	1:B:1547:ARG:HH21	1.78	0.48
1:D:682:SER:O	1:D:683:SER:C	2.57	0.48
1:D:785:ARG:HG2	1:D:790:LEU:HG	1.95	0.48
1:D:1360:LYS:C	1:D:1362:GLU:N	2.69	0.48
1:A:2293:TYR:HB2	1:A:2294:ASN:OD1	2.13	0.48
1:A:2435:LEU:HD13	1:A:2435:LEU:HA	1.76	0.48
1:A:2435:LEU:HB3	1:A:2438:TYR:H	1.78	0.48
1:B:688:GLY:O	1:B:692:LEU:HG	2.14	0.48
1:B:2045:MET:O	1:B:2048:ILE:CD1	2.41	0.48
1:B:2175:MET:SD	2:F:239:GLU:HB2	2.53	0.48
1:B:2435:LEU:HB3	1:B:2438:TYR:H	1.78	0.48
1:D:688:GLY:O	1:D:692:LEU:HG	2.14	0.48
1:D:2171:VAL:HG11	2:E:239:GLU:OE2	2.12	0.48
1:D:2185:ALA:HA	1:D:2189:PHE:HB2	1.96	0.48
1:B:978:ASP:HA	1:B:1155:LEU:HG	1.96	0.47
1:B:1358:ARG:HE	1:B:1358:ARG:HB2	1.46	0.47
1:A:682:SER:O	1:A:683:SER:C	2.57	0.47
1:A:984:LYS:HD2	1:A:984:LYS:HA	1.47	0.47
1:A:2284:SER:HB3	1:B:2273:SER:OG	2.14	0.47
1:B:847:LYS:HA	1:B:847:LYS:HD3	1.56	0.47
1:B:1554:LEU:HB3	1:B:1555:LEU:H	1.51	0.47
1:B:2185:ALA:HA	1:B:2189:PHE:HB2	1.96	0.47
1:B:2238:GLN:H	1:B:2238:GLN:HG3	1.38	0.47
1:D:1171:LEU:HD13	1:D:1171:LEU:HA	1.55	0.47
1:A:1316:ALA:HA	1:A:1319:LEU:HB2	1.97	0.47
1:A:2302:ARG:HB3	1:A:2302:ARG:HE	1.42	0.47
1:A:2323:LYS:H	1:A:2323:LYS:HG2	1.40	0.47
1:B:1171:LEU:HD13	1:B:1171:LEU:HA	1.56	0.47
1:B:1562:ARG:NE	1:B:1566:ASP:CB	2.77	0.47
2:C:233:CYS:O	2:C:236:ILE:HB	2.14	0.47
1:A:587:MET:HE2	1:A:587:MET:HA	1.91	0.47
1:A:635:ALA:C	1:A:639:LEU:HD12	2.33	0.47
1:A:1028:ARG:HB3	1:A:1034:ILE:HG12	1.95	0.47
1:B:1699:HIS:CG	1:B:1707:SER:HB2	2.49	0.47
1:B:2341:LEU:HG	1:B:2348:GLN:HB2	1.97	0.47
1:D:635:ALA:C	1:D:639:LEU:HD12	2.33	0.47
1:D:2049:LEU:H	1:D:2049:LEU:CD2	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2417:LEU:HD23	1:A:2417:LEU:HA	1.79	0.47
2:C:229:GLU:H	2:C:229:GLU:HG3	1.42	0.47
1:D:1214:LEU:HD22	1:D:1214:LEU:HA	1.74	0.47
1:D:1797:ARG:HE	1:D:1797:ARG:HB3	1.40	0.47
1:D:2294:ASN:OD1	1:D:2294:ASN:N	2.47	0.47
1:D:2302:ARG:HE	1:D:2323:LYS:HZ2	1.63	0.47
1:A:688:GLY:O	1:A:692:LEU:HG	2.14	0.47
1:A:827:ARG:H	1:A:827:ARG:HG2	1.45	0.47
1:A:2138:CYS:HG	1:D:2466:ILE:HG21	1.78	0.47
1:A:2153:ARG:HA	1:A:2153:ARG:HD3	1.61	0.47
1:A:2341:LEU:HG	1:A:2348:GLN:HB2	1.97	0.47
1:B:1160:VAL:HG12	1:B:1550:LEU:CD2	2.41	0.47
1:B:1316:ALA:HA	1:B:1319:LEU:HB2	1.97	0.47
1:B:2153:ARG:HA	1:B:2153:ARG:HD3	1.61	0.47
1:B:2293:TYR:CB	1:B:2294:ASN:OD1	2.63	0.47
1:A:602:ILE:H	1:A:602:ILE:HG13	1.47	0.47
1:A:1203:LEU:O	1:A:1207:ASP:HB2	2.15	0.47
1:A:1719:MET:HE2	1:A:1719:MET:HB2	1.64	0.47
1:B:1360:LYS:HB2	1:B:1360:LYS:HE2	1.52	0.47
1:B:1722:ILE:H	1:B:1722:ILE:HG13	1.24	0.47
1:B:2225:MET:HB2	1:B:2406:ILE:HD11	1.96	0.47
1:B:2294:ASN:OD1	1:B:2294:ASN:N	2.47	0.47
1:D:587:MET:HA	1:D:587:MET:CE	2.45	0.47
1:D:950:GLU:HB3	1:D:954:ARG:HH21	1.78	0.47
1:D:1203:LEU:O	1:D:1207:ASP:HB2	2.15	0.47
1:D:1699:HIS:CG	1:D:1707:SER:HB2	2.49	0.47
1:D:1722:ILE:H	1:D:1722:ILE:HG13	1.23	0.47
1:D:2225:MET:HB2	1:D:2406:ILE:HD11	1.96	0.47
1:D:2289:LYS:CA	1:D:2292:LEU:HD12	2.42	0.47
1:D:2307:PHE:HE2	1:D:2360:ILE:HG21	1.80	0.47
1:A:2222:LEU:HD13	1:A:2222:LEU:HA	1.77	0.47
1:B:798:LEU:HD13	1:B:798:LEU:HA	1.68	0.47
1:B:1014:LEU:HD12	1:B:1014:LEU:HA	1.73	0.47
1:B:2142:ILE:HD13	1:B:2503:LEU:HD22	1.97	0.47
1:B:2354:ASN:HA	1:B:2384:GLY:HA2	1.97	0.47
1:D:1160:VAL:HA	1:D:1550:LEU:HD23	1.91	0.47
1:D:2010:ILE:O	1:D:2011:GLN:C	2.57	0.47
1:D:2513:MET:HE2	1:D:2513:MET:HB2	1.67	0.47
1:A:978:ASP:HA	1:A:1155:LEU:HG	1.96	0.47
1:A:2294:ASN:OD1	1:A:2294:ASN:N	2.47	0.47
1:B:785:ARG:HG2	1:B:790:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ARG:HE	1:B:786:ARG:HB3	1.55	0.47
1:B:1953:LYS:HB2	1:B:1954:TYR:H	1.47	0.47
1:B:2282:PRO:O	1:B:2286:ALA:HB3	2.15	0.47
1:B:2377:ASN:CB	1:B:2380:ALA:HB3	2.45	0.47
1:D:2065:LEU:HD13	1:D:2065:LEU:HA	1.71	0.47
1:D:2109:PHE:CE1	1:D:2116:VAL:HG13	2.49	0.47
1:A:2374:LEU:HD12	1:A:2374:LEU:HA	1.78	0.47
1:B:572:VAL:HA	1:B:575:VAL:HB	1.97	0.47
1:B:2265:ILE:HD13	1:B:2423:PHE:CB	2.44	0.47
1:B:2292:LEU:HD22	1:B:2338:LEU:HB3	1.95	0.47
1:A:2010:ILE:HG22	1:A:2011:GLN:H	1.77	0.46
1:A:2293:TYR:CB	1:A:2294:ASN:OD1	2.63	0.46
1:A:2302:ARG:HE	1:A:2323:LYS:HZ2	1.63	0.46
1:B:680:LEU:H	1:B:680:LEU:HG	1.50	0.46
1:D:807:GLU:H	1:D:807:GLU:HG2	1.45	0.46
1:D:2147:PHE:CE1	1:D:2151:CYS:SG	3.08	0.46
1:A:1562:ARG:NE	1:A:1566:ASP:CB	2.77	0.46
1:A:2222:LEU:HB3	1:A:2223:PHE:H	1.50	0.46
1:B:587:MET:HA	1:B:587:MET:CE	2.45	0.46
1:B:1365:ARG:HA	1:B:1368:ARG:HE	1.80	0.46
1:D:2045:MET:O	1:D:2048:ILE:CD1	2.41	0.46
1:D:2401:LEU:HD22	1:D:2403:TRP:CH2	2.51	0.46
1:A:1351:LYS:HD2	1:A:1351:LYS:HA	1.28	0.46
1:A:2147:PHE:CE1	1:A:2151:CYS:SG	3.08	0.46
1:A:2168:LYS:HB3	1:A:2171:VAL:HG23	1.97	0.46
1:B:1203:LEU:O	1:B:1207:ASP:HB2	2.15	0.46
1:D:786:ARG:HE	1:D:786:ARG:HB3	1.55	0.46
1:D:2293:TYR:CB	1:D:2294:ASN:OD1	2.63	0.46
1:D:2377:ASN:CB	1:D:2380:ALA:HB3	2.45	0.46
1:A:1365:ARG:HA	1:A:1368:ARG:HE	1.80	0.46
1:A:1744:LYS:NZ	1:A:1744:LYS:CB	2.78	0.46
1:A:1744:LYS:HD2	1:A:1782:TYR:HB2	1.98	0.46
1:A:2468:PHE:HE1	1:A:2510:PRO:HG3	1.79	0.46
1:B:1157:MET:HA	1:B:1160:VAL:HG22	1.98	0.46
1:B:2010:ILE:O	1:B:2011:GLN:C	2.57	0.46
1:B:2094:LEU:CB	1:B:2106:PHE:CB	2.89	0.46
1:B:2147:PHE:CE1	1:B:2151:CYS:SG	3.08	0.46
1:B:2208:ILE:HG23	1:B:2229:GLN:HG2	1.97	0.46
1:D:1157:MET:HA	1:D:1160:VAL:HG22	1.98	0.46
1:D:1365:ARG:HA	1:D:1368:ARG:HE	1.81	0.46
1:D:1744:LYS:NZ	1:D:1744:LYS:CB	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2308:GLN:HG3	1:D:2319:TYR:HD2	1.81	0.46
1:A:1219:ILE:HG13	1:A:1295:LEU:HB3	1.98	0.46
1:A:2185:ALA:HA	1:A:2189:PHE:HB2	1.96	0.46
1:A:2252:LEU:H	1:A:2252:LEU:HG	1.39	0.46
1:A:2256:PHE:CD2	1:A:2371:VAL:HG13	2.51	0.46
1:A:2401:LEU:HD22	1:A:2403:TRP:CH2	2.51	0.46
1:B:2465:SER:C	1:B:2467:MET:N	2.72	0.46
1:D:849:LEU:H	1:D:849:LEU:HG	1.58	0.46
1:D:2341:LEU:HG	1:D:2348:GLN:HB2	1.97	0.46
1:A:1408:ASP:N	1:A:1412:VAL:HB	2.29	0.46
1:A:2157:LYS:HB2	1:A:2157:LYS:HE2	1.56	0.46
1:A:2377:ASN:CB	1:A:2380:ALA:HB3	2.45	0.46
1:B:2307:PHE:HE2	1:B:2360:ILE:HG21	1.80	0.46
1:D:1728:ARG:H	1:D:1728:ARG:HG3	1.37	0.46
1:D:2142:ILE:HD13	1:D:2503:LEU:HD22	1.97	0.46
1:D:2313:LYS:H	1:D:2313:LYS:HG3	1.51	0.46
1:A:1157:MET:HA	1:A:1160:VAL:HG22	1.98	0.46
1:A:2100:HIS:CE1	2:C:238:MET:CB	2.99	0.46
1:A:2167:LYS:O	1:A:2168:LYS:HB2	2.15	0.46
1:A:2225:MET:HB2	1:A:2406:ILE:HD11	1.96	0.46
1:B:2103:LEU:HG	1:B:2151:CYS:CB	2.46	0.46
1:D:827:ARG:H	1:D:827:ARG:HG2	1.45	0.46
1:D:984:LYS:HD2	1:D:984:LYS:HA	1.47	0.46
1:D:1316:ALA:HA	1:D:1319:LEU:HB2	1.97	0.46
1:D:1562:ARG:NE	1:D:1566:ASP:CB	2.77	0.46
1:D:2103:LEU:HG	1:D:2151:CYS:CB	2.46	0.46
1:A:806:LYS:HB3	1:A:807:GLU:H	1.55	0.46
1:A:1953:LYS:HB2	1:A:1954:TYR:H	1.47	0.46
1:B:800:THR:HG23	1:B:815:LEU:HD21	1.98	0.46
1:B:2408:LEU:H	1:B:2411:CYS:HB2	1.81	0.46
1:D:1744:LYS:HD2	1:D:1782:TYR:HB2	1.97	0.46
1:D:2354:ASN:HA	1:D:2384:GLY:HA2	1.97	0.46
1:B:682:SER:O	1:B:683:SER:C	2.57	0.46
1:B:1744:LYS:HD2	1:B:1782:TYR:HB2	1.97	0.46
1:B:1949:ILE:HD12	1:B:1949:ILE:HA	1.80	0.46
1:D:572:VAL:HA	1:D:575:VAL:HB	1.97	0.46
1:A:572:VAL:HA	1:A:575:VAL:HB	1.97	0.46
1:A:798:LEU:HD13	1:A:798:LEU:HA	1.68	0.46
1:A:1555:LEU:HB2	1:A:1556:GLN:H	1.45	0.46
1:A:2307:PHE:HE2	1:A:2360:ILE:HG21	1.80	0.46
1:A:596:ARG:HD2	1:A:596:ARG:HA	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:LEU:HD22	1:A:787:LEU:HA	1.77	0.45
1:A:2208:ILE:HG23	1:A:2229:GLN:HG2	1.97	0.45
1:B:2401:LEU:HD22	1:B:2403:TRP:CH2	2.51	0.45
1:B:2513:MET:HE2	1:B:2513:MET:HB2	1.67	0.45
1:D:2208:ILE:HG23	1:D:2229:GLN:HG2	1.97	0.45
1:D:2256:PHE:CD2	1:D:2371:VAL:HG13	2.51	0.45
1:A:1568:LEU:C	1:A:1653:ARG:CB	2.88	0.45
1:A:2308:GLN:HG3	1:A:2319:TYR:HD2	1.81	0.45
1:B:1744:LYS:NZ	1:B:1744:LYS:CB	2.78	0.45
1:B:2358:LYS:HZ2	1:B:2383:LEU:HD22	1.76	0.45
1:D:1104:LEU:HD13	1:D:1104:LEU:HA	1.73	0.45
1:A:1014:LEU:HD12	1:A:1014:LEU:HA	1.73	0.45
1:A:2354:ASN:HA	1:A:2384:GLY:HA2	1.97	0.45
1:A:2468:PHE:CE2	1:D:2467:MET:SD	3.10	0.45
1:B:1719:MET:HE2	1:B:1719:MET:HB2	1.64	0.45
1:B:2256:PHE:CD2	1:B:2371:VAL:HG13	2.51	0.45
1:B:2308:GLN:HG3	1:B:2319:TYR:HD2	1.81	0.45
1:D:2189:PHE:HD1	1:D:2189:PHE:HA	1.63	0.45
1:D:2426:LYS:HB3	1:D:2426:LYS:HE2	1.61	0.45
1:A:609:LEU:HD12	1:A:609:LEU:HA	1.80	0.45
1:A:2142:ILE:HD13	1:A:2503:LEU:HD22	1.97	0.45
1:A:2408:LEU:H	1:A:2411:CYS:HB2	1.81	0.45
1:B:684:ILE:O	1:B:685:LEU:C	2.60	0.45
1:B:1515:TRP:HE3	1:B:1516:MET:CE	2.08	0.45
1:D:1205:GLN:H	1:D:1205:GLN:HG3	1.69	0.45
1:D:2302:ARG:H	1:D:2302:ARG:HG2	1.35	0.45
1:A:2010:ILE:HD12	1:A:2010:ILE:HA	1.63	0.45
1:A:2187:ILE:H	1:A:2187:ILE:HG12	1.60	0.45
1:A:2265:ILE:HD11	1:A:2423:PHE:CE2	2.51	0.45
1:B:708:LEU:HD23	1:B:708:LEU:HA	1.84	0.45
1:B:1037:LEU:HD23	1:B:1037:LEU:HA	1.73	0.45
1:B:1562:ARG:HD2	1:B:1562:ARG:HA	1.36	0.45
1:D:622:TRP:HB2	1:D:711:MET:HE2	1.99	0.45
1:D:853:LYS:CE	1:D:853:LYS:H	2.29	0.45
1:D:1562:ARG:HD2	1:D:1562:ARG:HA	1.36	0.45
1:D:1649:LEU:HB2	1:D:1650:LEU:H	1.47	0.45
1:D:2248:ASP:HA	1:D:2254:MET:HB2	1.99	0.45
1:D:2408:LEU:H	1:D:2411:CYS:HB2	1.81	0.45
1:A:853:LYS:H	1:A:853:LYS:CE	2.29	0.45
1:A:1037:LEU:HD23	1:A:1037:LEU:HA	1.73	0.45
1:B:785:ARG:HB3	1:B:945:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1187:LEU:HD23	1:B:1187:LEU:HA	1.87	0.45
1:B:1797:ARG:HE	1:B:1797:ARG:HB3	1.40	0.45
1:B:2094:LEU:HB3	1:B:2106:PHE:HB2	1.98	0.45
1:D:1219:ILE:HG13	1:D:1295:LEU:HB3	1.98	0.45
1:D:2203:VAL:HB	1:D:2430:PRO:HG2	1.99	0.45
1:A:1568:LEU:HD13	1:A:1659:LEU:CD2	2.47	0.45
1:A:2094:LEU:HB3	1:A:2106:PHE:HB2	1.98	0.45
1:A:2103:LEU:HG	1:A:2151:CYS:CB	2.46	0.45
1:A:2174:GLY:HA3	2:C:236:ILE:CG2	2.41	0.45
1:A:847:LYS:CG	1:A:928:TYR:CE2	2.95	0.45
1:A:979:LEU:HD13	1:A:979:LEU:HA	1.80	0.45
1:A:1940:ARG:N	1:A:1941:PRO:HD3	2.32	0.45
1:A:2383:LEU:HD12	1:A:2383:LEU:HA	1.84	0.45
1:B:1940:ARG:N	1:B:1941:PRO:HD3	2.32	0.45
1:B:2465:SER:O	1:B:2466:ILE:C	2.58	0.45
1:A:683:SER:O	1:A:684:ILE:C	2.61	0.45
1:A:847:LYS:HA	1:A:847:LYS:HD3	1.56	0.45
1:A:1100:ILE:H	1:A:1100:ILE:HG12	1.55	0.45
1:A:1160:VAL:HA	1:A:1550:LEU:HD23	1.91	0.45
1:A:1214:LEU:HD22	1:A:1214:LEU:HA	1.74	0.45
1:A:1552:GLN:OE1	1:A:1552:GLN:N	2.45	0.45
1:A:2254:MET:HE3	1:A:2254:MET:HB3	1.58	0.45
1:B:1219:ILE:HG13	1:B:1295:LEU:HB3	1.98	0.45
1:B:1549:LEU:HD13	1:B:1549:LEU:HA	1.84	0.45
1:B:2203:VAL:HB	1:B:2430:PRO:HG2	1.99	0.45
1:D:596:ARG:HA	1:D:596:ARG:HD2	1.63	0.45
1:D:623:ARG:HE	1:D:623:ARG:HB2	1.48	0.45
1:A:2030:LYS:HD2	1:A:2030:LYS:HA	1.58	0.44
1:B:853:LYS:CE	1:B:853:LYS:H	2.29	0.44
1:B:1214:LEU:HD22	1:B:1214:LEU:HA	1.74	0.44
1:A:2341:LEU:HB3	1:A:2389:LEU:HD23	1.99	0.44
1:A:2467:MET:C	1:A:2468:PHE:CG	2.95	0.44
1:B:1568:LEU:HD13	1:B:1659:LEU:CD2	2.47	0.44
1:B:2011:GLN:HE21	1:B:2011:GLN:HB2	1.44	0.44
1:B:2092:ASN:CG	1:B:2106:PHE:HE1	2.25	0.44
1:D:847:LYS:CG	1:D:928:TYR:CE2	2.95	0.44
1:D:1940:ARG:N	1:D:1941:PRO:HD3	2.32	0.44
1:D:2222:LEU:HB3	1:D:2223:PHE:H	1.50	0.44
1:A:785:ARG:HB3	1:A:945:VAL:HG21	1.99	0.44
1:A:2273:SER:HB3	1:D:2283:PRO:HB2	1.98	0.44
1:A:2282:PRO:HB2	1:A:2283:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1656:ILE:HB	1:B:1657:PRO:HD3	1.99	0.44
1:B:2323:LYS:H	1:B:2323:LYS:HG2	1.40	0.44
1:B:2418:LEU:HA	1:B:2419:PRO:HD3	1.88	0.44
1:B:2426:LYS:HB3	1:B:2426:LYS:HE2	1.61	0.44
1:D:1218:LEU:HD22	1:D:1218:LEU:HA	1.68	0.44
1:A:800:THR:HG23	1:A:815:LEU:HD21	1.98	0.44
1:A:1099:LEU:HD12	1:A:1099:LEU:HA	1.84	0.44
1:A:1656:ILE:HB	1:A:1657:PRO:HD3	1.99	0.44
1:B:678:SER:O	1:B:682:SER:N	2.50	0.44
1:B:683:SER:O	1:B:684:ILE:C	2.61	0.44
1:B:1555:LEU:HB2	1:B:1556:GLN:H	1.45	0.44
1:D:1553:GLU:HB2	1:D:1554:LEU:H	1.58	0.44
1:D:1744:LYS:O	1:D:1747:PHE:CD1	2.71	0.44
1:A:684:ILE:O	1:A:685:LEU:C	2.60	0.44
1:A:2203:VAL:HB	1:A:2430:PRO:HG2	1.99	0.44
1:B:2222:LEU:HB3	1:B:2223:PHE:H	1.50	0.44
1:B:2280:ILE:C	1:D:2275:GLY:HA3	2.43	0.44
1:B:2302:ARG:HE	1:B:2323:LYS:HZ2	1.66	0.44
1:D:573:LYS:HA	1:D:573:LYS:HD3	1.51	0.44
1:D:587:MET:CA	1:D:587:MET:CE	2.89	0.44
1:D:800:THR:HG23	1:D:815:LEU:HD21	1.98	0.44
1:A:1220:LEU:HD13	1:A:1220:LEU:HA	1.76	0.44
1:A:1409:HIS:O	1:A:1411:THR:N	2.51	0.44
1:A:1797:ARG:HE	1:A:1797:ARG:HB3	1.40	0.44
1:A:2248:ASP:HA	1:A:2254:MET:HB2	1.99	0.44
1:A:2274:SER:CB	1:A:2404:TRP:H	2.30	0.44
1:A:2289:LYS:CA	1:A:2292:LEU:CD1	2.90	0.44
1:B:1744:LYS:O	1:B:1747:PHE:CD1	2.71	0.44
1:B:2341:LEU:HB3	1:B:2389:LEU:HD23	1.99	0.44
1:D:785:ARG:HB3	1:D:945:VAL:HG21	1.99	0.44
1:D:2265:ILE:HD13	1:D:2423:PHE:CB	2.44	0.44
1:D:2502:LYS:HE3	1:D:2502:LYS:HB3	1.39	0.44
1:A:1744:LYS:O	1:A:1747:PHE:CD1	2.71	0.44
1:B:596:ARG:HA	1:B:596:ARG:HD2	1.63	0.44
1:B:1650:LEU:HD11	1:B:1654:LEU:HD12	1.99	0.44
1:B:2157:LYS:HB2	1:B:2157:LYS:HE2	1.56	0.44
1:D:678:SER:O	1:D:682:SER:N	2.50	0.44
1:D:684:ILE:O	1:D:685:LEU:C	2.60	0.44
1:A:1160:VAL:HG12	1:A:1550:LEU:CD2	2.41	0.44
1:A:1562:ARG:HD2	1:A:1562:ARG:HA	1.36	0.44
1:A:2213:THR:CG2	1:A:2224:THR:HG23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:853:LYS:N	1:B:853:LYS:CE	2.81	0.44
1:D:847:LYS:HA	1:D:847:LYS:HD3	1.56	0.44
1:D:1568:LEU:HD13	1:D:1659:LEU:CD2	2.47	0.44
1:D:1744:LYS:HZ3	1:D:1744:LYS:CB	2.31	0.44
1:D:1942:LEU:HD13	1:D:1942:LEU:HA	1.90	0.44
1:A:1112:GLN:O	1:A:1116:PHE:HB2	2.18	0.44
1:A:1699:HIS:CG	1:A:1707:SER:HB2	2.49	0.44
1:A:2112:VAL:HB	1:A:2115:LEU:HB2	1.99	0.44
1:A:2309:ARG:H	1:A:2318:GLU:HB2	1.83	0.44
1:B:1552:GLN:OE1	1:B:1552:GLN:N	2.45	0.44
1:B:2252:LEU:H	1:B:2252:LEU:HG	1.39	0.44
1:B:2280:ILE:HG22	1:B:2284:SER:HB2	1.99	0.44
1:D:609:LEU:HD12	1:D:609:LEU:HA	1.80	0.44
1:D:635:ALA:O	1:D:639:LEU:CD1	2.45	0.44
1:D:1568:LEU:C	1:D:1653:ARG:CB	2.88	0.44
1:A:622:TRP:HB2	1:A:711:MET:HE2	1.99	0.43
1:A:849:LEU:H	1:A:849:LEU:HG	1.58	0.43
1:B:768:GLU:HB2	1:B:769:LEU:H	1.64	0.43
1:B:1649:LEU:HB2	1:B:1650:LEU:H	1.56	0.43
1:B:2291:GLU:HB3	1:B:2335:ARG:NH2	2.33	0.43
1:B:2374:LEU:HD12	1:B:2374:LEU:HA	1.78	0.43
1:D:683:SER:O	1:D:684:ILE:C	2.61	0.43
1:D:2383:LEU:HD12	1:D:2383:LEU:HA	1.84	0.43
1:A:853:LYS:N	1:A:853:LYS:CE	2.81	0.43
1:A:1744:LYS:HZ3	1:A:1744:LYS:CB	2.31	0.43
1:A:2223:PHE:CE1	1:A:2406:ILE:HG12	2.53	0.43
1:B:806:LYS:HA	1:B:806:LYS:HD3	1.64	0.43
1:B:1559:GLU:H	1:B:1559:GLU:HG3	1.51	0.43
1:D:814:LEU:HD23	1:D:814:LEU:HA	1.68	0.43
1:A:2502:LYS:HB3	1:A:2502:LYS:HE3	1.39	0.43
1:B:807:GLU:H	1:B:807:GLU:HG2	1.44	0.43
1:B:823:LEU:HD12	1:B:823:LEU:HA	1.91	0.43
1:B:1975:ILE:HD13	1:B:1975:ILE:HA	1.91	0.43
1:B:2098:TYR:HA	1:B:2151:CYS:SG	2.58	0.43
1:B:2248:ASP:HA	1:B:2254:MET:HB2	1.99	0.43
1:D:587:MET:N	1:D:587:MET:CE	2.66	0.43
1:D:785:ARG:HA	1:D:790:LEU:CB	2.46	0.43
1:D:1112:GLN:O	1:D:1116:PHE:HB2	2.18	0.43
1:D:2120:ALA:HB1	1:D:2137:MET:SD	2.58	0.43
1:D:2284:SER:O	1:D:2288:MET:N	2.50	0.43
1:A:1360:LYS:O	1:A:1362:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1555:LEU:HB2	1:D:1556:GLN:H	1.45	0.43
1:D:1656:ILE:HB	1:D:1657:PRO:HD3	1.99	0.43
1:D:2030:LYS:HD2	1:D:2030:LYS:HA	1.58	0.43
1:A:678:SER:O	1:A:682:SER:N	2.50	0.43
1:A:823:LEU:HD12	1:A:823:LEU:HA	1.91	0.43
1:A:1649:LEU:HB2	1:A:1650:LEU:H	1.47	0.43
1:B:814:LEU:HA	1:B:814:LEU:HD23	1.68	0.43
1:B:849:LEU:H	1:B:849:LEU:HG	1.58	0.43
1:B:2384:GLY:O	1:B:2408:LEU:HG	2.19	0.43
1:D:818:LEU:HD23	1:D:818:LEU:HA	1.90	0.43
1:D:1099:LEU:HD12	1:D:1099:LEU:HA	1.84	0.43
1:D:1197:LEU:HD12	1:D:1197:LEU:HA	1.91	0.43
1:D:2098:TYR:HA	1:D:2151:CYS:SG	2.58	0.43
1:A:1218:LEU:HD22	1:A:1218:LEU:HA	1.68	0.43
1:A:2098:TYR:HA	1:A:2151:CYS:SG	2.58	0.43
1:B:636:TYR:HA	1:B:639:LEU:HD12	2.01	0.43
1:D:925:ASN:HD22	1:D:925:ASN:HA	1.65	0.43
1:D:2157:LYS:HB2	1:D:2157:LYS:HE2	1.56	0.43
1:D:2223:PHE:CE1	1:D:2406:ILE:HG12	2.53	0.43
1:D:2309:ARG:H	1:D:2318:GLU:HB2	1.83	0.43
1:A:1043:LEU:HD23	1:A:1043:LEU:HA	1.77	0.43
1:A:1942:LEU:HD13	1:A:1942:LEU:HA	1.90	0.43
1:A:2467:MET:SD	1:B:2468:PHE:CE2	3.12	0.43
1:B:1043:LEU:HD23	1:B:1043:LEU:HA	1.77	0.43
1:B:1112:GLN:O	1:B:1116:PHE:HB2	2.18	0.43
1:B:2120:ALA:HB1	1:B:2137:MET:SD	2.59	0.43
1:B:2223:PHE:CE1	1:B:2406:ILE:HG12	2.53	0.43
1:B:2265:ILE:HD11	1:B:2423:PHE:CE2	2.51	0.43
1:D:798:LEU:HD13	1:D:798:LEU:HA	1.68	0.43
1:D:1360:LYS:HB2	1:D:1360:LYS:HE2	1.52	0.43
1:D:2384:GLY:O	1:D:2408:LEU:HG	2.19	0.43
1:D:2435:LEU:HD13	1:D:2435:LEU:HA	1.76	0.43
2:E:229:GLU:H	2:E:229:GLU:HG3	1.42	0.43
1:A:627:LYS:HA	1:A:627:LYS:HD2	1.88	0.43
1:A:1408:ASP:O	1:A:1409:HIS:C	2.62	0.43
1:A:2172:LYS:NZ	1:B:2127:THR:O	2.50	0.43
1:A:2238:GLN:H	1:A:2238:GLN:HG3	1.38	0.43
1:B:622:TRP:HB2	1:B:711:MET:HE2	1.99	0.43
1:B:1555:LEU:H	1:B:1555:LEU:HG	1.47	0.43
1:B:2222:LEU:HD13	1:B:2222:LEU:HA	1.77	0.43
1:B:2282:PRO:HD2	1:D:2403:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2502:LYS:HE3	1:B:2502:LYS:HB3	1.39	0.43
1:D:602:ILE:H	1:D:602:ILE:HG13	1.47	0.43
1:D:2341:LEU:HB3	1:D:2389:LEU:HD23	2.00	0.43
1:A:768:GLU:HB2	1:A:769:LEU:H	1.64	0.43
1:B:1733:ALA:HB3	1:B:1793:LEU:CD2	2.48	0.43
1:B:2302:ARG:HB3	1:B:2302:ARG:HE	1.42	0.43
1:D:1733:ALA:HB3	1:D:1793:LEU:CD2	2.48	0.43
1:A:1197:LEU:HD12	1:A:1197:LEU:HA	1.91	0.43
1:A:1319:LEU:HD12	1:A:1319:LEU:HA	1.85	0.43
1:A:1733:ALA:HB3	1:A:1793:LEU:CD2	2.48	0.43
1:A:2121:VAL:HA	1:A:2133:LEU:HD21	2.01	0.43
1:B:951:HIS:HA	1:B:954:ARG:HB2	2.01	0.43
1:B:1650:LEU:HD22	1:B:1650:LEU:HA	1.89	0.43
1:D:610:LEU:HD12	1:D:610:LEU:HA	1.77	0.43
1:A:1649:LEU:H	1:A:1649:LEU:HG	1.75	0.42
1:B:573:LYS:HA	1:B:573:LYS:HD3	1.52	0.42
1:B:1568:LEU:C	1:B:1653:ARG:CB	2.88	0.42
1:D:2010:ILE:HA	1:D:2010:ILE:HD12	1.63	0.42
1:D:2170:ILE:H	1:D:2170:ILE:HG12	1.32	0.42
2:E:243:ILE:HA	2:E:247:SER:CA	2.38	0.42
1:A:1345:LYS:HB2	1:A:1345:LYS:HE2	1.81	0.42
1:A:2019:ARG:HE	1:A:2023:LEU:CD2	2.32	0.42
1:A:2291:GLU:HB3	1:A:2335:ARG:NH2	2.33	0.42
1:B:597:LEU:HD23	1:B:848:MET:O	2.19	0.42
1:B:806:LYS:HB3	1:B:807:GLU:H	1.55	0.42
1:B:2019:ARG:HE	1:B:2023:LEU:HD22	1.84	0.42
1:B:2309:ARG:H	1:B:2318:GLU:HB2	1.83	0.42
1:D:787:LEU:HD22	1:D:787:LEU:HA	1.77	0.42
1:D:951:HIS:HA	1:D:954:ARG:HB2	2.01	0.42
1:D:2153:ARG:HA	1:D:2153:ARG:HD3	1.61	0.42
1:D:2291:GLU:HB3	1:D:2335:ARG:NH2	2.33	0.42
1:B:1360:LYS:O	1:B:1362:GLU:N	2.52	0.42
1:B:1363:LYS:HB3	1:B:1363:LYS:HE3	1.28	0.42
1:B:2080:GLN:NE2	1:B:2080:GLN:CA	2.65	0.42
1:D:1186:GLY:HA3	1:D:1745:TYR:OH	2.20	0.42
1:D:2019:ARG:HE	1:D:2023:LEU:CD2	2.32	0.42
1:A:807:GLU:H	1:A:807:GLU:HG2	1.44	0.42
1:A:951:HIS:HA	1:A:954:ARG:HB2	2.01	0.42
1:B:2172:LYS:NZ	1:D:2127:THR:O	2.50	0.42
1:D:597:LEU:HD23	1:D:848:MET:O	2.19	0.42
1:D:614:LEU:HD23	1:D:614:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1710:LEU:HD23	1:D:1710:LEU:HA	1.76	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.85	0.42
1:A:1186:GLY:HA3	1:A:1745:TYR:OH	2.20	0.42
1:A:2503:LEU:HD23	1:A:2503:LEU:HA	1.82	0.42
1:B:1710:LEU:HD23	1:B:1710:LEU:HA	1.76	0.42
1:B:2254:MET:HE3	1:B:2254:MET:HB3	1.58	0.42
1:B:2288:MET:O	1:B:2292:LEU:CG	2.64	0.42
1:D:853:LYS:N	1:D:853:LYS:CE	2.81	0.42
1:D:947:ARG:HA	1:D:950:GLU:HB2	2.02	0.42
1:D:2121:VAL:HA	1:D:2133:LEU:HD21	2.01	0.42
1:A:2107:GLN:HE22	2:C:242:GLY:HA2	1.83	0.42
1:A:2121:VAL:HG22	1:A:2133:LEU:HD11	2.02	0.42
1:B:710:ASP:HB2	1:B:712:GLU:OE1	2.20	0.42
1:B:2101:LEU:HD22	1:B:2101:LEU:HA	1.72	0.42
1:D:636:TYR:HA	1:D:639:LEU:HD12	2.01	0.42
1:D:955:GLN:O	1:D:956:HIS:C	2.63	0.42
1:D:2121:VAL:HG22	1:D:2133:LEU:HD11	2.02	0.42
1:D:2341:LEU:HD23	1:D:2341:LEU:HA	1.90	0.42
1:A:947:ARG:HA	1:A:950:GLU:HB2	2.02	0.42
1:A:2170:ILE:HB	2:C:232:ASP:OD2	2.20	0.42
1:A:2281:SER:HB3	1:B:2275:GLY:CA	2.31	0.42
1:A:2418:LEU:HA	1:A:2419:PRO:HD3	1.89	0.42
1:B:1102:ASP:OD1	1:B:1102:ASP:O	2.38	0.42
1:B:1408:ASP:HB2	1:B:1411:THR:HG23	2.01	0.42
1:B:2459:PHE:HE1	2:F:243:ILE:C	2.28	0.42
1:D:710:ASP:HB2	1:D:712:GLU:OE1	2.20	0.42
1:D:1102:ASP:OD1	1:D:1102:ASP:O	2.38	0.42
1:D:1559:GLU:H	1:D:1559:GLU:HG3	1.51	0.42
1:D:1722:ILE:O	1:D:1723:PRO:C	2.63	0.42
1:A:573:LYS:HD3	1:A:573:LYS:HA	1.51	0.42
1:A:1940:ARG:HA	1:A:1943:ARG:NE	2.35	0.42
1:A:2019:ARG:HE	1:A:2023:LEU:HD22	1.84	0.42
1:B:947:ARG:HA	1:B:950:GLU:HB2	2.02	0.42
1:B:1409:HIS:CD2	1:B:2497:GLU:OE1	2.58	0.42
1:D:1161:ALA:CA	1:D:1165:TYR:CE2	2.88	0.42
1:D:1358:ARG:HE	1:D:1358:ARG:HB2	1.46	0.42
1:A:597:LEU:HD23	1:A:848:MET:O	2.19	0.42
1:A:623:ARG:HE	1:A:623:ARG:HB2	1.48	0.42
1:A:710:ASP:HB2	1:A:712:GLU:OE1	2.20	0.42
1:A:1360:LYS:HB2	1:A:1360:LYS:HE2	1.52	0.42
1:A:2065:LEU:HD13	1:A:2065:LEU:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2120:ALA:HB3	1:A:2137:MET:CE	2.50	0.42
1:A:2120:ALA:HB1	1:A:2137:MET:SD	2.59	0.42
1:D:1656:ILE:H	1:D:1656:ILE:HG12	1.51	0.42
1:D:2011:GLN:HE21	1:D:2011:GLN:HB2	1.44	0.42
1:D:2120:ALA:HB3	1:D:2137:MET:CE	2.50	0.42
1:D:2213:THR:CG2	1:D:2224:THR:HG23	2.42	0.42
1:D:2289:LYS:CA	1:D:2292:LEU:CD1	2.90	0.42
2:F:245:PHE:O	2:F:246:PRO:C	2.62	0.42
1:A:587:MET:HA	1:A:587:MET:CE	2.45	0.42
1:A:777:LEU:O	1:A:778:SER:C	2.62	0.42
1:A:853:LYS:HE2	1:A:853:LYS:H	1.85	0.42
1:A:1205:GLN:H	1:A:1205:GLN:HG3	1.69	0.42
1:A:2023:LEU:HD13	1:A:2023:LEU:HA	1.84	0.42
1:B:626:LEU:O	1:B:630:TRP:N	2.53	0.42
1:B:1722:ILE:O	1:B:1723:PRO:C	2.63	0.42
1:B:2120:ALA:HB3	1:B:2137:MET:CE	2.50	0.42
1:D:849:LEU:O	1:D:850:TYR:C	2.63	0.42
1:D:2302:ARG:HB3	1:D:2302:ARG:HE	1.42	0.42
1:A:1658:GLU:HB3	1:A:1661:GLU:HB2	2.02	0.41
1:A:2274:SER:HB3	1:A:2403:TRP:HB3	2.02	0.41
1:A:2513:MET:HE2	1:A:2513:MET:HB2	1.67	0.41
1:B:1186:GLY:HA3	1:B:1745:TYR:OH	2.20	0.41
1:B:2025:LYS:HD2	1:B:2085:TYR:HB3	2.02	0.41
1:B:2121:VAL:HG22	1:B:2133:LEU:HD11	2.02	0.41
1:B:2170:ILE:HB	2:F:232:ASP:OD2	2.20	0.41
1:B:2443:LEU:HD22	1:B:2444:TYR:HA	2.01	0.41
1:D:853:LYS:HE2	1:D:853:LYS:H	1.85	0.41
1:D:1360:LYS:O	1:D:1362:GLU:N	2.52	0.41
1:D:1408:ASP:HB2	1:D:1411:THR:HG23	2.01	0.41
1:D:2019:ARG:HE	1:D:2023:LEU:HD22	1.84	0.41
1:D:2094:LEU:HB2	1:D:2106:PHE:HD1	1.85	0.41
1:D:2305:TRP:HE3	1:D:2307:PHE:HZ	1.68	0.41
2:F:240:CYS:C	2:F:242:GLY:H	2.28	0.41
1:A:1943:ARG:H	1:A:1943:ARG:HG3	1.47	0.41
1:A:2384:GLY:O	1:A:2408:LEU:HG	2.19	0.41
1:A:2472:PRO:HB2	1:A:2473:CYS:H	1.62	0.41
1:B:2115:LEU:HD23	1:B:2115:LEU:HA	1.86	0.41
1:B:2121:VAL:HA	1:B:2133:LEU:HD21	2.01	0.41
1:B:2325:MET:HE3	1:B:2325:MET:HB3	1.65	0.41
1:D:680:LEU:H	1:D:680:LEU:HG	1.49	0.41
1:D:1658:GLU:HB3	1:D:1661:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2123:ASP:HB3	1:D:2136:TRP:CZ2	2.55	0.41
1:D:2170:ILE:HB	2:E:232:ASP:OD2	2.20	0.41
1:A:571:LEU:H	1:A:571:LEU:HG	1.65	0.41
1:A:849:LEU:O	1:A:850:TYR:C	2.63	0.41
1:A:955:GLN:O	1:A:956:HIS:C	2.63	0.41
1:A:1102:ASP:O	1:A:1102:ASP:OD1	2.38	0.41
1:A:2443:LEU:HD22	1:A:2444:TYR:HA	2.01	0.41
1:B:2019:ARG:HE	1:B:2023:LEU:CD2	2.32	0.41
1:B:2503:LEU:HA	1:B:2503:LEU:HD23	1.82	0.41
1:A:636:TYR:HA	1:A:639:LEU:HD12	2.01	0.41
1:A:2127:THR:O	1:D:2172:LYS:NZ	2.50	0.41
1:B:849:LEU:O	1:B:850:TYR:C	2.63	0.41
1:B:955:GLN:O	1:B:956:HIS:C	2.63	0.41
1:B:2407:GLU:HB3	1:B:2415:CYS:SG	2.61	0.41
1:B:581:ILE:H	1:B:581:ILE:HG12	1.57	0.41
1:B:636:TYR:N	1:B:636:TYR:CD1	2.88	0.41
1:B:1099:LEU:HD12	1:B:1099:LEU:HA	1.84	0.41
1:B:1940:ARG:HA	1:B:1943:ARG:NE	2.35	0.41
1:B:2187:ILE:H	1:B:2187:ILE:HG12	1.60	0.41
1:D:2281:SER:O	1:D:2282:PRO:C	2.60	0.41
1:D:2472:PRO:HB2	1:D:2473:CYS:H	1.67	0.41
1:A:936:LEU:HD22	1:A:936:LEU:HA	1.87	0.41
1:A:2171:VAL:HG22	2:C:232:ASP:OD1	2.21	0.41
1:A:2341:LEU:HD23	1:A:2341:LEU:HA	1.90	0.41
1:B:703:ARG:H	1:B:703:ARG:HG3	1.51	0.41
1:B:1218:LEU:HA	1:B:1218:LEU:HD22	1.68	0.41
1:B:1658:GLU:HB3	1:B:1661:GLU:HB2	2.02	0.41
1:D:578:LYS:HE3	1:D:578:LYS:HB2	1.58	0.41
1:D:2025:LYS:HD2	1:D:2085:TYR:HB3	2.02	0.41
1:D:2088:ARG:HA	1:D:2489:GLU:OE1	2.21	0.41
1:A:636:TYR:N	1:A:636:TYR:CD1	2.88	0.41
1:B:1345:LYS:HB2	1:B:1345:LYS:HE2	1.81	0.41
1:B:2163:LYS:O	1:B:2164:GLY:C	2.63	0.41
1:B:2213:THR:CG2	1:B:2224:THR:HG23	2.42	0.41
1:B:2274:SER:HB3	1:B:2403:TRP:HB3	2.03	0.41
1:B:2471:LEU:HA	1:B:2472:PRO:HD3	1.95	0.41
1:D:636:TYR:N	1:D:636:TYR:CD1	2.87	0.41
1:D:1550:LEU:O	1:D:1550:LEU:HG	2.21	0.41
1:A:695:ILE:HD12	1:A:695:ILE:HA	1.78	0.41
1:A:1697:LEU:HD22	1:A:1697:LEU:HA	1.81	0.41
1:A:1722:ILE:H	1:A:1722:ILE:HG13	1.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:ARG:HA	1:A:2489:GLU:OE1	2.21	0.41
1:A:2163:LYS:O	1:A:2164:GLY:C	2.64	0.41
1:A:2270:ILE:HD13	1:A:2418:LEU:HD13	2.03	0.41
1:A:2309:ARG:HB2	1:A:2310:ASP:H	1.60	0.41
1:A:2313:LYS:H	1:A:2313:LYS:HG3	1.50	0.41
1:B:1347:LEU:HD12	1:B:1347:LEU:HA	1.81	0.41
1:B:1724:ARG:O	1:B:1725:PRO:C	2.64	0.41
1:B:2172:LYS:HE2	1:D:2124:TRP:O	2.21	0.41
1:D:853:LYS:H	1:D:853:LYS:HG2	1.61	0.41
1:D:1036:ARG:H	1:D:1036:ARG:HG3	1.71	0.41
1:D:1940:ARG:HA	1:D:1943:ARG:NE	2.35	0.41
1:D:2171:VAL:HG22	2:E:232:ASP:OD1	2.21	0.41
1:D:2282:PRO:O	1:D:2286:ALA:HB3	2.21	0.41
1:A:814:LEU:HD23	1:A:814:LEU:HA	1.68	0.41
1:A:1722:ILE:O	1:A:1723:PRO:C	2.63	0.41
1:A:2098:TYR:HB3	1:A:2151:CYS:HA	2.03	0.41
1:A:2123:ASP:HB3	1:A:2136:TRP:CZ2	2.55	0.41
1:A:2268:ALA:HB2	1:A:2422:ILE:HG13	2.03	0.41
1:A:2273:SER:HA	1:A:2405:VAL:HG22	2.03	0.41
1:B:2015:MET:HE2	1:B:2015:MET:HB2	1.86	0.41
1:B:2270:ILE:HD13	1:B:2418:LEU:HD13	2.03	0.41
1:B:2305:TRP:HE3	1:B:2307:PHE:HZ	1.68	0.41
1:B:2435:LEU:HD13	1:B:2435:LEU:HA	1.76	0.41
1:B:2497:GLU:H	1:B:2497:GLU:HG3	1.74	0.41
1:D:1697:LEU:HA	1:D:1697:LEU:HD22	1.81	0.41
1:D:2170:ILE:O	2:E:236:ILE:CD1	2.69	0.41
1:D:2198:ARG:HE	1:D:2198:ARG:HB2	1.73	0.41
1:D:2274:SER:HB3	1:D:2403:TRP:HB3	2.02	0.41
1:D:2459:PHE:HE1	2:E:243:ILE:C	2.28	0.41
1:B:2024:ARG:HD2	1:B:2024:ARG:HA	1.77	0.41
1:B:2467:MET:HA	1:D:2508:ARG:HA	2.03	0.41
1:D:615:PHE:HB2	1:D:621:LEU:O	2.21	0.41
1:D:1363:LYS:HE3	1:D:1363:LYS:HB3	1.28	0.41
1:D:1975:ILE:HD13	1:D:1975:ILE:HA	1.91	0.41
1:D:2268:ALA:HB2	1:D:2422:ILE:HG13	2.03	0.41
2:E:245:PHE:O	2:E:246:PRO:C	2.63	0.41
1:A:2121:VAL:O	1:A:2125:VAL:HG23	2.21	0.40
1:A:2172:LYS:HE2	1:B:2124:TRP:O	2.21	0.40
1:B:615:PHE:HB2	1:B:621:LEU:O	2.21	0.40
1:B:1565:LEU:H	1:B:1565:LEU:HG	1.68	0.40
1:B:2123:ASP:HB3	1:B:2136:TRP:CZ2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2341:LEU:HD23	1:B:2341:LEU:HA	1.90	0.40
1:D:627:LYS:HA	1:D:627:LYS:CE	2.20	0.40
1:D:1514:LEU:H	1:D:1514:LEU:HG	1.63	0.40
1:D:1801:LEU:HD12	1:D:1801:LEU:HA	1.89	0.40
1:A:587:MET:CA	1:A:587:MET:CE	2.89	0.40
1:A:615:PHE:HB2	1:A:621:LEU:O	2.21	0.40
1:B:596:ARG:O	1:B:600:TYR:HB2	2.21	0.40
1:B:610:LEU:HD12	1:B:610:LEU:HA	1.77	0.40
1:B:624:LYS:HA	1:B:706:MET:O	2.22	0.40
1:B:2417:LEU:HA	1:B:2417:LEU:HD23	1.79	0.40
1:D:1187:LEU:HD23	1:D:1187:LEU:HA	1.87	0.40
1:D:1354:MET:SD	1:D:2490:THR:HG21	2.61	0.40
1:D:2121:VAL:O	1:D:2125:VAL:HG23	2.21	0.40
1:D:2407:GLU:HB3	1:D:2415:CYS:SG	2.61	0.40
1:A:818:LEU:HD23	1:A:818:LEU:HA	1.90	0.40
1:A:1354:MET:SD	1:A:2490:THR:HG21	2.61	0.40
1:A:2025:LYS:HD2	1:A:2085:TYR:HB3	2.02	0.40
1:A:2459:PHE:HE1	2:C:243:ILE:C	2.30	0.40
1:B:777:LEU:O	1:B:778:SER:C	2.62	0.40
1:B:1354:MET:SD	1:B:2490:THR:HG21	2.61	0.40
1:D:2037:LEU:HD23	1:D:2037:LEU:HA	1.79	0.40
1:D:2187:ILE:H	1:D:2187:ILE:HG12	1.60	0.40
1:D:2222:LEU:HA	1:D:2222:LEU:HD13	1.77	0.40
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.93	0.40
1:A:791:HIS:CB	1:A:946:TYR:HE2	2.34	0.40
1:A:1171:LEU:HD13	1:A:1171:LEU:HA	1.56	0.40
1:A:1550:LEU:O	1:A:1550:LEU:HG	2.21	0.40
1:A:1559:GLU:H	1:A:1559:GLU:HG3	1.51	0.40
1:A:2318:GLU:H	1:A:2318:GLU:HG3	1.61	0.40
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.89	0.40
1:B:1697:LEU:HD22	1:B:1697:LEU:HA	1.81	0.40
1:B:1725:PRO:HG2	1:B:1730:TRP:CZ2	2.57	0.40
1:B:1728:ARG:H	1:B:1728:ARG:HG3	1.37	0.40
1:B:1744:LYS:HZ3	1:B:1744:LYS:CB	2.33	0.40
1:B:2037:LEU:HD23	1:B:2037:LEU:HA	1.79	0.40
1:D:624:LYS:HA	1:D:706:MET:O	2.22	0.40
1:D:2292:LEU:HG	1:D:2292:LEU:H	1.40	0.40
1:A:624:LYS:HA	1:A:706:MET:O	2.22	0.40
1:A:626:LEU:O	1:A:630:TRP:N	2.53	0.40
1:A:679:GLU:H	1:A:679:GLU:HG3	1.63	0.40
1:A:686:VAL:CB	1:A:687:PRO:HD3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2275:GLY:HA3	1:D:2280:ILE:CA	2.52	0.40
1:A:2407:GLU:HB3	1:A:2415:CYS:SG	2.61	0.40
1:B:577:ALA:HB1	1:B:701:PHE:HB3	2.03	0.40
1:B:602:ILE:H	1:B:602:ILE:HG13	1.47	0.40
1:B:785:ARG:HA	1:B:790:LEU:CB	2.46	0.40
1:B:1327:LEU:HD12	1:B:1539:MET:HG2	2.03	0.40
1:B:2189:PHE:HD1	1:B:2189:PHE:HA	1.63	0.40
1:D:1351:LYS:HA	1:D:1351:LYS:HD2	1.28	0.40
1:D:1719:MET:HE2	1:D:1719:MET:HB2	1.64	0.40
1:D:1725:PRO:HG2	1:D:1730:TRP:CZ2	2.57	0.40
1:D:2207:PRO:HB3	1:D:2307:PHE:HB3	2.04	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	1248/2521 (50%)	1063 (85%)	144 (12%)	41 (3%)	3	21
1	B	1248/2521 (50%)	1071 (86%)	137 (11%)	40 (3%)	3	21
1	D	1248/2521 (50%)	1072 (86%)	139 (11%)	37 (3%)	3	22
2	C	19/246 (8%)	14 (74%)	3 (16%)	2 (10%)	0	6
2	E	19/246 (8%)	17 (90%)	0	2 (10%)	0	6
2	F	19/246 (8%)	17 (90%)	1 (5%)	1 (5%)	1	15
All	All	3801/8301 (46%)	3254 (86%)	424 (11%)	123 (3%)	5	21

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1409	HIS

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Mol	Chain	Res	Type
1	A	1723	PRO
1	A	1725	PRO
1	A	1953	LYS
1	A	2316	THR
1	A	2379	GLU
1	A	2429	PRO
1	A	2430	PRO
1	B	1723	PRO
1	B	1725	PRO
1	B	1953	LYS
1	B	2316	THR
1	B	2379	GLU
1	B	2429	PRO
1	B	2430	PRO
1	B	2472	PRO
2	C	246	PRO
1	D	1723	PRO
1	D	1725	PRO
1	D	1953	LYS
1	D	2316	THR
1	D	2379	GLU
1	D	2429	PRO
1	D	2430	PRO
1	D	2472	PRO
2	E	246	PRO
2	F	246	PRO
1	A	1029	ARG
1	A	1941	PRO
1	A	2168	LYS
1	A	2295	GLY
1	A	2363	PRO
1	A	2382	TYR
1	A	2472	PRO
1	B	1029	ARG
1	B	1941	PRO
1	B	2168	LYS
1	B	2283	PRO
1	B	2295	GLY
1	B	2363	PRO
1	B	2382	TYR
1	B	2466	ILE
1	D	1029	ARG

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Mol	Chain	Res	Type
1	D	1941	PRO
1	D	2168	LYS
1	D	2295	GLY
1	D	2363	PRO
1	D	2382	TYR
1	A	850	TYR
1	A	921	LYS
1	A	1164	ARG
1	A	1410	ALA
1	A	1555	LEU
1	A	1672	ALA
1	A	1726	SER
1	A	2166	LYS
1	B	850	TYR
1	B	921	LYS
1	B	1164	ARG
1	B	1555	LEU
1	B	1672	ALA
1	B	1726	SER
1	D	850	TYR
1	D	921	LYS
1	D	1164	ARG
1	D	1555	LEU
1	D	1672	ALA
1	D	1726	SER
1	D	2166	LYS
2	E	244	CYS
1	A	684	ILE
1	A	1200	GLY
1	A	1658	GLU
1	A	2283	PRO
1	A	2466	ILE
1	B	620	SER
1	B	684	ILE
1	B	1200	GLY
1	B	1658	GLU
1	B	2166	LYS
2	C	244	CYS
1	D	620	SER
1	D	684	ILE
1	D	1200	GLY
1	D	1658	GLU

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Mol	Chain	Res	Type
1	D	2466	ILE
1	A	620	SER
1	A	851	GLN
1	A	971	THR
1	A	1361	GLN
1	A	2113	PRO
1	B	851	GLN
1	B	971	THR
1	B	1361	GLN
1	B	2113	PRO
1	D	851	GLN
1	D	971	THR
1	D	1361	GLN
1	A	1954	TYR
1	A	2419	PRO
1	B	1954	TYR
1	B	2169	LYS
1	B	2419	PRO
1	D	1954	TYR
1	D	2419	PRO
1	A	599	VAL
1	A	808	VAL
1	A	2353	PRO
1	B	599	VAL
1	B	808	VAL
1	B	2353	PRO
1	D	599	VAL
1	D	808	VAL
1	D	2353	PRO
1	A	2344	GLY
1	B	2344	GLY
1	D	2344	GLY
1	A	598	VAL
1	A	854	VAL
1	B	598	VAL
1	B	854	VAL
1	D	598	VAL
1	D	854	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1108/2172 (51%)	634 (57%)	474 (43%)	0	0
1	B	1107/2172 (51%)	630 (57%)	477 (43%)	0	0
1	D	1108/2172 (51%)	639 (58%)	469 (42%)	0	0
2	C	18/203 (9%)	10 (56%)	8 (44%)	0	0
2	E	18/203 (9%)	11 (61%)	7 (39%)	0	1
2	F	18/203 (9%)	12 (67%)	6 (33%)	0	2
All	All	3377/7125 (47%)	1936 (57%)	1441 (43%)	0	0

All (1441) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	GLU
1	A	571	LEU
1	A	572	VAL
1	A	573	LYS
1	A	578	LYS
1	A	579	TYR
1	A	580	TRP
1	A	581	ILE
1	A	583	VAL
1	A	587	MET
1	A	589	ILE
1	A	591	VAL
1	A	592	SER
1	A	593	PHE
1	A	596	ARG
1	A	597	LEU
1	A	598	VAL
1	A	602	ILE
1	A	608	PHE
1	A	609	LEU
1	A	610	LEU
1	A	611	CYS

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Mol	Chain	Res	Type
1	A	612	LEU
1	A	617	VAL
1	A	621	LEU
1	A	623	ARG
1	A	626	LEU
1	A	627	LYS
1	A	631	TRP
1	A	638	MET
1	A	644	VAL
1	A	679	GLU
1	A	680	LEU
1	A	682	SER
1	A	685	LEU
1	A	687	PRO
1	A	691	LEU
1	A	694	CYS
1	A	695	ILE
1	A	696	LEU
1	A	700	TYR
1	A	703	ARG
1	A	706	MET
1	A	707	GLN
1	A	708	LEU
1	A	709	THR
1	A	768	GLU
1	A	769	LEU
1	A	781	GLN
1	A	784	LEU
1	A	786	ARG
1	A	787	LEU
1	A	788	LEU
1	A	792	VAL
1	A	794	LYS
1	A	798	LEU
1	A	799	TYR
1	A	805	LEU
1	A	806	LYS
1	A	807	GLU
1	A	808	VAL
1	A	809	SER
1	A	813	LEU
1	A	817	VAL

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Mol	Chain	Res	Type
1	A	823	LEU
1	A	827	ARG
1	A	828	PHE
1	A	831	MET
1	A	833	SER
1	A	836	SER
1	A	837	THR
1	A	839	TRP
1	A	841	CYS
1	A	843	ILE
1	A	844	ILE
1	A	848	MET
1	A	849	LEU
1	A	851	GLN
1	A	852	LEU
1	A	853	LYS
1	A	854	VAL
1	A	855	VAL
1	A	856	ASN
1	A	917	PHE
1	A	919	VAL
1	A	920	ARG
1	A	921	LYS
1	A	925	ASN
1	A	930	GLN
1	A	932	HIS
1	A	933	LEU
1	A	935	VAL
1	A	936	LEU
1	A	938	LEU
1	A	946	TYR
1	A	949	GLN
1	A	953	ARG
1	A	954	ARG
1	A	971	THR
1	A	973	GLN
1	A	974	GLN
1	A	975	LEU
1	A	976	ASP
1	A	978	ASP
1	A	979	LEU
1	A	980	LEU

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Mol	Chain	Res	Type
1	A	983	LEU
1	A	984	LYS
1	A	990	PHE
1	A	993	LYS
1	A	999	CYS
1	A	1002	MET
1	A	1007	ILE
1	A	1010	ARG
1	A	1014	LEU
1	A	1015	VAL
1	A	1025	ILE
1	A	1026	LEU
1	A	1028	ARG
1	A	1030	HIS
1	A	1031	ARG
1	A	1032	GLN
1	A	1034	ILE
1	A	1036	ARG
1	A	1037	LEU
1	A	1043	LEU
1	A	1048	PHE
1	A	1050	LEU
1	A	1052	GLN
1	A	1055	LEU
1	A	1057	LEU
1	A	1097	THR
1	A	1099	LEU
1	A	1100	ILE
1	A	1101	SER
1	A	1103	PHE
1	A	1104	LEU
1	A	1112	GLN
1	A	1116	PHE
1	A	1119	GLU
1	A	1155	LEU
1	A	1156	ASP
1	A	1158	LEU
1	A	1162	VAL
1	A	1165	TYR
1	A	1171	LEU
1	A	1175	PHE
1	A	1181	ARG

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Mol	Chain	Res	Type
1	A	1182	ILE
1	A	1184	ILE
1	A	1187	LEU
1	A	1191	LEU
1	A	1198	LEU
1	A	1201	THR
1	A	1203	LEU
1	A	1204	LEU
1	A	1205	GLN
1	A	1206	ARG
1	A	1208	THR
1	A	1209	ARG
1	A	1211	ARG
1	A	1212	LEU
1	A	1214	LEU
1	A	1216	ASP
1	A	1217	CYS
1	A	1218	LEU
1	A	1219	ILE
1	A	1220	LEU
1	A	1227	ILE
1	A	1231	MET
1	A	1232	LEU
1	A	1233	SER
1	A	1285	ILE
1	A	1286	ILE
1	A	1296	LEU
1	A	1299	ARG
1	A	1300	ARG
1	A	1303	LEU
1	A	1304	SER
1	A	1307	TYR
1	A	1308	LEU
1	A	1310	VAL
1	A	1319	LEU
1	A	1322	SER
1	A	1323	ARG
1	A	1327	LEU
1	A	1328	TYR
1	A	1333	LEU
1	A	1336	ILE
1	A	1340	ARG

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Mol	Chain	Res	Type
1	A	1343	GLU
1	A	1344	GLU
1	A	1345	LYS
1	A	1347	LEU
1	A	1349	GLN
1	A	1351	LYS
1	A	1355	GLU
1	A	1356	ARG
1	A	1358	ARG
1	A	1360	LYS
1	A	1362	GLU
1	A	1363	LYS
1	A	1365	ARG
1	A	1366	GLN
1	A	1408	ASP
1	A	1409	HIS
1	A	1411	THR
1	A	1423	SER
1	A	1424	ASP
1	A	1426	GLU
1	A	1427	GLU
1	A	1514	LEU
1	A	1524	GLU
1	A	1533	THR
1	A	1534	ARG
1	A	1536	HIS
1	A	1539	MET
1	A	1543	LEU
1	A	1544	ARG
1	A	1546	GLU
1	A	1547	ARG
1	A	1549	LEU
1	A	1551	THR
1	A	1553	GLU
1	A	1554	LEU
1	A	1555	LEU
1	A	1556	GLN
1	A	1559	GLU
1	A	1560	VAL
1	A	1562	ARG
1	A	1564	VAL
1	A	1565	LEU

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Mol	Chain	Res	Type
1	A	1566	ASP
1	A	1567	GLN
1	A	1646	SER
1	A	1647	GLU
1	A	1649	LEU
1	A	1650	LEU
1	A	1651	ASP
1	A	1653	ARG
1	A	1654	LEU
1	A	1655	ARG
1	A	1656	ILE
1	A	1659	LEU
1	A	1660	GLU
1	A	1663	GLU
1	A	1665	PHE
1	A	1667	GLU
1	A	1669	GLN
1	A	1673	LEU
1	A	1674	ARG
1	A	1675	LEU
1	A	1676	LEU
1	A	1677	ARG
1	A	1681	GLN
1	A	1687	SER
1	A	1689	LEU
1	A	1690	LEU
1	A	1695	ILE
1	A	1696	ILE
1	A	1697	LEU
1	A	1699	HIS
1	A	1707	SER
1	A	1708	LEU
1	A	1722	ILE
1	A	1724	ARG
1	A	1727	LYS
1	A	1728	ARG
1	A	1731	MET
1	A	1741	VAL
1	A	1744	LYS
1	A	1779	THR
1	A	1780	ASP
1	A	1783	ILE

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Mol	Chain	Res	Type
1	A	1786	ASP
1	A	1787	LEU
1	A	1793	LEU
1	A	1797	ARG
1	A	1801	LEU
1	A	1802	CYS
1	A	1803	TYR
1	A	1940	ARG
1	A	1942	LEU
1	A	1943	ARG
1	A	1949	ILE
1	A	1950	LEU
1	A	1953	LYS
1	A	1954	TYR
1	A	1955	ARG
1	A	1958	THR
1	A	1960	VAL
1	A	1972	PHE
1	A	1974	ILE
1	A	1976	ILE
1	A	1977	PHE
1	A	1979	PHE
1	A	1980	TRP
1	A	1999	GLN
1	A	2000	VAL
1	A	2004	PHE
1	A	2006	VAL
1	A	2007	MET
1	A	2008	LEU
1	A	2009	LEU
1	A	2010	ILE
1	A	2011	GLN
1	A	2023	LEU
1	A	2026	THR
1	A	2027	VAL
1	A	2028	LEU
1	A	2030	LYS
1	A	2031	LEU
1	A	2037	LEU
1	A	2043	LEU
1	A	2045	MET
1	A	2048	ILE

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Mol	Chain	Res	Type
1	A	2049	LEU
1	A	2061	VAL
1	A	2065	LEU
1	A	2066	TRP
1	A	2070	LYS
1	A	2077	SER
1	A	2080	GLN
1	A	2082	ARG
1	A	2083	CYS
1	A	2087	THR
1	A	2088	ARG
1	A	2089	ILE
1	A	2090	LEU
1	A	2094	LEU
1	A	2096	LYS
1	A	2097	LYS
1	A	2099	ASN
1	A	2100	HIS
1	A	2101	LEU
1	A	2103	LEU
1	A	2116	VAL
1	A	2117	GLU
1	A	2122	MET
1	A	2129	THR
1	A	2133	LEU
1	A	2134	SER
1	A	2137	MET
1	A	2140	GLU
1	A	2152	SER
1	A	2153	ARG
1	A	2154	GLU
1	A	2159	TYR
1	A	2168	LYS
1	A	2169	LYS
1	A	2170	ILE
1	A	2171	VAL
1	A	2184	ILE
1	A	2187	ILE
1	A	2189	PHE
1	A	2198	ARG
1	A	2201	VAL
1	A	2203	VAL

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Mol	Chain	Res	Type
1	A	2204	VAL
1	A	2205	ASN
1	A	2210	VAL
1	A	2211	THR
1	A	2215	LYS
1	A	2216	LEU
1	A	2222	LEU
1	A	2223	PHE
1	A	2224	THR
1	A	2228	GLN
1	A	2229	GLN
1	A	2231	SER
1	A	2232	ILE
1	A	2236	THR
1	A	2238	GLN
1	A	2242	GLU
1	A	2243	LEU
1	A	2244	SER
1	A	2248	ASP
1	A	2250	GLN
1	A	2252	LEU
1	A	2254	MET
1	A	2259	GLN
1	A	2263	GLU
1	A	2265	ILE
1	A	2266	VAL
1	A	2269	GLN
1	A	2270	ILE
1	A	2271	GLU
1	A	2273	SER
1	A	2280	ILE
1	A	2284	SER
1	A	2287	GLN
1	A	2291	GLU
1	A	2292	LEU
1	A	2294	ASN
1	A	2302	ARG
1	A	2306	ASN
1	A	2309	ARG
1	A	2310	ASP
1	A	2313	LYS
1	A	2316	THR

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Mol	Chain	Res	Type
1	A	2317	VAL
1	A	2318	GLU
1	A	2319	TYR
1	A	2321	ASN
1	A	2323	LYS
1	A	2325	MET
1	A	2326	LEU
1	A	2331	ASN
1	A	2340	SER
1	A	2342	LEU
1	A	2343	GLU
1	A	2345	THR
1	A	2346	SER
1	A	2347	ASP
1	A	2351	VAL
1	A	2354	ASN
1	A	2355	LEU
1	A	2356	PHE
1	A	2358	LYS
1	A	2360	ILE
1	A	2361	ARG
1	A	2364	ASN
1	A	2372	LYS
1	A	2374	LEU
1	A	2375	GLN
1	A	2381	ASP
1	A	2387	ILE
1	A	2389	LEU
1	A	2390	ARG
1	A	2400	PHE
1	A	2405	VAL
1	A	2406	ILE
1	A	2407	GLU
1	A	2408	LEU
1	A	2410	GLU
1	A	2412	ARG
1	A	2413	THR
1	A	2414	ASP
1	A	2420	MET
1	A	2421	VAL
1	A	2424	SER
1	A	2426	LYS

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Mol	Chain	Res	Type
1	A	2427	VAL
1	A	2432	LEU
1	A	2435	LEU
1	A	2441	MET
1	A	2443	LEU
1	A	2446	SER
1	A	2453	LYS
1	A	2462	ILE
1	A	2465	SER
1	A	2469	GLU
1	A	2471	LEU
1	A	2473	CYS
1	A	2477	ILE
1	A	2480	LEU
1	A	2486	LEU
1	A	2487	VAL
1	A	2489	GLU
1	A	2491	ARG
1	A	2492	GLU
1	A	2494	GLU
1	A	2498	GLU
1	A	2502	LYS
1	A	2504	ILE
1	A	2506	LEU
1	A	2508	ARG
1	A	2509	SER
1	A	2511	GLU
1	A	2512	THR
1	A	2513	MET
1	A	2516	TRP
1	A	2520	LYS
1	A	2521	GLU
1	B	570	GLU
1	B	571	LEU
1	B	572	VAL
1	B	573	LYS
1	B	578	LYS
1	B	579	TYR
1	B	580	TRP
1	B	581	ILE
1	B	583	VAL
1	B	587	MET

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Mol	Chain	Res	Type
1	B	589	ILE
1	B	591	VAL
1	B	592	SER
1	B	593	PHE
1	B	596	ARG
1	B	597	LEU
1	B	598	VAL
1	B	602	ILE
1	B	608	PHE
1	B	609	LEU
1	B	610	LEU
1	B	611	CYS
1	B	612	LEU
1	B	617	VAL
1	B	621	LEU
1	B	623	ARG
1	B	626	LEU
1	B	627	LYS
1	B	631	TRP
1	B	638	MET
1	B	644	VAL
1	B	679	GLU
1	B	680	LEU
1	B	682	SER
1	B	685	LEU
1	B	687	PRO
1	B	691	LEU
1	B	694	CYS
1	B	695	ILE
1	B	696	LEU
1	B	700	TYR
1	B	703	ARG
1	B	706	MET
1	B	707	GLN
1	B	708	LEU
1	B	709	THR
1	B	768	GLU
1	B	769	LEU
1	B	781	GLN
1	B	784	LEU
1	B	786	ARG
1	B	787	LEU

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Mol	Chain	Res	Type
1	B	788	LEU
1	B	792	VAL
1	B	794	LYS
1	B	798	LEU
1	B	799	TYR
1	B	805	LEU
1	B	806	LYS
1	B	807	GLU
1	B	808	VAL
1	B	809	SER
1	B	813	LEU
1	B	817	VAL
1	B	823	LEU
1	B	827	ARG
1	B	828	PHE
1	B	831	MET
1	B	833	SER
1	B	836	SER
1	B	837	THR
1	B	839	TRP
1	B	841	CYS
1	B	843	ILE
1	B	844	ILE
1	B	848	MET
1	B	849	LEU
1	B	851	GLN
1	B	852	LEU
1	B	853	LYS
1	B	854	VAL
1	B	855	VAL
1	B	856	ASN
1	B	917	PHE
1	B	919	VAL
1	B	920	ARG
1	B	921	LYS
1	B	925	ASN
1	B	930	GLN
1	B	932	HIS
1	B	933	LEU
1	B	935	VAL
1	B	936	LEU
1	B	938	LEU

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Mol	Chain	Res	Type
1	B	946	TYR
1	B	949	GLN
1	B	953	ARG
1	B	954	ARG
1	B	971	THR
1	B	973	GLN
1	B	974	GLN
1	B	975	LEU
1	B	976	ASP
1	B	978	ASP
1	B	979	LEU
1	B	980	LEU
1	B	983	LEU
1	B	984	LYS
1	B	990	PHE
1	B	993	LYS
1	B	999	CYS
1	B	1002	MET
1	B	1007	ILE
1	B	1010	ARG
1	B	1014	LEU
1	B	1015	VAL
1	B	1025	ILE
1	B	1026	LEU
1	B	1028	ARG
1	B	1030	HIS
1	B	1031	ARG
1	B	1032	GLN
1	B	1034	ILE
1	B	1036	ARG
1	B	1037	LEU
1	B	1043	LEU
1	B	1048	PHE
1	B	1050	LEU
1	B	1052	GLN
1	B	1055	LEU
1	B	1057	LEU
1	B	1097	THR
1	B	1099	LEU
1	B	1100	ILE
1	B	1101	SER
1	B	1103	PHE

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Mol	Chain	Res	Type
1	B	1104	LEU
1	B	1112	GLN
1	B	1116	PHE
1	B	1119	GLU
1	B	1155	LEU
1	B	1156	ASP
1	B	1158	LEU
1	B	1162	VAL
1	B	1165	TYR
1	B	1171	LEU
1	B	1175	PHE
1	B	1181	ARG
1	B	1182	ILE
1	B	1184	ILE
1	B	1187	LEU
1	B	1191	LEU
1	B	1198	LEU
1	B	1201	THR
1	B	1203	LEU
1	B	1204	LEU
1	B	1205	GLN
1	B	1206	ARG
1	B	1208	THR
1	B	1209	ARG
1	B	1211	ARG
1	B	1212	LEU
1	B	1214	LEU
1	B	1216	ASP
1	B	1217	CYS
1	B	1218	LEU
1	B	1219	ILE
1	B	1220	LEU
1	B	1227	ILE
1	B	1231	MET
1	B	1232	LEU
1	B	1233	SER
1	B	1285	ILE
1	B	1286	ILE
1	B	1296	LEU
1	B	1299	ARG
1	B	1300	ARG
1	B	1303	LEU

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Mol	Chain	Res	Type
1	B	1304	SER
1	B	1307	TYR
1	B	1308	LEU
1	B	1310	VAL
1	B	1319	LEU
1	B	1322	SER
1	B	1323	ARG
1	B	1327	LEU
1	B	1328	TYR
1	B	1333	LEU
1	B	1336	ILE
1	B	1340	ARG
1	B	1343	GLU
1	B	1344	GLU
1	B	1345	LYS
1	B	1347	LEU
1	B	1349	GLN
1	B	1351	LYS
1	B	1355	GLU
1	B	1356	ARG
1	B	1358	ARG
1	B	1360	LYS
1	B	1362	GLU
1	B	1363	LYS
1	B	1365	ARG
1	B	1366	GLN
1	B	1411	THR
1	B	1423	SER
1	B	1424	ASP
1	B	1426	GLU
1	B	1427	GLU
1	B	1514	LEU
1	B	1524	GLU
1	B	1533	THR
1	B	1534	ARG
1	B	1536	HIS
1	B	1539	MET
1	B	1543	LEU
1	B	1544	ARG
1	B	1546	GLU
1	B	1547	ARG
1	B	1549	LEU

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Mol	Chain	Res	Type
1	B	1551	THR
1	B	1553	GLU
1	B	1554	LEU
1	B	1555	LEU
1	B	1556	GLN
1	B	1559	GLU
1	B	1560	VAL
1	B	1562	ARG
1	B	1564	VAL
1	B	1565	LEU
1	B	1566	ASP
1	B	1567	GLN
1	B	1646	SER
1	B	1647	GLU
1	B	1649	LEU
1	B	1650	LEU
1	B	1651	ASP
1	B	1652	ARG
1	B	1653	ARG
1	B	1654	LEU
1	B	1655	ARG
1	B	1656	ILE
1	B	1659	LEU
1	B	1660	GLU
1	B	1663	GLU
1	B	1665	PHE
1	B	1667	GLU
1	B	1669	GLN
1	B	1673	LEU
1	B	1674	ARG
1	B	1675	LEU
1	B	1676	LEU
1	B	1677	ARG
1	B	1681	GLN
1	B	1687	SER
1	B	1689	LEU
1	B	1690	LEU
1	B	1695	ILE
1	B	1696	ILE
1	B	1697	LEU
1	B	1699	HIS
1	B	1707	SER

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Mol	Chain	Res	Type
1	B	1708	LEU
1	B	1722	ILE
1	B	1724	ARG
1	B	1727	LYS
1	B	1728	ARG
1	B	1731	MET
1	B	1741	VAL
1	B	1744	LYS
1	B	1779	THR
1	B	1780	ASP
1	B	1783	ILE
1	B	1786	ASP
1	B	1787	LEU
1	B	1793	LEU
1	B	1797	ARG
1	B	1801	LEU
1	B	1802	CYS
1	B	1803	TYR
1	B	1940	ARG
1	B	1942	LEU
1	B	1943	ARG
1	B	1949	ILE
1	B	1950	LEU
1	B	1953	LYS
1	B	1954	TYR
1	B	1955	ARG
1	B	1958	THR
1	B	1960	VAL
1	B	1972	PHE
1	B	1974	ILE
1	B	1976	ILE
1	B	1977	PHE
1	B	1979	PHE
1	B	1980	TRP
1	B	1999	GLN
1	B	2000	VAL
1	B	2004	PHE
1	B	2006	VAL
1	B	2007	MET
1	B	2008	LEU
1	B	2009	LEU
1	B	2010	ILE

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Mol	Chain	Res	Type
1	B	2011	GLN
1	B	2023	LEU
1	B	2026	THR
1	B	2027	VAL
1	B	2028	LEU
1	B	2030	LYS
1	B	2031	LEU
1	B	2037	LEU
1	B	2043	LEU
1	B	2045	MET
1	B	2048	ILE
1	B	2049	LEU
1	B	2061	VAL
1	B	2065	LEU
1	B	2066	TRP
1	B	2070	LYS
1	B	2077	SER
1	B	2080	GLN
1	B	2082	ARG
1	B	2083	CYS
1	B	2087	THR
1	B	2088	ARG
1	B	2089	ILE
1	B	2090	LEU
1	B	2094	LEU
1	B	2096	LYS
1	B	2097	LYS
1	B	2099	ASN
1	B	2100	HIS
1	B	2101	LEU
1	B	2103	LEU
1	B	2109	PHE
1	B	2112	VAL
1	B	2115	LEU
1	B	2116	VAL
1	B	2117	GLU
1	B	2122	MET
1	B	2129	THR
1	B	2133	LEU
1	B	2134	SER
1	B	2137	MET
1	B	2140	GLU

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Mol	Chain	Res	Type
1	B	2152	SER
1	B	2153	ARG
1	B	2154	GLU
1	B	2159	TYR
1	B	2169	LYS
1	B	2170	ILE
1	B	2171	VAL
1	B	2184	ILE
1	B	2187	ILE
1	B	2189	PHE
1	B	2198	ARG
1	B	2201	VAL
1	B	2203	VAL
1	B	2204	VAL
1	B	2205	ASN
1	B	2210	VAL
1	B	2211	THR
1	B	2215	LYS
1	B	2216	LEU
1	B	2222	LEU
1	B	2223	PHE
1	B	2224	THR
1	B	2228	GLN
1	B	2229	GLN
1	B	2231	SER
1	B	2232	ILE
1	B	2236	THR
1	B	2238	GLN
1	B	2242	GLU
1	B	2243	LEU
1	B	2244	SER
1	B	2248	ASP
1	B	2250	GLN
1	B	2252	LEU
1	B	2254	MET
1	B	2259	GLN
1	B	2263	GLU
1	B	2265	ILE
1	B	2266	VAL
1	B	2269	GLN
1	B	2270	ILE
1	B	2271	GLU

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Mol	Chain	Res	Type
1	B	2280	ILE
1	B	2281	SER
1	B	2284	SER
1	B	2287	GLN
1	B	2291	GLU
1	B	2292	LEU
1	B	2294	ASN
1	B	2302	ARG
1	B	2306	ASN
1	B	2309	ARG
1	B	2310	ASP
1	B	2313	LYS
1	B	2316	THR
1	B	2317	VAL
1	B	2318	GLU
1	B	2319	TYR
1	B	2321	ASN
1	B	2323	LYS
1	B	2325	MET
1	B	2326	LEU
1	B	2331	ASN
1	B	2340	SER
1	B	2342	LEU
1	B	2343	GLU
1	B	2345	THR
1	B	2346	SER
1	B	2347	ASP
1	B	2351	VAL
1	B	2354	ASN
1	B	2355	LEU
1	B	2356	PHE
1	B	2358	LYS
1	B	2360	ILE
1	B	2361	ARG
1	B	2364	ASN
1	B	2372	LYS
1	B	2374	LEU
1	B	2375	GLN
1	B	2381	ASP
1	B	2387	ILE
1	B	2389	LEU
1	B	2390	ARG

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Mol	Chain	Res	Type
1	B	2400	PHE
1	B	2404	TRP
1	B	2405	VAL
1	B	2406	ILE
1	B	2407	GLU
1	B	2408	LEU
1	B	2410	GLU
1	B	2412	ARG
1	B	2413	THR
1	B	2414	ASP
1	B	2420	MET
1	B	2421	VAL
1	B	2424	SER
1	B	2426	LYS
1	B	2427	VAL
1	B	2432	LEU
1	B	2435	LEU
1	B	2441	MET
1	B	2443	LEU
1	B	2446	SER
1	B	2453	LYS
1	B	2462	ILE
1	B	2465	SER
1	B	2466	ILE
1	B	2467	MET
1	B	2469	GLU
1	B	2473	CYS
1	B	2477	ILE
1	B	2480	LEU
1	B	2486	LEU
1	B	2487	VAL
1	B	2489	GLU
1	B	2491	ARG
1	B	2492	GLU
1	B	2494	GLU
1	B	2498	GLU
1	B	2502	LYS
1	B	2504	ILE
1	B	2506	LEU
1	B	2508	ARG
1	B	2509	SER
1	B	2511	GLU

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Mol	Chain	Res	Type
1	B	2512	THR
1	B	2513	MET
1	B	2516	TRP
1	B	2520	LYS
1	B	2521	GLU
2	C	228	CYS
2	C	229	GLU
2	C	230	SER
2	C	233	CYS
2	C	235	GLU
2	C	243	ILE
2	C	244	CYS
2	C	247	SER
1	D	570	GLU
1	D	571	LEU
1	D	572	VAL
1	D	573	LYS
1	D	578	LYS
1	D	579	TYR
1	D	580	TRP
1	D	581	ILE
1	D	583	VAL
1	D	587	MET
1	D	589	ILE
1	D	591	VAL
1	D	592	SER
1	D	593	PHE
1	D	596	ARG
1	D	597	LEU
1	D	598	VAL
1	D	602	ILE
1	D	608	PHE
1	D	609	LEU
1	D	610	LEU
1	D	611	CYS
1	D	612	LEU
1	D	617	VAL
1	D	621	LEU
1	D	623	ARG
1	D	626	LEU
1	D	627	LYS
1	D	631	TRP

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Mol	Chain	Res	Type
1	D	638	MET
1	D	644	VAL
1	D	679	GLU
1	D	680	LEU
1	D	682	SER
1	D	685	LEU
1	D	687	PRO
1	D	691	LEU
1	D	694	CYS
1	D	695	ILE
1	D	696	LEU
1	D	700	TYR
1	D	703	ARG
1	D	706	MET
1	D	707	GLN
1	D	708	LEU
1	D	709	THR
1	D	768	GLU
1	D	769	LEU
1	D	781	GLN
1	D	784	LEU
1	D	786	ARG
1	D	787	LEU
1	D	788	LEU
1	D	792	VAL
1	D	794	LYS
1	D	798	LEU
1	D	799	TYR
1	D	805	LEU
1	D	806	LYS
1	D	807	GLU
1	D	808	VAL
1	D	809	SER
1	D	813	LEU
1	D	817	VAL
1	D	823	LEU
1	D	827	ARG
1	D	828	PHE
1	D	831	MET
1	D	833	SER
1	D	836	SER
1	D	837	THR

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Mol	Chain	Res	Type
1	D	839	TRP
1	D	841	CYS
1	D	843	ILE
1	D	844	ILE
1	D	848	MET
1	D	849	LEU
1	D	851	GLN
1	D	852	LEU
1	D	853	LYS
1	D	854	VAL
1	D	855	VAL
1	D	856	ASN
1	D	917	PHE
1	D	919	VAL
1	D	920	ARG
1	D	921	LYS
1	D	925	ASN
1	D	930	GLN
1	D	932	HIS
1	D	933	LEU
1	D	935	VAL
1	D	936	LEU
1	D	938	LEU
1	D	946	TYR
1	D	949	GLN
1	D	953	ARG
1	D	954	ARG
1	D	971	THR
1	D	973	GLN
1	D	974	GLN
1	D	975	LEU
1	D	976	ASP
1	D	978	ASP
1	D	979	LEU
1	D	980	LEU
1	D	983	LEU
1	D	984	LYS
1	D	990	PHE
1	D	993	LYS
1	D	999	CYS
1	D	1002	MET
1	D	1007	ILE

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Mol	Chain	Res	Type
1	D	1010	ARG
1	D	1014	LEU
1	D	1015	VAL
1	D	1025	ILE
1	D	1026	LEU
1	D	1028	ARG
1	D	1030	HIS
1	D	1031	ARG
1	D	1032	GLN
1	D	1034	ILE
1	D	1036	ARG
1	D	1037	LEU
1	D	1043	LEU
1	D	1048	PHE
1	D	1050	LEU
1	D	1052	GLN
1	D	1055	LEU
1	D	1057	LEU
1	D	1097	THR
1	D	1099	LEU
1	D	1100	ILE
1	D	1101	SER
1	D	1103	PHE
1	D	1104	LEU
1	D	1112	GLN
1	D	1116	PHE
1	D	1119	GLU
1	D	1155	LEU
1	D	1156	ASP
1	D	1158	LEU
1	D	1162	VAL
1	D	1165	TYR
1	D	1171	LEU
1	D	1175	PHE
1	D	1181	ARG
1	D	1182	ILE
1	D	1184	ILE
1	D	1187	LEU
1	D	1191	LEU
1	D	1198	LEU
1	D	1201	THR
1	D	1203	LEU

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Mol	Chain	Res	Type
1	D	1204	LEU
1	D	1205	GLN
1	D	1206	ARG
1	D	1208	THR
1	D	1209	ARG
1	D	1211	ARG
1	D	1212	LEU
1	D	1214	LEU
1	D	1216	ASP
1	D	1217	CYS
1	D	1218	LEU
1	D	1219	ILE
1	D	1220	LEU
1	D	1227	ILE
1	D	1231	MET
1	D	1232	LEU
1	D	1233	SER
1	D	1285	ILE
1	D	1286	ILE
1	D	1296	LEU
1	D	1299	ARG
1	D	1300	ARG
1	D	1303	LEU
1	D	1304	SER
1	D	1307	TYR
1	D	1308	LEU
1	D	1310	VAL
1	D	1319	LEU
1	D	1322	SER
1	D	1323	ARG
1	D	1327	LEU
1	D	1328	TYR
1	D	1333	LEU
1	D	1336	ILE
1	D	1340	ARG
1	D	1343	GLU
1	D	1344	GLU
1	D	1345	LYS
1	D	1347	LEU
1	D	1349	GLN
1	D	1351	LYS
1	D	1355	GLU

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Mol	Chain	Res	Type
1	D	1356	ARG
1	D	1358	ARG
1	D	1360	LYS
1	D	1362	GLU
1	D	1363	LYS
1	D	1365	ARG
1	D	1366	GLN
1	D	1411	THR
1	D	1423	SER
1	D	1424	ASP
1	D	1426	GLU
1	D	1427	GLU
1	D	1514	LEU
1	D	1524	GLU
1	D	1533	THR
1	D	1534	ARG
1	D	1536	HIS
1	D	1539	MET
1	D	1543	LEU
1	D	1544	ARG
1	D	1546	GLU
1	D	1547	ARG
1	D	1549	LEU
1	D	1551	THR
1	D	1553	GLU
1	D	1554	LEU
1	D	1555	LEU
1	D	1556	GLN
1	D	1559	GLU
1	D	1560	VAL
1	D	1562	ARG
1	D	1564	VAL
1	D	1565	LEU
1	D	1566	ASP
1	D	1567	GLN
1	D	1646	SER
1	D	1647	GLU
1	D	1649	LEU
1	D	1650	LEU
1	D	1651	ASP
1	D	1653	ARG
1	D	1654	LEU

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Mol	Chain	Res	Type
1	D	1655	ARG
1	D	1656	ILE
1	D	1659	LEU
1	D	1660	GLU
1	D	1663	GLU
1	D	1665	PHE
1	D	1667	GLU
1	D	1669	GLN
1	D	1673	LEU
1	D	1674	ARG
1	D	1675	LEU
1	D	1676	LEU
1	D	1677	ARG
1	D	1681	GLN
1	D	1687	SER
1	D	1689	LEU
1	D	1690	LEU
1	D	1695	ILE
1	D	1696	ILE
1	D	1697	LEU
1	D	1699	HIS
1	D	1707	SER
1	D	1708	LEU
1	D	1722	ILE
1	D	1724	ARG
1	D	1727	LYS
1	D	1728	ARG
1	D	1731	MET
1	D	1741	VAL
1	D	1744	LYS
1	D	1779	THR
1	D	1780	ASP
1	D	1783	ILE
1	D	1786	ASP
1	D	1787	LEU
1	D	1793	LEU
1	D	1797	ARG
1	D	1801	LEU
1	D	1802	CYS
1	D	1803	TYR
1	D	1940	ARG
1	D	1942	LEU

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Mol	Chain	Res	Type
1	D	1943	ARG
1	D	1949	ILE
1	D	1950	LEU
1	D	1953	LYS
1	D	1954	TYR
1	D	1955	ARG
1	D	1958	THR
1	D	1960	VAL
1	D	1972	PHE
1	D	1974	ILE
1	D	1976	ILE
1	D	1977	PHE
1	D	1979	PHE
1	D	1980	TRP
1	D	1999	GLN
1	D	2000	VAL
1	D	2004	PHE
1	D	2006	VAL
1	D	2007	MET
1	D	2008	LEU
1	D	2009	LEU
1	D	2010	ILE
1	D	2011	GLN
1	D	2023	LEU
1	D	2026	THR
1	D	2027	VAL
1	D	2028	LEU
1	D	2030	LYS
1	D	2031	LEU
1	D	2037	LEU
1	D	2043	LEU
1	D	2045	MET
1	D	2048	ILE
1	D	2049	LEU
1	D	2061	VAL
1	D	2065	LEU
1	D	2066	TRP
1	D	2070	LYS
1	D	2077	SER
1	D	2080	GLN
1	D	2082	ARG
1	D	2083	CYS

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Mol	Chain	Res	Type
1	D	2087	THR
1	D	2088	ARG
1	D	2089	ILE
1	D	2090	LEU
1	D	2094	LEU
1	D	2096	LYS
1	D	2097	LYS
1	D	2099	ASN
1	D	2100	HIS
1	D	2101	LEU
1	D	2103	LEU
1	D	2111	LEU
1	D	2116	VAL
1	D	2117	GLU
1	D	2122	MET
1	D	2129	THR
1	D	2133	LEU
1	D	2134	SER
1	D	2137	MET
1	D	2140	GLU
1	D	2152	SER
1	D	2153	ARG
1	D	2154	GLU
1	D	2159	TYR
1	D	2169	LYS
1	D	2170	ILE
1	D	2171	VAL
1	D	2184	ILE
1	D	2187	ILE
1	D	2189	PHE
1	D	2198	ARG
1	D	2201	VAL
1	D	2203	VAL
1	D	2204	VAL
1	D	2205	ASN
1	D	2210	VAL
1	D	2211	THR
1	D	2215	LYS
1	D	2216	LEU
1	D	2222	LEU
1	D	2223	PHE
1	D	2224	THR

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Mol	Chain	Res	Type
1	D	2228	GLN
1	D	2229	GLN
1	D	2231	SER
1	D	2232	ILE
1	D	2236	THR
1	D	2238	GLN
1	D	2242	GLU
1	D	2243	LEU
1	D	2244	SER
1	D	2248	ASP
1	D	2250	GLN
1	D	2252	LEU
1	D	2254	MET
1	D	2259	GLN
1	D	2263	GLU
1	D	2265	ILE
1	D	2266	VAL
1	D	2269	GLN
1	D	2270	ILE
1	D	2271	GLU
1	D	2280	ILE
1	D	2284	SER
1	D	2287	GLN
1	D	2291	GLU
1	D	2292	LEU
1	D	2294	ASN
1	D	2302	ARG
1	D	2306	ASN
1	D	2309	ARG
1	D	2310	ASP
1	D	2313	LYS
1	D	2316	THR
1	D	2317	VAL
1	D	2318	GLU
1	D	2319	TYR
1	D	2321	ASN
1	D	2323	LYS
1	D	2325	MET
1	D	2326	LEU
1	D	2331	ASN
1	D	2340	SER
1	D	2342	LEU

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Mol	Chain	Res	Type
1	D	2343	GLU
1	D	2345	THR
1	D	2346	SER
1	D	2347	ASP
1	D	2351	VAL
1	D	2354	ASN
1	D	2355	LEU
1	D	2356	PHE
1	D	2358	LYS
1	D	2360	ILE
1	D	2361	ARG
1	D	2364	ASN
1	D	2372	LYS
1	D	2374	LEU
1	D	2375	GLN
1	D	2381	ASP
1	D	2387	ILE
1	D	2389	LEU
1	D	2390	ARG
1	D	2400	PHE
1	D	2405	VAL
1	D	2406	ILE
1	D	2407	GLU
1	D	2408	LEU
1	D	2410	GLU
1	D	2412	ARG
1	D	2413	THR
1	D	2414	ASP
1	D	2420	MET
1	D	2421	VAL
1	D	2424	SER
1	D	2426	LYS
1	D	2427	VAL
1	D	2432	LEU
1	D	2435	LEU
1	D	2441	MET
1	D	2443	LEU
1	D	2446	SER
1	D	2453	LYS
1	D	2462	ILE
1	D	2465	SER
1	D	2471	LEU

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Mol	Chain	Res	Type
1	D	2473	CYS
1	D	2477	ILE
1	D	2480	LEU
1	D	2486	LEU
1	D	2487	VAL
1	D	2489	GLU
1	D	2491	ARG
1	D	2492	GLU
1	D	2494	GLU
1	D	2498	GLU
1	D	2502	LYS
1	D	2504	ILE
1	D	2506	LEU
1	D	2509	SER
1	D	2511	GLU
1	D	2512	THR
1	D	2513	MET
1	D	2516	TRP
1	D	2520	LYS
1	D	2521	GLU
2	E	228	CYS
2	E	229	GLU
2	E	230	SER
2	E	233	CYS
2	E	234	LEU
2	E	237	CYS
2	E	243	ILE
2	F	228	CYS
2	F	229	GLU
2	F	230	SER
2	F	233	CYS
2	F	234	LEU
2	F	237	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	699	HIS
1	A	702	HIS
1	A	851	GLN
1	A	925	ASN
1	A	1040	ASN

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Mol	Chain	Res	Type
1	A	1052	GLN
1	A	1222	ASN
1	A	1305	HIS
1	A	1309	HIS
1	A	1409	HIS
1	A	1536	HIS
1	A	1561	HIS
1	A	1698	ASN
1	A	1796	HIS
1	A	1999	GLN
1	A	2064	GLN
1	A	2080	GLN
1	A	2100	HIS
1	A	2145	ASN
1	A	2165	GLN
1	A	2229	GLN
1	A	2287	GLN
1	A	2331	ASN
1	A	2354	ASN
1	A	2364	ASN
1	A	2464	HIS
1	B	699	HIS
1	B	702	HIS
1	B	851	GLN
1	B	925	ASN
1	B	1040	ASN
1	B	1052	GLN
1	B	1222	ASN
1	B	1305	HIS
1	B	1309	HIS
1	B	1409	HIS
1	B	1536	HIS
1	B	1561	HIS
1	B	1698	ASN
1	B	1796	HIS
1	B	1999	GLN
1	B	2080	GLN
1	B	2100	HIS
1	B	2206	GLN
1	B	2229	GLN
1	B	2331	ASN
1	B	2354	ASN

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Mol	Chain	Res	Type
1	B	2364	ASN
1	B	2464	HIS
1	D	699	HIS
1	D	702	HIS
1	D	851	GLN
1	D	925	ASN
1	D	1040	ASN
1	D	1222	ASN
1	D	1305	HIS
1	D	1309	HIS
1	D	1409	HIS
1	D	1536	HIS
1	D	1561	HIS
1	D	1698	ASN
1	D	1796	HIS
1	D	1999	GLN
1	D	2080	GLN
1	D	2100	HIS
1	D	2107	GLN
1	D	2206	GLN
1	D	2229	GLN
1	D	2331	ASN
1	D	2354	ASN
1	D	2364	ASN
1	D	2464	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

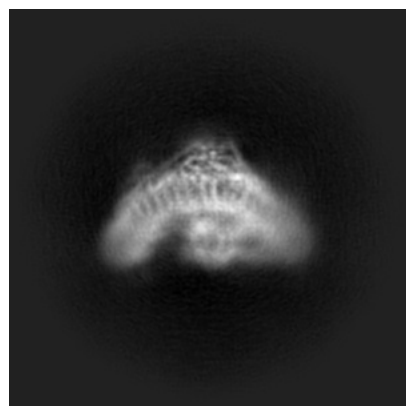
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39223. These allow visual inspection of the internal detail of the map and identification of artifacts.

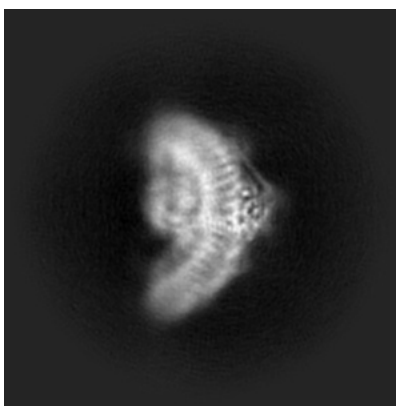
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

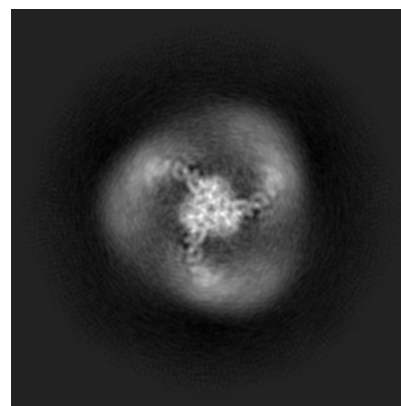
6.1.1 Primary map



X

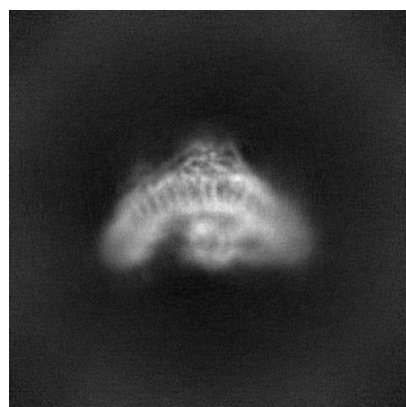


Y

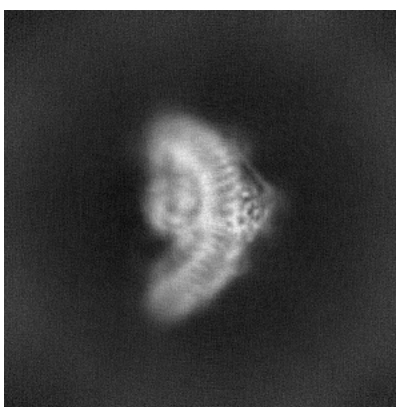


Z

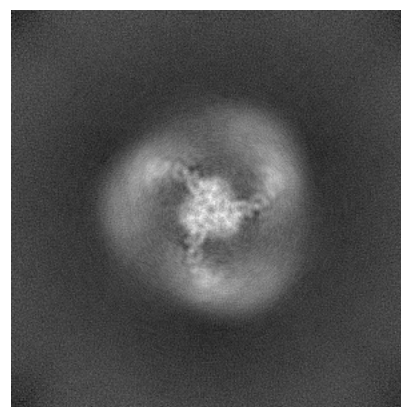
6.1.2 Raw map



X



Y

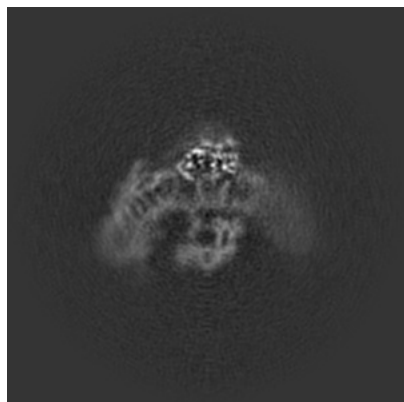


Z

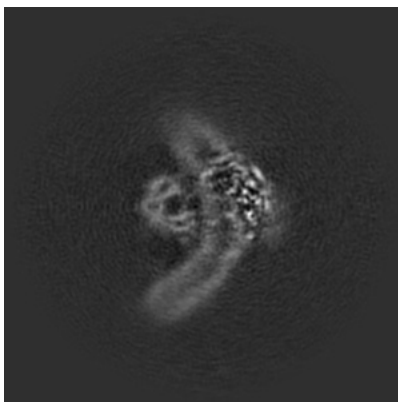
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

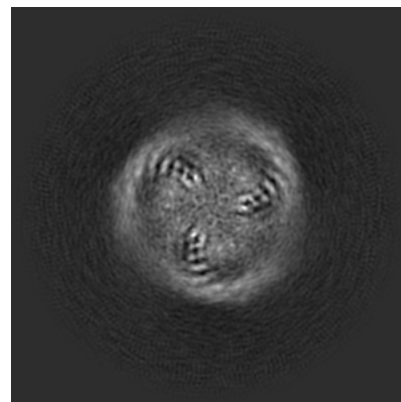
6.2.1 Primary map



X Index: 360

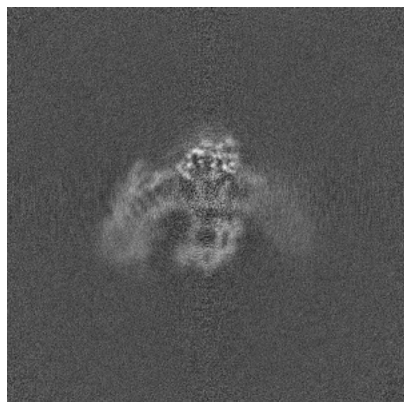


Y Index: 360

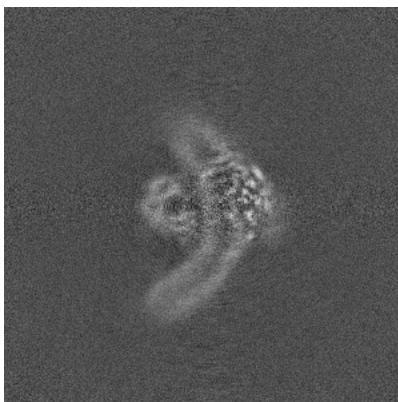


Z Index: 360

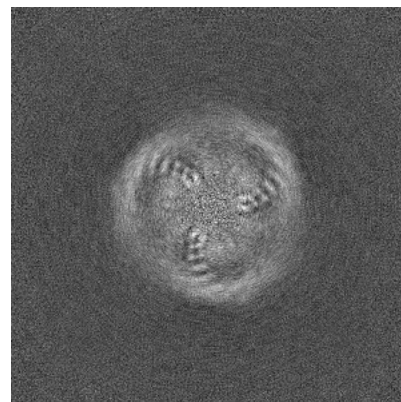
6.2.2 Raw map



X Index: 360



Y Index: 360

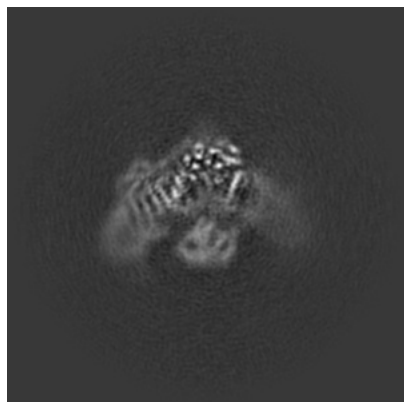


Z Index: 360

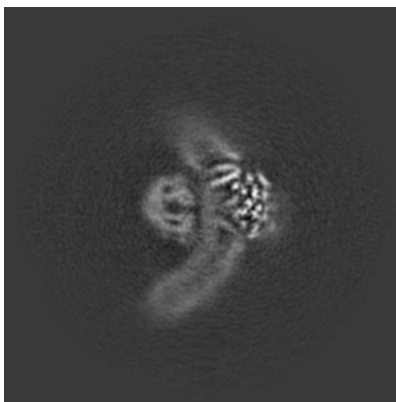
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

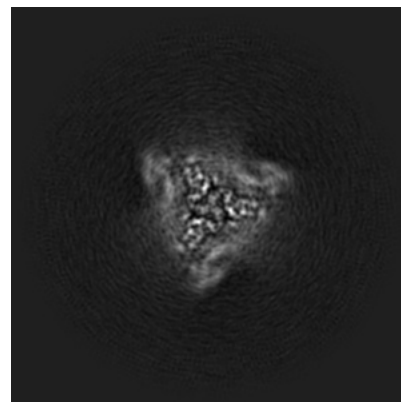
6.3.1 Primary map



X Index: 341

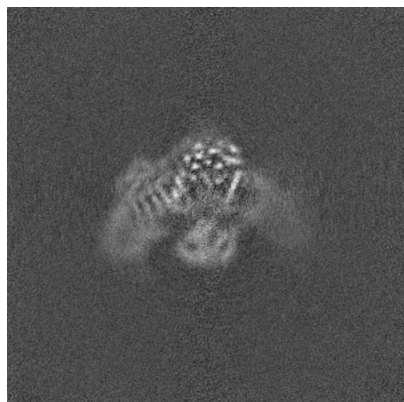


Y Index: 350

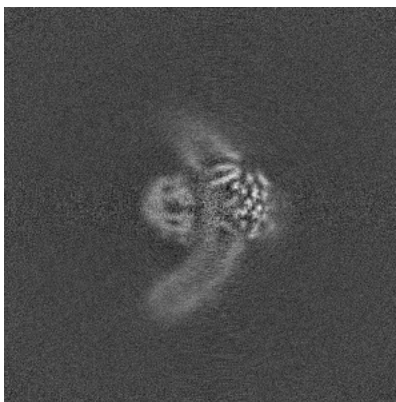


Z Index: 415

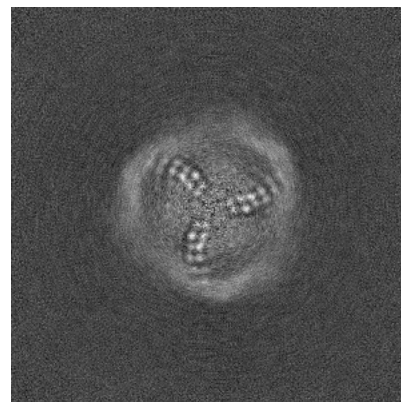
6.3.2 Raw map



X Index: 342



Y Index: 350



Z Index: 371

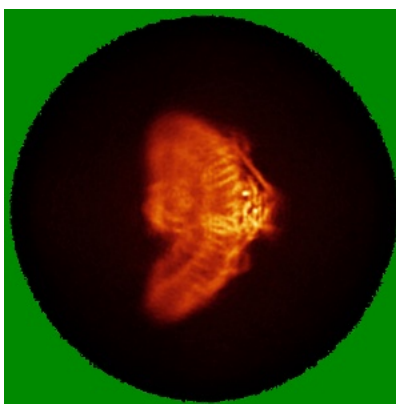
The images above show the largest variance slices of the map in three orthogonal directions.

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

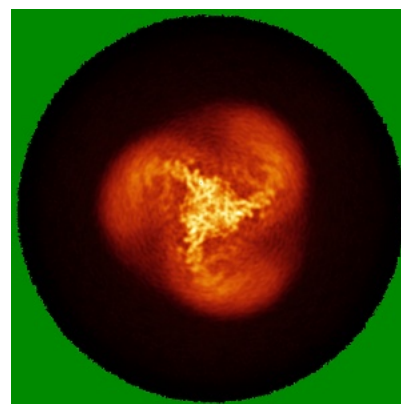
6.4.1 Primary map



X

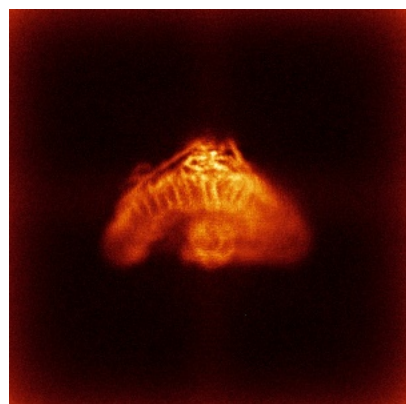


Y

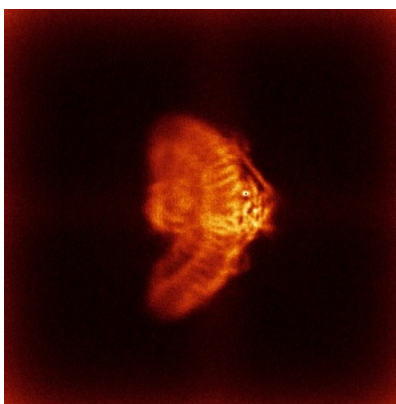


Z

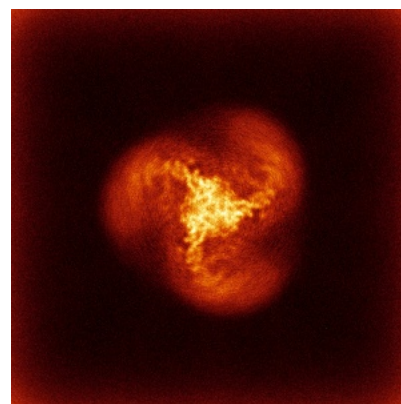
6.4.2 Raw map



X



Y

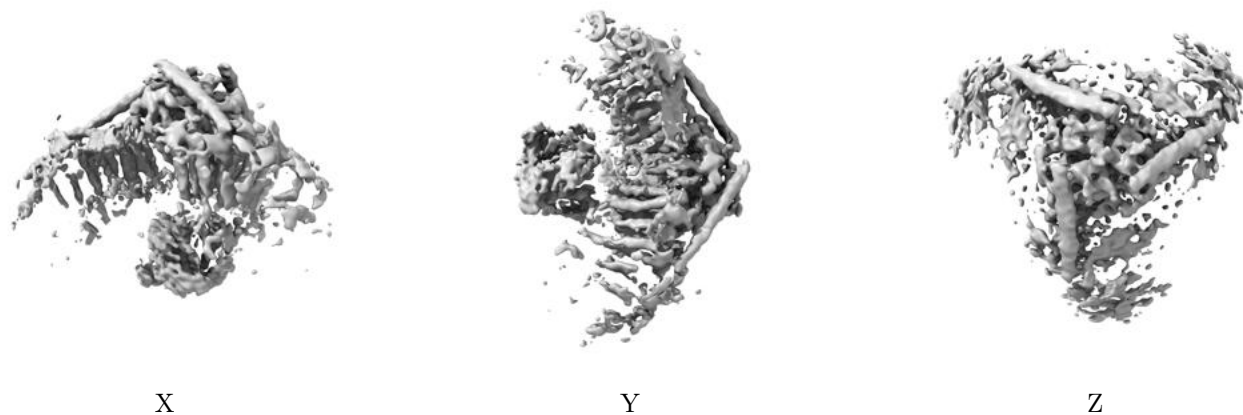


Z

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.

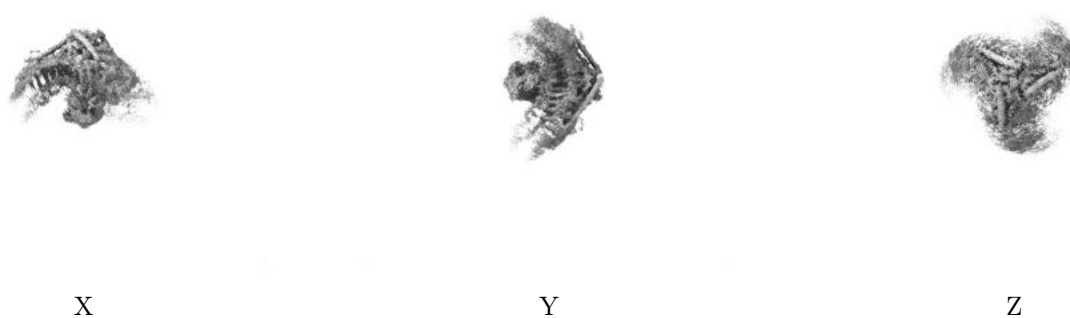
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

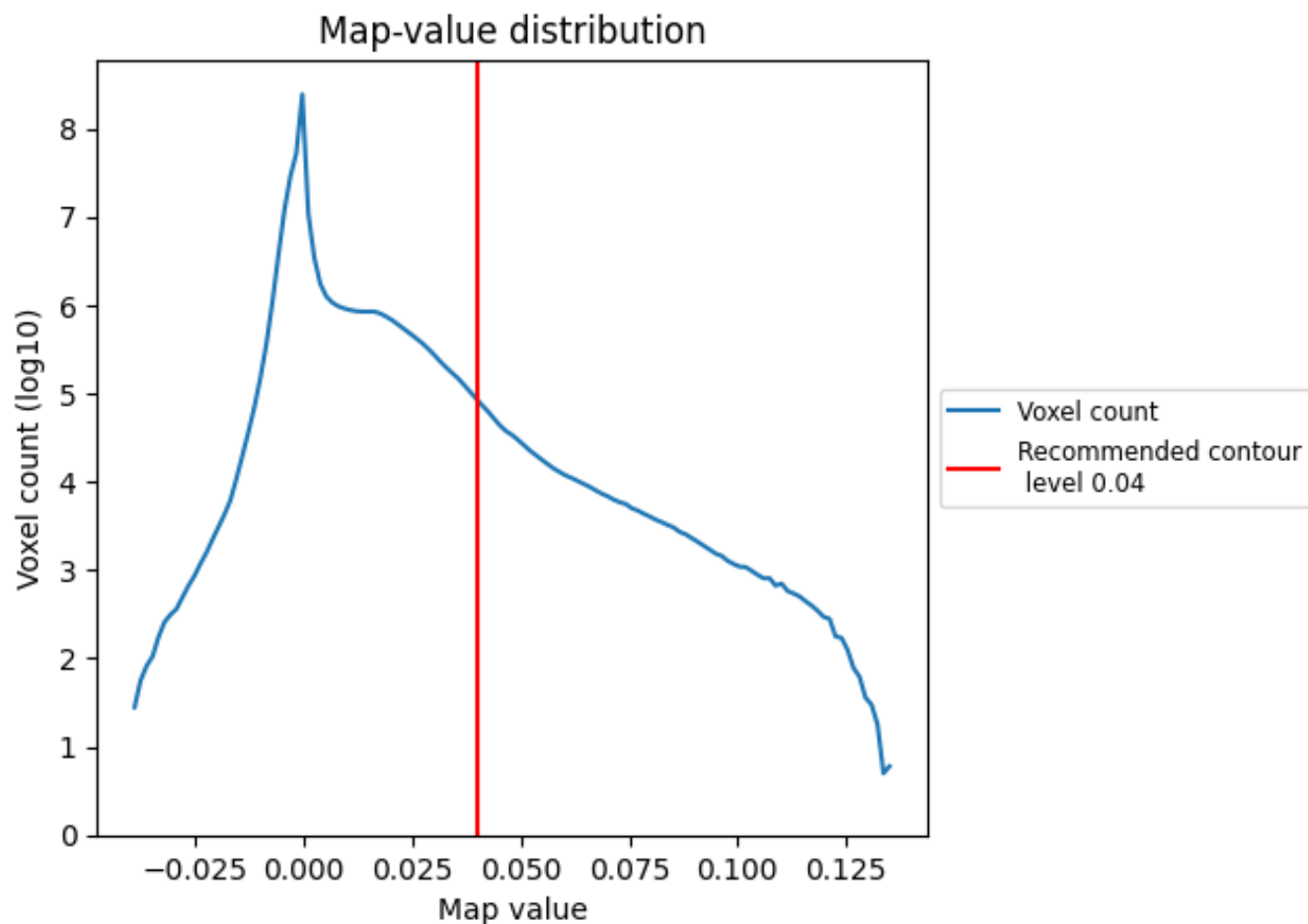
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

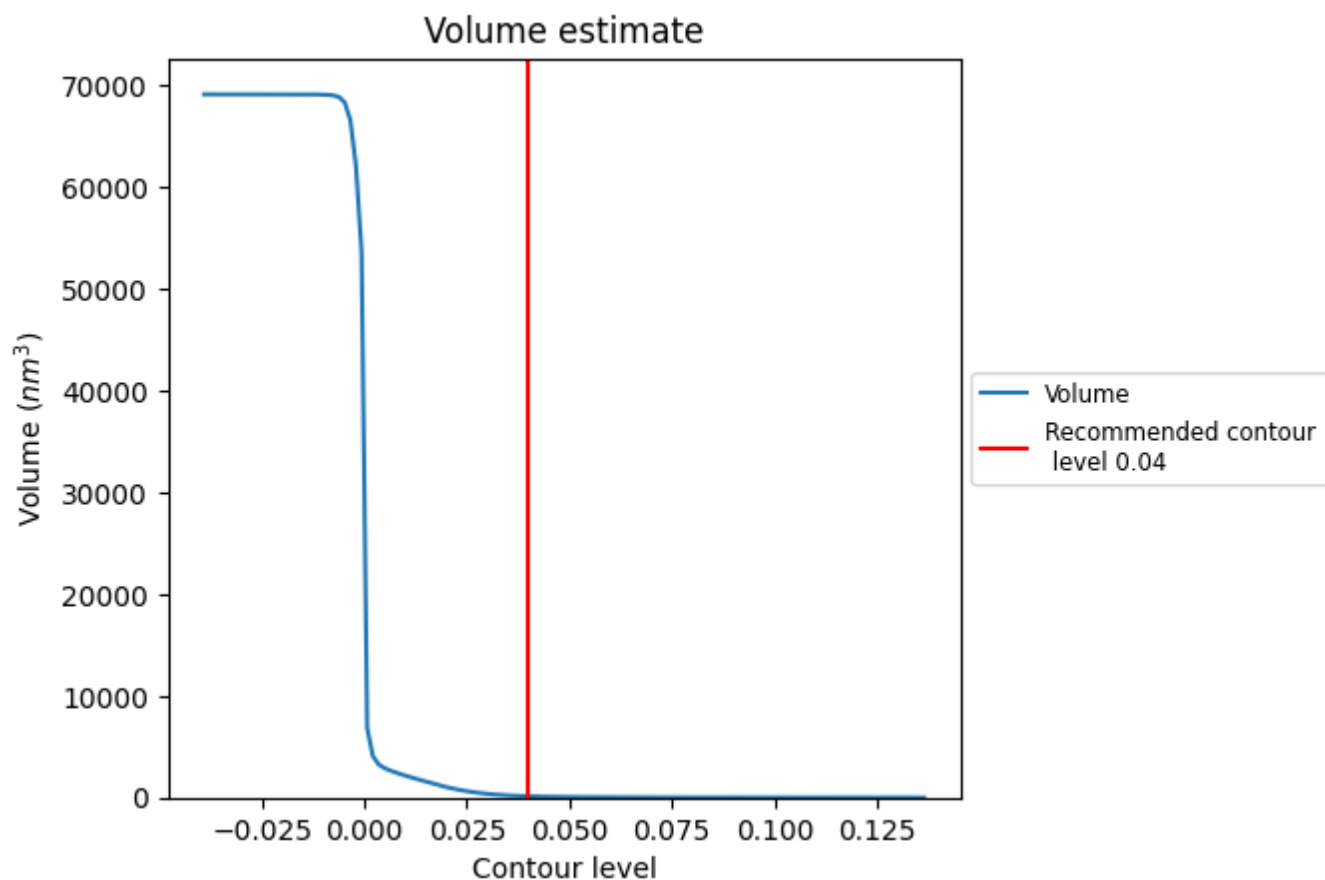
This section contains the results of statistical analysis of the map.

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.

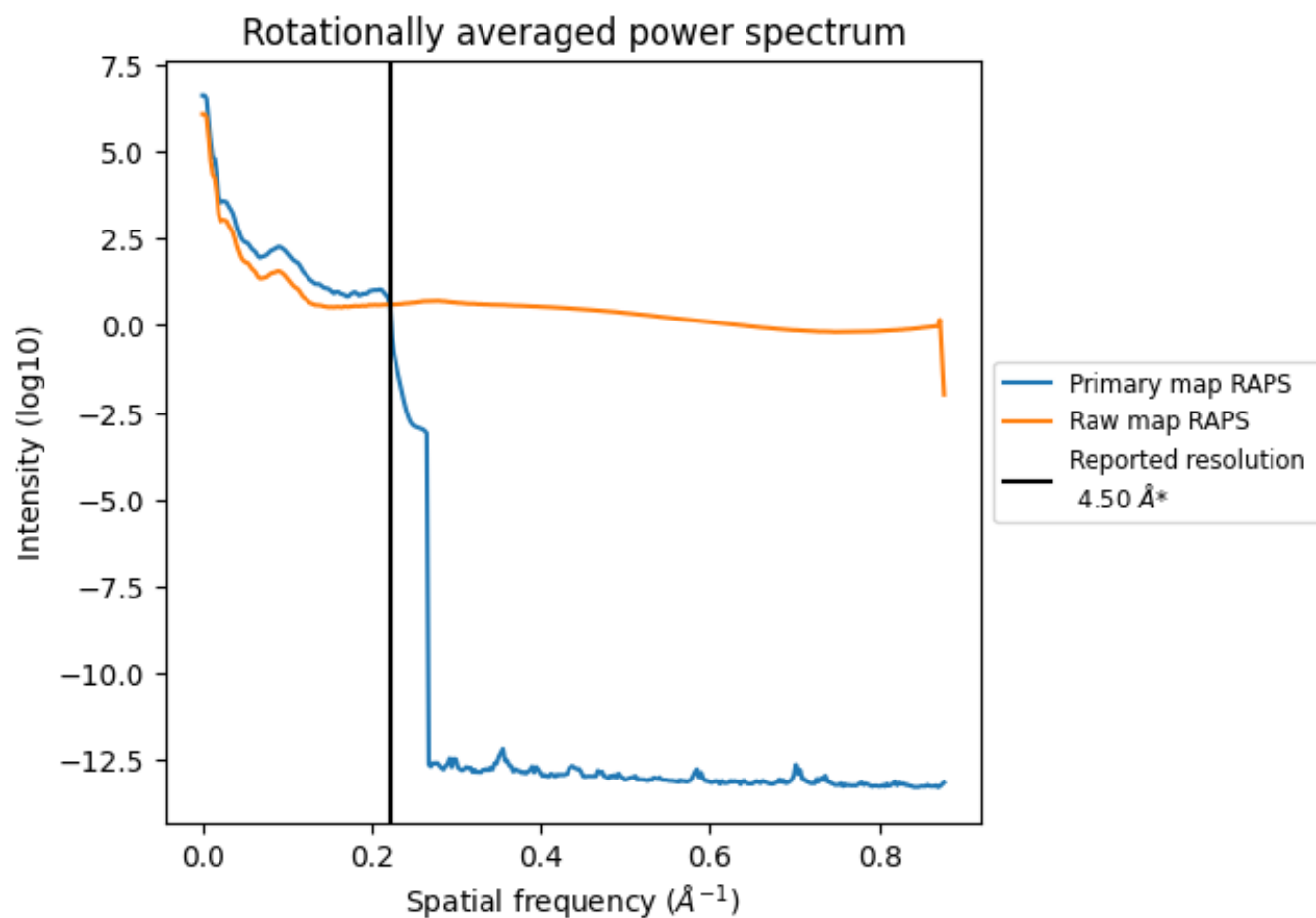
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 114 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 ⓘ

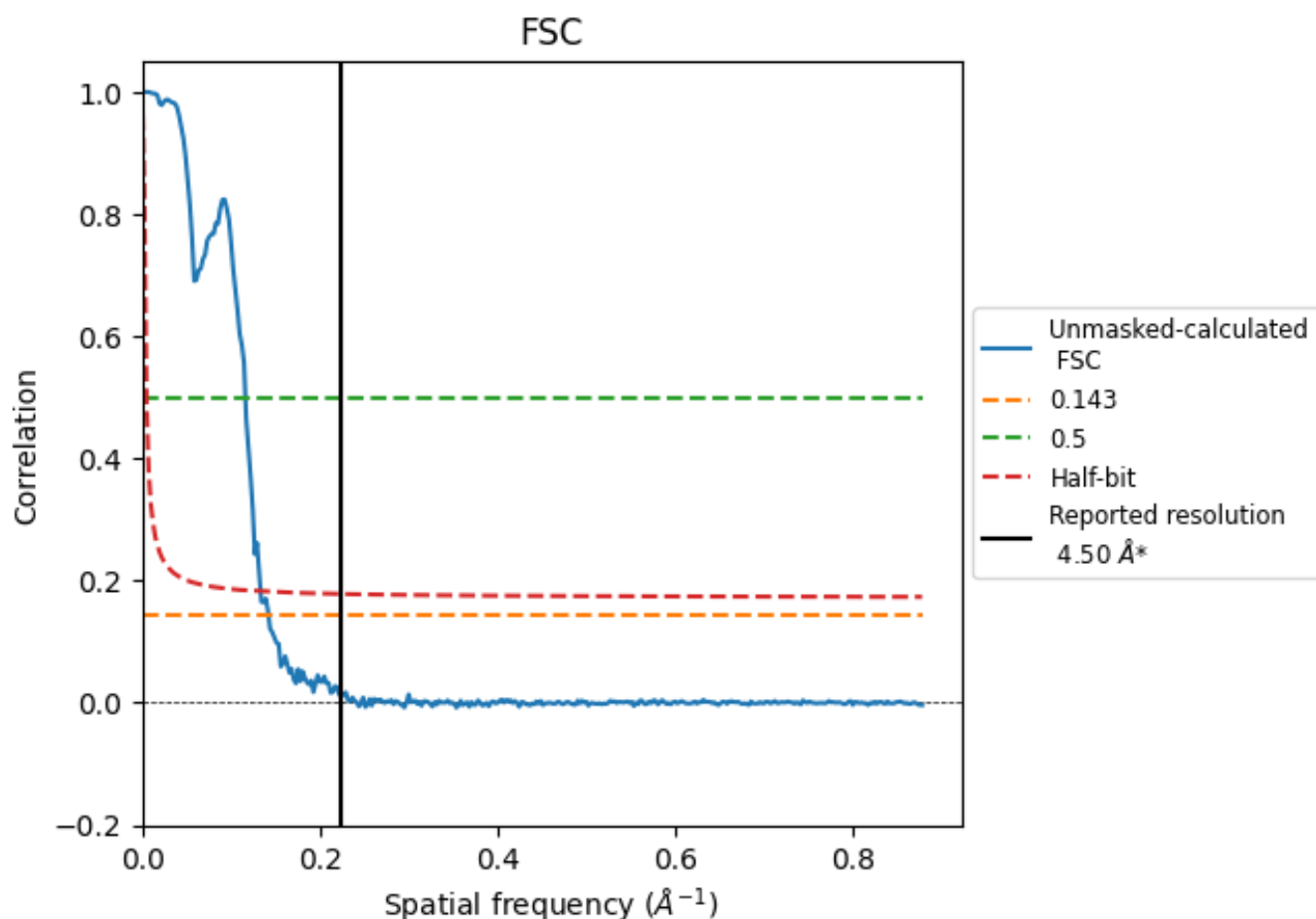


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

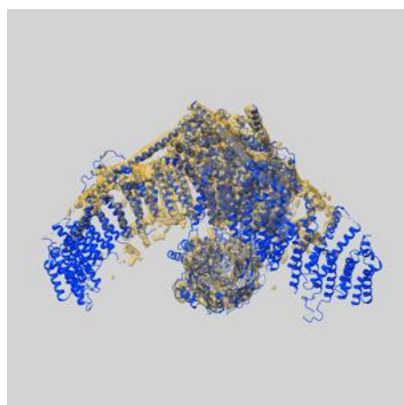
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.04	8.62	7.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.04 differs from the reported value 4.5 by more than 10 %

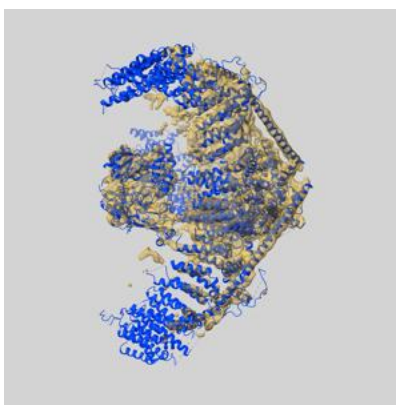
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39223 and PDB model 8YFG. Per-residue inclusion information can be found in section [3](#) on page [5](#).

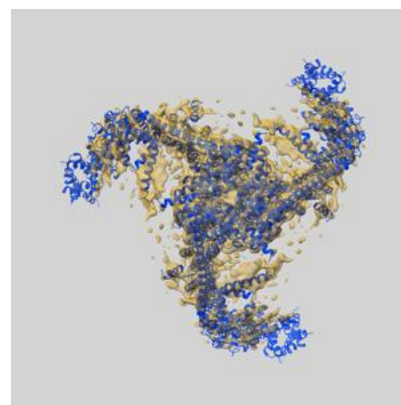
9.1 Map-model overlay [i](#)



X



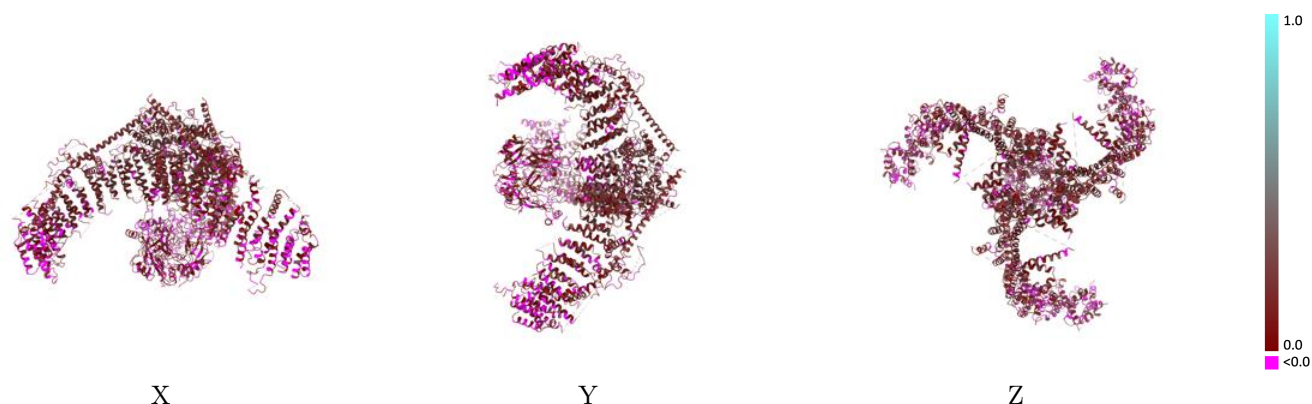
Y



Z

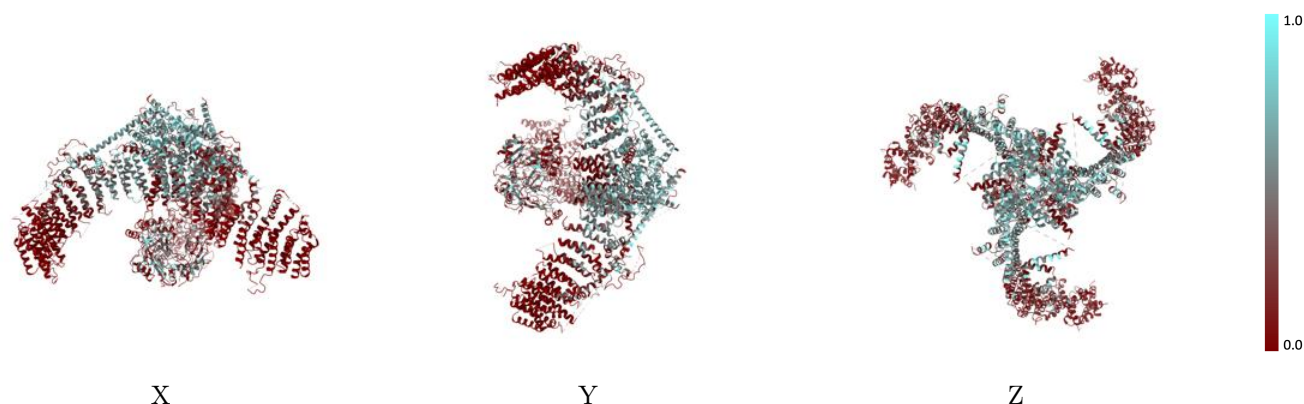
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



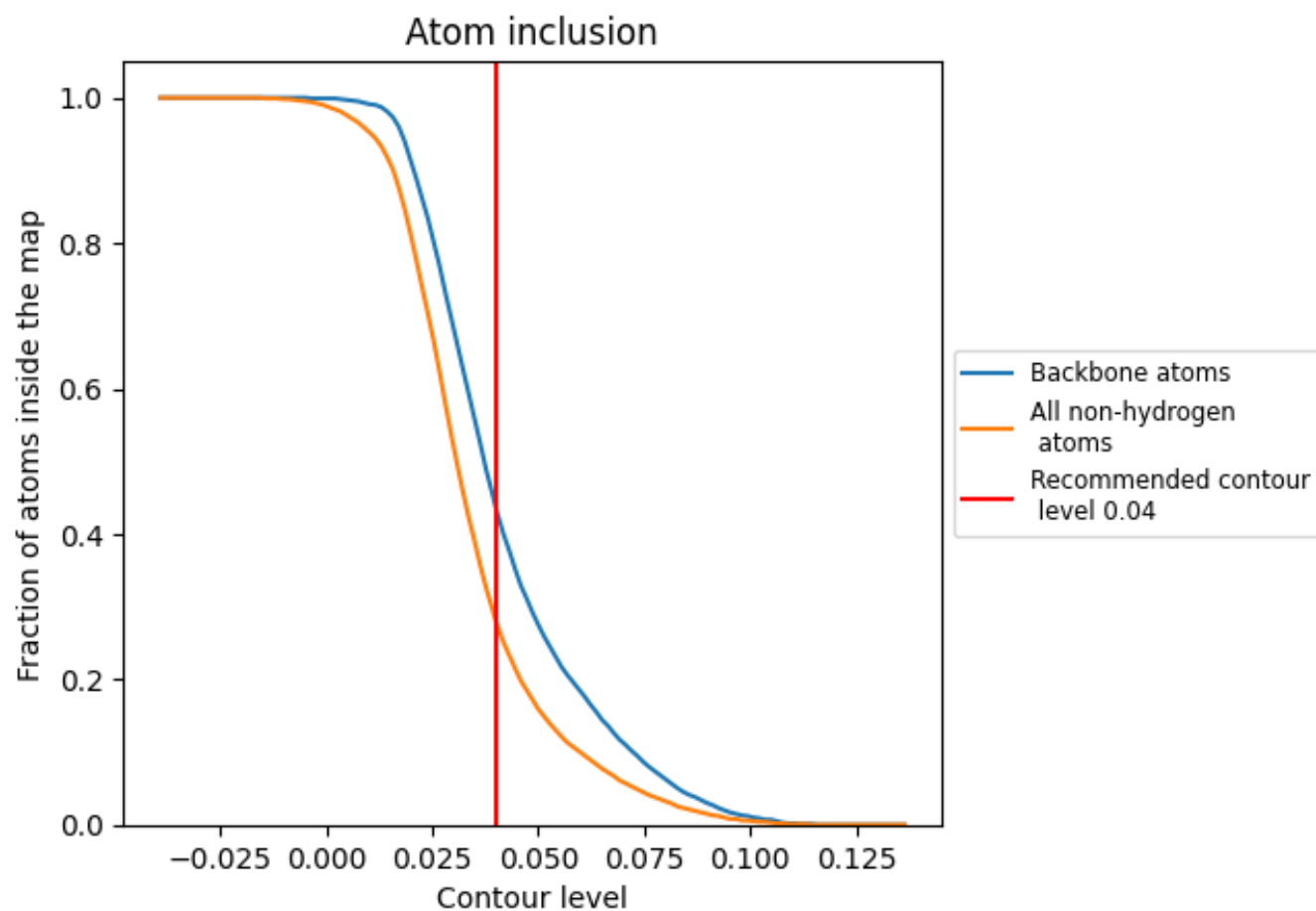
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 28% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2810	0.1280
A	0.2840	0.1280
B	0.2840	0.1290
C	0.0710	0.1130
D	0.2840	0.1290
E	0.0850	0.1200
F	0.0920	0.1240

1.0

0.0

<0.0