



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:11 PM UTC

PDB ID : 7YXX / pdb_00007yxx
EMDB ID : EMD-14368
Title : Cryo-EM structure of USP9X
Authors : Deme, J.C.; Halabelian, L.; Arrowsmith, C.H.; Lea, S.M.; Structural Genomics Consortium (SGC)
Deposited on : 2022-02-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

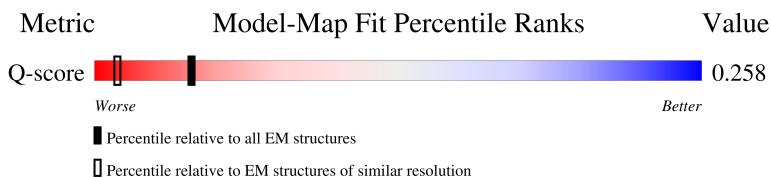
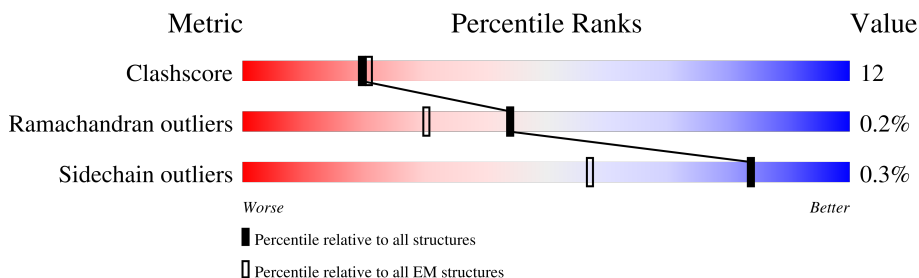
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

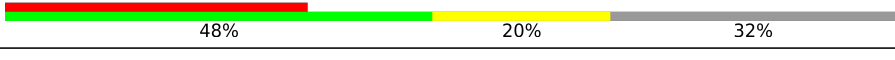
The reported resolution of this entry is 3.30 Å.

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	15087 (2.80 - 3.80)

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	2579	
1	B	2579	
1	C	2579	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 42357 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 Probable ubiquitin carboxyl-terminal hydrolase FAF-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1754	Total 14155	C 9062	N 2426	O 2571	S 96	1	0
1	B	1754	Total 14155	C 9062	N 2426	O 2571	S 96	1	0
1	C	1741	Total 14047	C 8997	N 2407	O 2547	S 96	1	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q93008
A	-16	HIS	-	expression tag	UNP Q93008
A	-15	HIS	-	expression tag	UNP Q93008
A	-14	HIS	-	expression tag	UNP Q93008
A	-13	HIS	-	expression tag	UNP Q93008
A	-12	HIS	-	expression tag	UNP Q93008
A	-11	HIS	-	expression tag	UNP Q93008
A	-10	SER	-	expression tag	UNP Q93008
A	-9	SER	-	expression tag	UNP Q93008
A	-8	GLY	-	expression tag	UNP Q93008
A	-7	ARG	-	expression tag	UNP Q93008
A	-6	GLU	-	expression tag	UNP Q93008
A	-5	ASN	-	expression tag	UNP Q93008
A	-4	LEU	-	expression tag	UNP Q93008
A	-3	TYR	-	expression tag	UNP Q93008
A	-2	PHE	-	expression tag	UNP Q93008
A	-1	GLN	-	expression tag	UNP Q93008
A	0	GLY	-	expression tag	UNP Q93008
A	2555	ASP	-	expression tag	UNP Q93008
A	2556	TYR	-	expression tag	UNP Q93008
A	2557	LYS	-	expression tag	UNP Q93008
A	2558	ASP	-	expression tag	UNP Q93008
A	2559	ASP	-	expression tag	UNP Q93008
A	2560	ASP	-	expression tag	UNP Q93008

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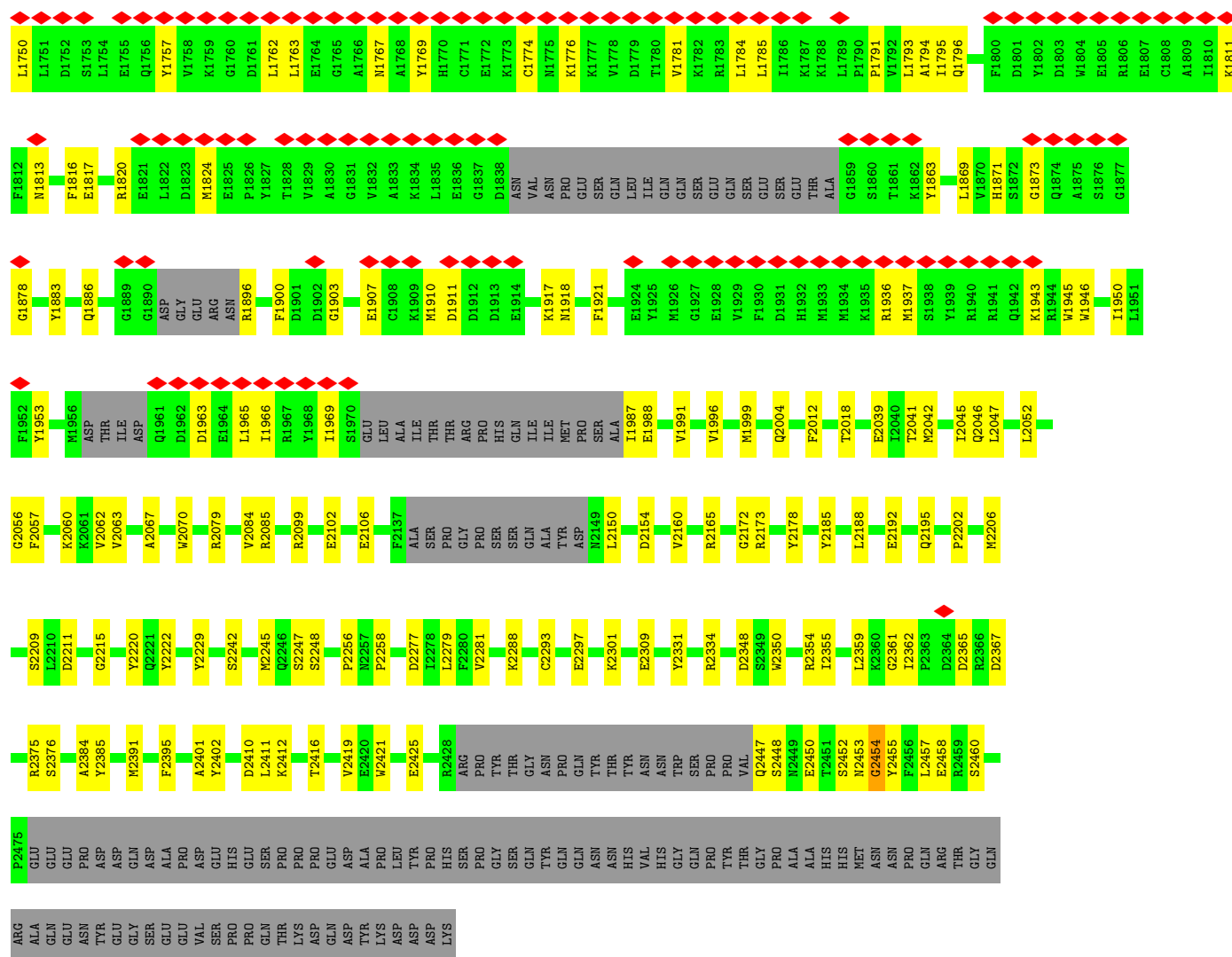
Chain	Residue	Modelled	Actual	Comment	Reference
A	2561	LYS	-	expression tag	UNP Q93008
B	-17	MET	-	initiating methionine	UNP Q93008
B	-16	HIS	-	expression tag	UNP Q93008
B	-15	HIS	-	expression tag	UNP Q93008
B	-14	HIS	-	expression tag	UNP Q93008
B	-13	HIS	-	expression tag	UNP Q93008
B	-12	HIS	-	expression tag	UNP Q93008
B	-11	HIS	-	expression tag	UNP Q93008
B	-10	SER	-	expression tag	UNP Q93008
B	-9	SER	-	expression tag	UNP Q93008
B	-8	GLY	-	expression tag	UNP Q93008
B	-7	ARG	-	expression tag	UNP Q93008
B	-6	GLU	-	expression tag	UNP Q93008
B	-5	ASN	-	expression tag	UNP Q93008
B	-4	LEU	-	expression tag	UNP Q93008
B	-3	TYR	-	expression tag	UNP Q93008
B	-2	PHE	-	expression tag	UNP Q93008
B	-1	GLN	-	expression tag	UNP Q93008
B	0	GLY	-	expression tag	UNP Q93008
B	2555	ASP	-	expression tag	UNP Q93008
B	2556	TYR	-	expression tag	UNP Q93008
B	2557	LYS	-	expression tag	UNP Q93008
B	2558	ASP	-	expression tag	UNP Q93008
B	2559	ASP	-	expression tag	UNP Q93008
B	2560	ASP	-	expression tag	UNP Q93008
B	2561	LYS	-	expression tag	UNP Q93008
C	-17	MET	-	initiating methionine	UNP Q93008
C	-16	HIS	-	expression tag	UNP Q93008
C	-15	HIS	-	expression tag	UNP Q93008
C	-14	HIS	-	expression tag	UNP Q93008
C	-13	HIS	-	expression tag	UNP Q93008
C	-12	HIS	-	expression tag	UNP Q93008
C	-11	HIS	-	expression tag	UNP Q93008
C	-10	SER	-	expression tag	UNP Q93008
C	-9	SER	-	expression tag	UNP Q93008
C	-8	GLY	-	expression tag	UNP Q93008
C	-7	ARG	-	expression tag	UNP Q93008
C	-6	GLU	-	expression tag	UNP Q93008
C	-5	ASN	-	expression tag	UNP Q93008
C	-4	LEU	-	expression tag	UNP Q93008
C	-3	TYR	-	expression tag	UNP Q93008
C	-2	PHE	-	expression tag	UNP Q93008

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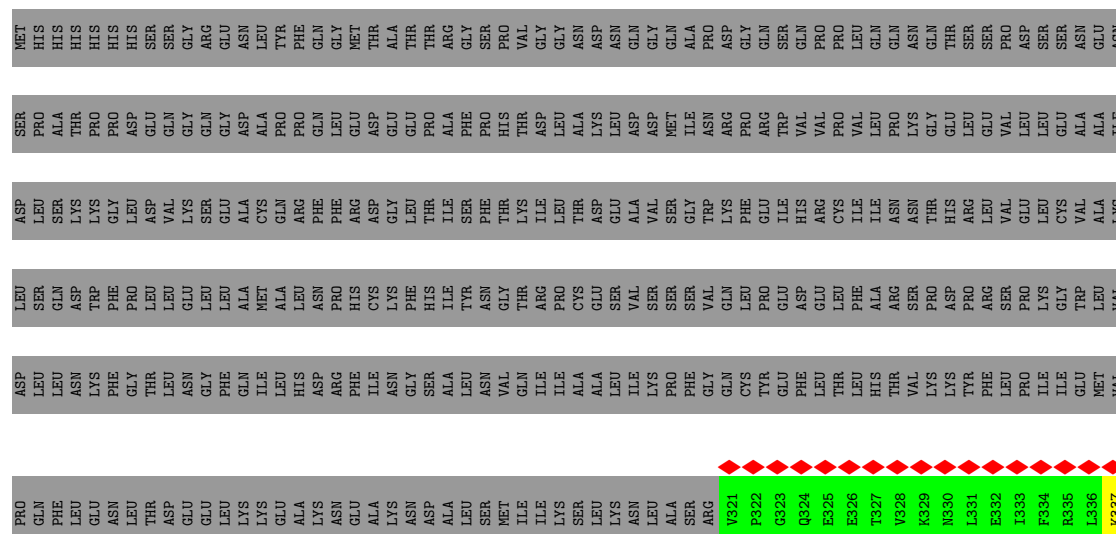
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLN	-	expression tag	UNP Q93008
C	0	GLY	-	expression tag	UNP Q93008
C	2555	ASP	-	expression tag	UNP Q93008
C	2556	TYR	-	expression tag	UNP Q93008
C	2557	LYS	-	expression tag	UNP Q93008
C	2558	ASP	-	expression tag	UNP Q93008
C	2559	ASP	-	expression tag	UNP Q93008
C	2560	ASP	-	expression tag	UNP Q93008
C	2561	LYS	-	expression tag	UNP Q93008



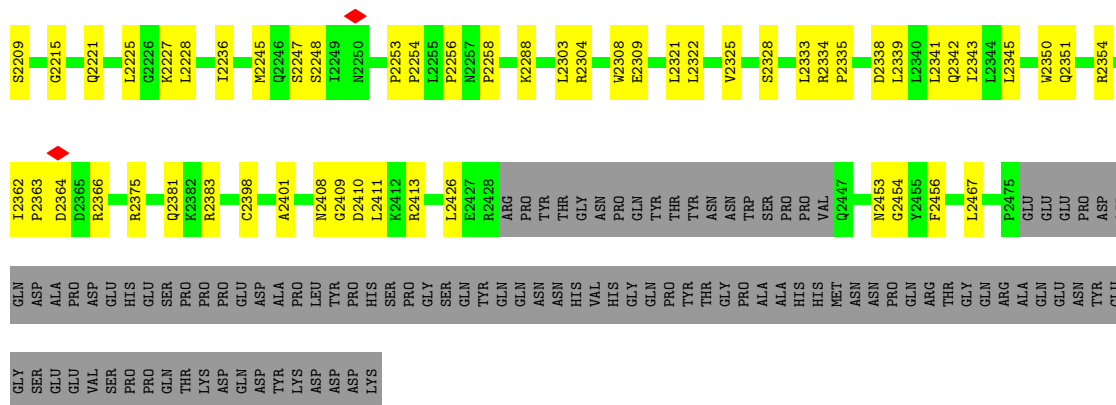


• Molecule 1: Probable ubiquitin carboxyl-terminal hydrolase FAF-X

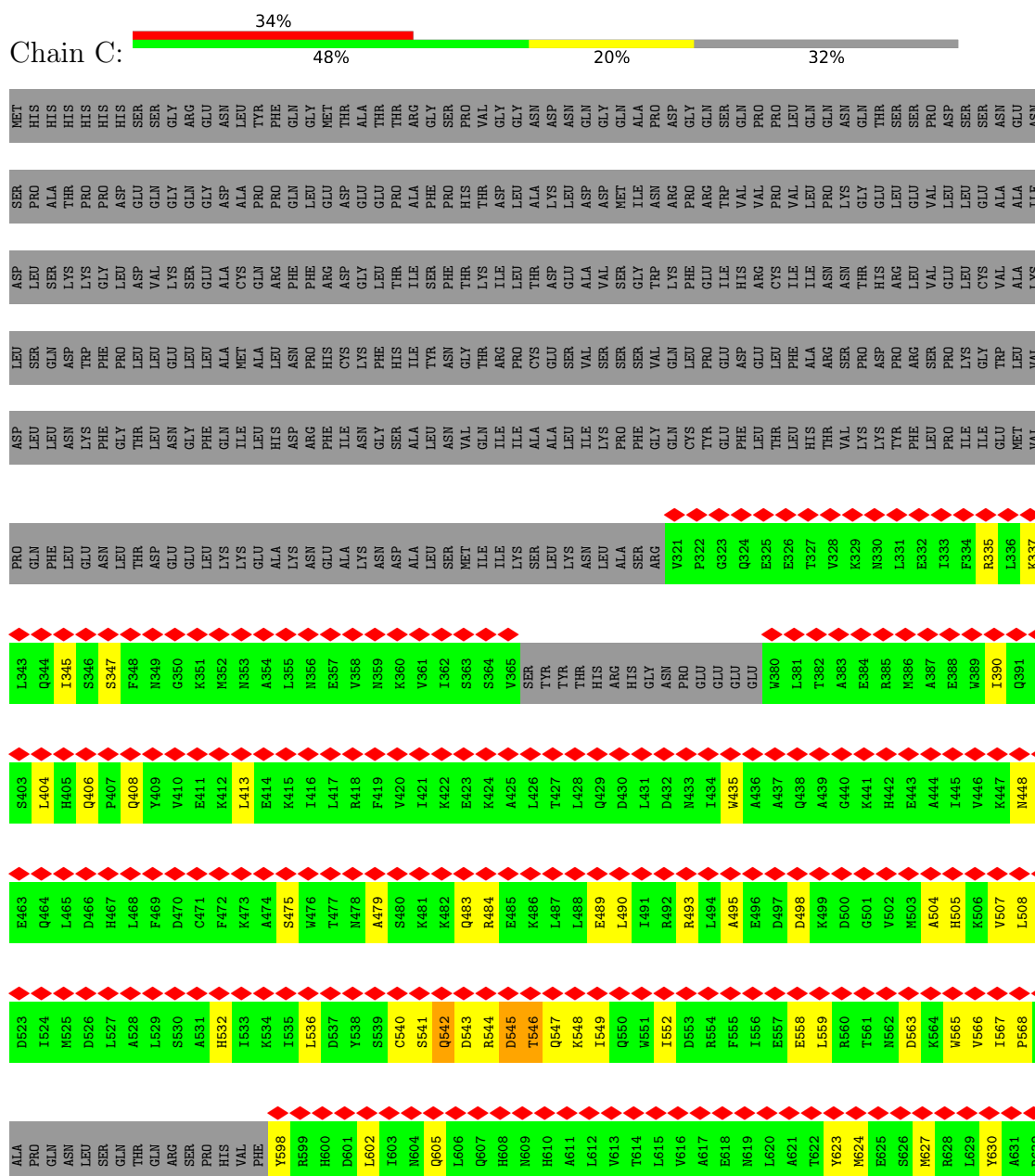


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H1064	A1065	K1066	LEU	GLY	GLU	SER	SER	SER	LEU	PRO	SER	L1076	D1077	F1080	F1081	G1082	P1083	S1084	Q1087	V1088	L1089	Y1090	L1091	T1092	E1093	K1094	V1095	Y1096	A1097	L1098	L1099	M1100	P1101	ALA	GLY	ALA	PRO	LEU	ALA	ASP	ASP	S1110	S1111	D1112	F1113	Q1114	F1115	H1116	K1119	S1120	G1121	L1123	P1124	L1125	V1126				
SER	CYS	LEU	PRO	GLY	VAL	ILE	MET	S1012	L1013	P1015	R1016	Y1017	I1018	S1019	F1020	L1021	W1022	Q1023	V1024	A1025	D1026	L1027	G1028	S1029	S1030	L1031	N1032	M1033	P1034	P1035	L1036	R1037	D1038	G1039	A1040	R1041	V1042	L1043	M1044	K1045	L1046	M1047	P1048	P1049	D1050	S1051	T1052	T1053	I1054	E1055	K1056	L1057	R1058	A1059	I1060	C1061	L1062	D1063	
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ALA	ASP	ARG	LYS	LEU	VAL	ILE	GLY	GLN	LEU	ASN	GLY	ASP	LYS	ASP	ILE	THR	ALA	LYS	LEU	TRP	ASN	THR	ASN	THR	ILE	GLY	VAL	ARG	ASP	SER	ILE	GLY	ASN	GLY	VAL	ALA	HIS	THR	LYS	ILE	GLY	LEU	PHE	VAL	GLY	GLY	GLY	ASN	PRO	GLU	ILE	ASP	PRO	GLU					
ALA	ASP	ARG	LYS	LEU	VAL	ILE	GLY	GLN	LEU	ASN	GLY	ASP	LYS	ASP	ILE	THR	ALA	LYS	LEU	TRP	ASN	THR	ASN	THR	ILE	GLY	VAL	ARG	ASP	SER	ILE	GLY	ASN	GLY	VAL	ALA	HIS	THR	LYS	ILE	GLY	LEU	PHE	VAL	GLY	GLY	GLY	ASN	PRO	GLU	ILE	ASP	PRO	GLU					
ALA	ASP	ARG	LYS	LEU	VAL	ILE	GLY	GLN	LEU	ASN	GLY	ASP	LYS	ASP	ILE	THR	ALA	LYS	LEU	TRP	ASN	THR	ASN	THR	ILE	GLY	VAL	ARG	ASP	SER	ILE	GLY	ASN	GLY	VAL	ALA	HIS	THR	LYS	ILE	GLY	LEU	PHE	VAL	GLY	GLY	GLY	ASN	PRO	GLU	ILE	ASP	PRO	GLU					
ALA	ASP	ARG	LYS	LEU	VAL	ILE	GLY	GLN	LEU	ASN	GLY	ASP	LYS	ASP	ILE	THR	ALA	LYS	LEU	TRP	ASN	THR	ASN	THR	ILE	GLY	VAL	ARG	ASP	SER	ILE	GLY	ASN	GLY</																									





• Molecule 1: Probable ubiquitin carboxyl-terminal hydrolase FAF-X



ARG	LEU	GLY	SER	ARG	TYR	SER	H650	V651	Q652	E653	V654	Q655	E656	R657	L658	N659	F660	L661	R662	F663	L664	L665	K666	D667	G668	Q669	L670	V671	L672	C673	A674	P675	Q676	A677	K678	Q679	I680	V681	K682	C683	L684	A685	E686	N687	A688	V689	Y690	L691	C692	D693	R694	E695	A696	C697	F698	K699	W700	Y701	S702		
K703	L704	M705	G706	D707	E708	P709	D710	L711	D712	P713	D714	E715	N716	K717	D718	F719	F720	E721	S722	N723	V724	L725	Q726	G668	L727	Q669	D728	P729	S730	L731	L732	T733	E734	N735	G736	M737	K738	C739	F740	E741	R742	F743	F744	K745	A746	A688	V747	N748	C749	R750	E751	G752	K753	L754	V755	A756	K757	R758	R759	Y761	M762
M763	D764	D765	L766	E767	L768	I769	G770	D771	L771	D772	Y773	L774	W775	R776	V777	V778	I779	Q780	S781	D782	D783	D784	I785	A786	S787	R788	A789	I790	D791	L792	L793	K794	E795	I796	Y797	T798	N799	L800	G801	P802	R803	L804	Q805	V806	A746	N807	Q808	V809	I810	I811	H812	E813	D814	F815	I816	Q817	S818	C819	F820	D821	R822
L823	K824	A825	S826	Y827	D828	T829	L830	C831	VAL	LEU	ASP	GLY	ASP	GLN	LYS	ASP	ASP	SER	ASN	VAL	C842	A843	R844	Q845	E846	A847	V848	R849	M850	V851	R852	V853	L854	T855	V856	L857	R858	E859	Y860	I861	N862	E863	C864	D865	S866	ASP	TYR	GLY	HIS	GLY	GLU	GLU	LEU	ASP							
GLY	LYS	HIS	ASP	ARG	SER	PHE	VAL	VAL	ARG	GLN	ASN	GLY	ASP	GLN	LYS	ASP	ASP	THR	ALA	LYS	THR	LEU	TRP	SER	HIS	THR	ASN	ASP	THR	ILE	GLY	SER	VAL	PRO	ASP	ARG	GLY	ASN	GLY	THR	LYS	ILE	GLU	THR	ASP	VAL	ASP	GLY	PRO	GLY	ASN	PRO	GLU	VAL							
PRO	ALA	ASP	GLY	ARG	LYS	LEU	ILE	GLN	ASN	LEU	LEU	LYS	ASP	GLN	LYS	ASP	ASP	THR	ALA	LYS	LEU	TRP	SER	HIS	THR	ASN	ASP	THR	ILE	GLY	SER	VAL	PRO	ASP	ARG	GLY	ASN	GLY	THR	LYS	ILE	GLU	THR	ASP	VAL	ASP	GLY	PRO	GLY	ASN	PRO	GLU	VAL								
GLU	SER	CYS	LEU	PRO	GLY	VAL	ILE	MET	S1012	L1013	H1014	P1015	R1016	Y1017	I1018	S1019	F1020	W1022	Q1023	V1024	A1025	D1026	L1027	L1031	N1032	M1033	P1034	P1035	L1036	R1037	D1038	G1039	A1040	R1041	V1042	L1043	M1044	K1045	L1046	M1047	P1048	D1050	S1051	T1052	T1053	T1054	E1055	L1056	R1058	A1059	C1060	L1062	D1063	H1064							
A1065	K1066	LEU	GLY	SER	SER	PRO	SER	L1076	D1077	S1078	L1079	F1081	G1082	P1083	S1084	A1085	S1086	Q1087	Y1090	L1091	T1092	E1093	V1094	A1095	Y1096	A1097	L1098	L1099	M1100	P1101	ALA	GLY	ALA	PRO	LEU	ALA	ASP	S1110	S1111	D1112	F1113	Q1114	F1115	H1116	L1117	L1118	K1119	S1120	G1121	G1122	L1123	P1124	L1125								
V1126	M1129	L1130	T1131	R1132	M1133	N1134	F1135	L1136	P1137	M1138	A1139	D1140	E1141	T1142	R1144	R1145	G1146	A1147	Y1148	L1149	M1150	A1151	L1152	K1153	I1154	A1155	K1156	L1157	L1158	L1159	T1160	A1161	I1162	G1163	Y1164	G1165	HIS	VAL	ARG	ALA	VAL	ALA	ALA	GLU	ALA	CYS	GLN	PRO	MET	THR	GLN										
ILE	ASN	GLN	VAL	THR	HIS	ASP	GLN	ALA	VAL	VAL	GLN	SER	ALA	GLN	ALA	GLN	SER	ILE	PRO	ASN	PRO	SER	SER	CYS	MET	LEU	ARG	ALA	GLN	ILE	ASP	GLY	ALA	ARG	Y1232	M1233	P1234	D1235	V1238	I1239	R1240	A1241	I1242	Q1243	K1244	I1245	I1246	W1247													
A1248	S1253	L1254	Q1255	L1256	V1257	P1260	N1261	E1262	E1263	I1264	T1265	Y1268	E1269	K1270	T1271	N1272	A1273	G1274	D1278	L1279	E1280	D1281	E1282	Q1283	C1286	E1287	E1290	V1291	M1292	T1293	L1294	C1295	F1296	A1297	L1298	I1299	A1302	S1307	K1308	E1309	Q1313	T1314	F1315	L1316	I1317	D1318	L1319	L1320	C1323												
H1324	S1325	K1326	T1327	V1328	R1329	Q1330	V1331	A1332	Q1333	E1334	Q1335	F1336	M1339	R1342	C1343	R1348	F1353	I1354	T1355	L1356	L1357	F1358	T1359	V1360	L1361	G1362	S1363	R1366	A1369	K1370	H1371	D1374	Y1375	F1376	T1377	L1378	L1379	R1380	H1381	L1382	L1383	A1386	Y1387	N1388	S1389	N1390	I1391	I1404	K1408												
D1412	D1413	V1414	K1415	I1426	L1427	H1430	G1432	V1433	T1434	K1435	E1436	L1437	L1438	Q1441	K1445	L1446	F1447	E1452	A1456	N1457	L1458	I1459	L1462	I1467	Y1474	M1478	ASN	GLY	GLY	LEU	PRO	ALA	GLU	GLN	ALA	I1489	P1490	V1491	I1498	N1499	A1500	G1501	F1502	ASP	VAL	ASP	ASP	ASP	MET												
L1508	N1515	V1520	D1521	S1522	L1523	T1524	E1525	M1526	Y1527	T1531	A1532	I1533	T1534	E1537	A1538	L1539	T1540	E1541	V1548	R1551	K1554	G1555	F1556	L1559	K1560	N1561	A1562	G1563	A1564	T1565	C1566	Y1567	Q1573	Q1574	I1585	I1588	E1589	G1590	T1591	G1592	SER	ASP	VAL	ASP	ASP	ASP	MET														

SER	GLN	THR	GLN	TYR	V2325	L2187	R2079	I1987	M1926	GLU	THR	ALA	L1797	C1733	G1666	SER
GLN	THR	THR	GLN	TYR	S2328	K2198	H2080	E1988	G1927	THR	ALA	GLI859	K1798	E1734	F1667	GLY
GLN	THR	TYR	GLN	TYR	V2200	L2199	V2084	R1989	E1928	GLI859	ALA	S1869	R1799	E1735	V1688	ASP
ASN	ASN	ASN	GLN	ASN	V2201	S2200	R2085	V1991	V1929	S1869		T1861	F1800	S1736	K1669	LYS
ASN	THR	THR	ASN	THR	V2202	P2202	F2088	K1993	F1930	T1861		K1862	D1801	F1737	Q1670	GLN
ASN	SER	A2203	F2088	A2089	A2203	A2203	Q1994	K1993	D1931	K1862		K1862	Y1802	T1739	F1671	ASP
HIS	PRO	M2206	A2089	H2090	M1999	M1999	M1995	K1993	H1932	K1863		R1864	D1803	T1739	R1672	ASN
VAL	PRO	L2207	H2091	M2092	M1999	M1999	M1995	K1993	H1932	K1863		R1864	D1803	T1739	L1673	GLU
GLY	VAL	V2208	M2091	M2092	M1999	M1999	M1995	K1993	H1932	K1863		R1864	D1803	T1739	V1674	ASN
GLN	GLN	S2209	L2093	M2092	M1999	M1999	M1995	K1993	H1932	K1863		R1864	D1803	T1739	G1675	VAL
PRO	GLN	L2210	L2093	M2092	M1999	M1999	M1995	K1993	H1932	K1863		R1864	D1803	T1739	E1676	ASP
TYR	ASN	D2211	E2102	R2002	R2002	R2002	E2102	K1935	R1936	V1866		V1866	E1805	M1742	P1677	PRO
THR	GLU	P2217	E2106	M2007	M2007	M2007	E2106	M1937	M1937	S1872		S1872	E1807	D1743	V1678	ARG
GLY	THR	P2217	E2106	E2008	E2008	E2008	E2106	M1937	M1937	S1872		S1872	E1807	D1743	V1678	ASP
SER	SER	P2217	E2106	E2008	E2008	E2008	E2106	M1937	M1937	S1872		S1872	E1807	D1743	V1678	VAL
ALA	ASN	L2235	K2118	Q2011	Q2011	Q2011	K2118	Y1939	Y1939	G1874		G1874	C1808	M1745	N1679	PHE
ALA	GLY	L2235	K2118	Q2011	Q2011	Q2011	K2118	Y1939	Y1939	G1874		G1874	C1808	M1745	N1679	GLY
THR	THR	L2236	F2122	F2012	F2012	F2012	F2122	A1875	A1875	A1875		A1875	I1810	H1747	R1680	TYR
HIS	PHE	R2237	F2122	M2013	M2013	M2013	F2122	S1876	S1876	S1876		S1876	K1811	Q1748	E1682	PRO
MET	LEU	N2240	D2130	K2015	K2015	K2015	D2130	G1877	G1877	G1877		G1877	F1812	M1749	Q1683	GLN
ASN	GLU	V2241	D2130	L2016	L2016	L2016	D2130	G1878	G1878	G1878		G1878	N1813	L1750	H1684	GLN
ARG	ARG	S2242	C2133	L2017	L2017	L2017	C2133	H1879	H1879	H1879		H1879	D1814	L1751	D1685	PHE
GLN	GLN	M2245	F2137	N2020	N2020	N2020	F2137	Y1880	Y1880	Y1880		Y1880	F1816	D1752	A1686	GLU
ARG	ARG	M2245	F2137	N2020	N2020	N2020	F2137	Y1880	Y1880	Y1880		Y1880	F1816	D1752	A1686	ASP
THR	THR	S2248	ALA	L2024	L2024	L2024	ALA	I1885	I1885	I1885		I1885	E1817	S1753	L1687	LYS
GLY	GLY	I2249	SER	L2024	L2024	L2024	SER	R1887	R1887	R1887		R1887	F1818	L1754	E1688	PRO
GLN	GLY	N2250	PRO	G2039	G2039	G2039	PRO	G1887	G1887	G1887		G1887	P1819	E1755	F1689	ALA
ALA	SER	D2261	SER	Q2030	Q2030	Q2030	SER	N1888	N1888	N1888		N1888	R1820	Q1756	L1693	LEU
GLU	GLU	D2271	SER	D2031	D2031	D2031	SER	G1889	G1889	G1889		G1889	E1821	Y1757	L1693	SER
ASN	ASN	I2271	GLN	H2032	H2032	H2032	GLN	G1890	G1890	G1890		G1890	L1822	Y1758	V1694	GLU
THR	ASP	D2277	ALA	L2033	L2033	L2033	ALA	ASP	ASP	ASP		ASP	D1823	K1759	D1695	ASP
GLN	GLN	D2277	TYR	A2037	A2037	A2037	TYR	GLY	GLY	GLY		GLY	M1824	G1760	A1700	GLU
ASP	ASP	F2280	ASP	E2038	E2038	E2038	ASP	GLY	GLY	GLY		GLY	E1825	D1761	L1701	ASP
ALA	ALA	R2281	ASP	M2042	M2042	M2042	ASP	ASN	ASN	ASN		ASN	P1826	L1762	L1701	LYS
ASP	ASP	T2283	D2154	M2042	M2042	M2042	D2154	ASP	ASP	ASP		ASP	Y1827	L1763	K1702	VAL
HIS	HIS	K2287	L2164	I2045	I2045	I2045	L2164	Q1961	Q1961	Q1961		Q1961	E1764	A1703	A1703	PRO
PRO	PRO	K2288	V2168	Q2046	Q2046	Q2046	V2168	D1962	D1962	D1962		D1962	G1765	L1704	E1638	PRO
GLU	GLU	I2289	G2172	A2048	A2048	A2048	G2172	D1963	D1963	D1963		D1963	G1766	G1705	Y1639	GLU
THR	THR	I2290	G2172	A2048	A2048	A2048	G2172	E1964	E1964	E1964		E1964	H1706	H1706	N1640	GLU
LYS	LYS	S2294	G2172	A2048	A2048	A2048	G2172	L1965	L1965	L1965		L1965	P1707	P1707	T1641	GLU
ASP	ASP	S2294	G2172	A2048	A2048	A2048	G2172	L1966	L1966	L1966		L1966	A1708	M1709	G1642	GLU
GLU	GLU	L2303	L2175	G2056	G2056	G2056	L2175	R1967	R1967	R1967		R1967	A1768	L1710	V1644	GLU
TYR	TYR	R2304	Q2176	F2057	F2057	F2057	Q2176	Y1968	Y1968	Y1968		Y1968	H1769	L1714	R1645	GLU
ALA	ALA	C2307	Q2177	V2062	V2062	V2062	Q2177	I1969	I1969	I1969		I1969	Y1770	G1715	H1646	GLU
PRO	PRO	C2307	N2180	V2062	V2062	V2062	N2180	GLU	GLU	GLU		GLU	S1717	G1716	Q1648	GLU
LEU	LEU	V2308	V2183	V2063	V2063	V2063	V2183	LEU	LEU	LEU		LEU	F1718	F1718	H1653	GLU
THR	THR	E2309	M2184	R2064	R2064	R2064	M2184	ALA	ALA	ALA		ALA	A1719	A1719	S1657	GLU
THR	THR	L2322	T2194	A2067	A2067	A2067	T2194	ILE	ILE	ILE		ILE	D1720	D1720	R1658	GLU
GLY	GLY	W2323	Q2195	A2067	A2067	A2067	Q2195	THR	THR	THR		THR	K1721	K1721	L1659	GLU
ASN	ASN	Q2324	L2196	W2070	W2070	W2070	L2196	ARG	ARG	ARG		ARG	V1778	V1778	Q1660	GLU
GLY	GLY							PRO	PRO	PRO		PRO	D1779	D1779	V1663	GLU
								HIS	HIS	HIS		HIS	T1780	T1780	P1664	GLU
								GLN	GLN	GLN		GLN	I1723	I1723	R1665	GLU
								ILE	ILE	ILE		ILE	C1724	C1724		GLU
								GLN	GLN	GLN		GLN	Q1725	Q1725		GLU
								GLN	GLN	GLN		GLN	G1726	G1726		GLU
								SER	SER	SER		SER	C1727	C1727		GLU
								GLU	GLU	GLU		GLU	P1728	P1728		GLU
								PRO	PRO	PRO		PRO	L1785	L1785		GLU
								GLU	GLU	GLU		GLU	I1786	I1786		GLU
								GLU	GLU	GLU		GLU	K1787	K1787		GLU
								GLU	GLU	GLU		GLU	K1788	K1788		GLU
								GLU	GLU	GLU		GLU	L1789	L1789		GLU
								GLU	GLU	GLU		GLU	L1793	L1793		GLU
								GLU	GLU	GLU		GLU	A1794	A1794		GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.330	Depositor
Minimum map value	-0.608	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.221	Depositor
Map size (Å)	372.73602, 372.73602, 372.73602	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/14461	0.35	3/19559 (0.0%)
1	B	0.16	0/14461	0.39	0/19559
1	C	0.16	0/14351	0.38	2/19411 (0.0%)
All	All	0.16	0/43273	0.37	5/58529 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2402	TYR	N-CA-C	-6.54	107.17	114.62
1	C	2404	ILE	N-CA-C	-5.41	107.16	111.81
1	C	1902	ASP	CB-CA-C	-5.36	110.37	116.54
1	A	1258	PHE	CA-C-N	5.09	131.86	121.48
1	A	1258	PHE	C-N-CA	5.09	131.86	121.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14155	0	14051	346	0
1	B	14155	0	14051	350	0
1	C	14047	0	13957	366	0
All	All	42357	0	42059	1054	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 12.

All (1054) 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:C:2413:ARG:O	1:C:2416:THR:HG22	1.31	1.24
1:C:1521:ASP:O	1:C:1524:THR:HG22	1.38	1.20
1:B:540:CYS:HB2	1:B:544:ARG:HA	1.29	1.07
1:C:1789:LEU:HB3	1:C:1863:TYR:OH	1.58	1.02
1:A:1265:THR:HA	1:A:1268:TYR:CD2	2.02	0.95
1:A:1264:ILE:HG22	1:A:1268:TYR:CZ	2.04	0.92
1:A:1265:THR:HA	1:A:1268:TYR:HD2	1.34	0.88
1:A:1264:ILE:HG22	1:A:1268:TYR:OH	1.73	0.87
1:C:2416:THR:HG23	1:C:2417:TRP:N	1.93	0.83
1:A:545:ASP:HB2	1:A:580:PHE:HE1	1.41	0.83
1:C:1248:ALA:HB1	1:C:1254:LEU:HA	1.62	0.81
1:A:1320:LEU:HD11	1:A:1333:GLN:HB3	1.62	0.80
1:A:406:GLN:HE21	1:A:408:GLN:HE22	1.31	0.79
1:A:846:GLU:HA	1:A:849:ARG:HD3	1.65	0.78
1:C:2049:ALA:HB1	1:C:2092:VAL:HG11	1.64	0.78
1:B:1653:HIS:HD2	1:B:1991:VAL:HG22	1.49	0.77
1:C:1376:PHE:HB3	1:C:1380:ARG:HH12	1.46	0.77
1:A:721:GLU:HA	1:A:725:LEU:HD12	1.66	0.77
1:C:2413:ARG:O	1:C:2416:THR:CG2	2.25	0.76
1:C:543:ASP:HB3	1:C:547:GLN:NE2	2.00	0.76
1:B:1368:ARG:HB3	1:B:1371:HIS:HB3	1.66	0.76
1:C:1041:ARG:HA	1:C:1044:MET:HE3	1.67	0.75
1:A:1333:GLN:HG2	1:A:1374:ASP:HB3	1.67	0.75
1:B:1917:LYS:HA	1:B:1921:PHE:HB2	1.66	0.75
1:B:557:GLU:HA	1:B:560:ARG:HD3	1.69	0.75
1:A:1811:LYS:NZ	1:A:1945:TRP:O	2.20	0.75
1:A:607:GLN:HA	1:A:611:ALA:HA	1.69	0.74
1:B:540:CYS:HB2	1:B:544:ARG:CA	2.12	0.74
1:C:406:GLN:HE21	1:C:408:GLN:HE22	1.33	0.74
1:A:1446:LYS:O	1:A:1515:ASN:ND2	2.20	0.74
1:C:2416:THR:HG23	1:C:2417:TRP:H	1.50	0.73
1:C:1033:MET:HG3	1:C:1035:PRO:HD2	1.69	0.73
1:B:2304:ARG:NH2	1:B:2342:GLN:OE1	2.21	0.73
1:C:858:ARG:HH22	1:C:1039:GLY:HA2	1.52	0.73
1:B:1444:GLU:O	1:B:1448:HIS:N	2.20	0.73
1:B:858:ARG:HH22	1:B:1039:GLY:HA2	1.54	0.72
1:A:545:ASP:HB2	1:A:580:PHE:CE1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:LEU:HD11	1:A:1526:MET:HA	1.70	0.72
1:B:1820:ARG:NH2	1:B:1911:ASP:O	2.22	0.72
1:B:1379:LEU:HD22	1:B:1433:VAL:HG22	1.71	0.71
1:B:1577:MET:HG3	1:B:1884:ILE:HG21	1.71	0.71
1:B:2007:MET:SD	1:B:2011:GLN:NE2	2.64	0.71
1:B:406:GLN:HE21	1:B:408:GLN:HE22	1.37	0.70
1:B:546:THR:HG23	1:B:547:GLN:OE1	1.91	0.70
1:C:729:PRO:HG3	1:C:776:ARG:HG3	1.72	0.70
1:C:1556:PHE:HB3	1:C:1905:VAL:HG11	1.73	0.70
1:A:547:GLN:HB2	1:A:551:TRP:CD1	2.25	0.70
1:B:1286:CYS:HB2	1:B:1331:VAL:HG11	1.74	0.70
1:B:1380:ARG:HH22	1:B:1428:GLU:HG3	1.57	0.70
1:C:630:TYR:HD2	1:C:634:HIS:HB2	1.57	0.70
1:C:1863:TYR:HB3	1:C:1953:TYR:HB3	1.74	0.70
1:B:1333:GLN:HE22	1:B:1377:THR:HB	1.57	0.70
1:A:1326:LYS:HG3	1:A:1329:ARG:HH12	1.57	0.69
1:B:2334:ARG:NH1	1:B:2338:ASP:OD1	2.25	0.69
1:A:2453:ASN:ND2	1:A:2458:GLU:OE2	2.26	0.69
1:B:547:GLN:CD	1:B:547:GLN:H	2.01	0.69
1:B:2209:SER:O	1:B:2288:LYS:NZ	2.23	0.69
1:C:624:MET:HE1	1:C:684:LEU:HG	1.74	0.69
1:A:1863:TYR:HB3	1:A:1953:TYR:HB3	1.74	0.69
1:B:543:ASP:O	1:B:546:THR:N	2.23	0.69
1:C:2030:GLN:NE2	1:C:2032:HIS:O	2.25	0.68
1:B:1707:PRO:HB3	1:B:1969:ILE:HD12	1.74	0.68
1:A:2211:ASP:OD2	1:C:2250:ASN:ND2	2.27	0.68
1:A:1264:ILE:CG2	1:A:1268:TYR:OH	2.40	0.68
1:B:536:LEU:HD23	1:B:546:THR:HG21	1.74	0.68
1:A:779:ILE:O	1:A:849:ARG:NH1	2.27	0.67
1:C:1244:LYS:HG3	1:C:1261:ASN:HD21	1.59	0.67
1:B:845:GLN:OE1	1:B:849:ARG:NH1	2.28	0.67
1:B:1811:LYS:NZ	1:B:1945:TRP:O	2.28	0.67
1:C:1446:LYS:O	1:C:1515:ASN:ND2	2.28	0.67
1:B:1333:GLN:HG3	1:B:1378:LEU:HG	1.77	0.67
1:B:540:CYS:CB	1:B:544:ARG:O	2.43	0.67
1:C:1377:THR:HG22	1:C:1381:HIS:NE2	2.09	0.67
1:C:1326:LYS:HG3	1:C:1329:ARG:HH22	1.60	0.66
1:C:2118:LYS:HG2	1:C:2184:MET:HE1	1.77	0.66
1:A:737:MET:HE3	1:A:785:ILE:HD12	1.77	0.66
1:C:489:GLU:OE2	1:C:493:ARG:NH1	2.28	0.66
1:C:1524:THR:CG2	1:C:1525:GLU:OE1	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1863:TYR:HB3	1:B:1953:TYR:HB3	1.78	0.66
1:C:1459:ILE:HG22	1:C:1508:LEU:HD13	1.76	0.66
1:A:2102:GLU:HA	1:A:2106:GLU:HB2	1.78	0.66
1:B:2007:MET:O	1:B:2011:GLN:NE2	2.28	0.66
1:C:2090:HIS:NE2	1:C:2133:CYS:SG	2.66	0.66
1:A:1037:ARG:NH1	1:A:1142:GLU:OE2	2.28	0.66
1:A:2067:ALA:HA	1:A:2070:TRP:HD1	1.61	0.66
1:A:2447:GLN:N	1:A:2458:GLU:OE1	2.28	0.66
1:A:1520:VAL:HG22	1:A:2047:LEU:HD13	1.78	0.66
1:C:1917:LYS:HA	1:C:1921:PHE:HB2	1.77	0.66
1:C:2202:PRO:O	1:C:2206:MET:HG3	1.95	0.66
1:C:2416:THR:CG2	1:C:2417:TRP:N	2.59	0.66
1:B:1321:LEU:HB3	1:B:1368:ARG:HG3	1.77	0.66
1:C:2089:ALA:HA	1:C:2093:LEU:HD12	1.78	0.66
1:C:1144:ARG:HG2	1:C:1145:ARG:HH22	1.61	0.66
1:A:1099:LEU:HD13	1:A:1157:LEU:HD11	1.78	0.66
1:B:1464:ASP:O	1:B:1472:ASN:ND2	2.29	0.66
1:B:1145:ARG:HG2	1:B:1254:LEU:HD13	1.78	0.65
1:B:540:CYS:HB3	1:B:544:ARG:O	1.96	0.65
1:A:1099:LEU:HD22	1:A:1114:GLN:HG3	1.77	0.65
1:C:2416:THR:CG2	1:C:2417:TRP:H	2.08	0.65
1:A:543:ASP:HB2	1:A:547:GLN:HE22	1.62	0.65
1:A:545:ASP:O	1:A:548:LYS:HB2	1.96	0.65
1:C:390:ILE:HG23	1:C:395:ILE:HB	1.78	0.64
1:C:1357:LEU:HB3	1:C:1375:TYR:OH	1.97	0.64
1:C:1037:ARG:NH1	1:C:1142:GLU:OE2	2.30	0.64
1:C:2304:ARG:HD3	1:C:2342:GLN:HB3	1.79	0.64
1:A:762:MET:SD	1:A:763:MET:N	2.71	0.64
1:A:1452:GLU:O	1:A:1457:ASN:ND2	2.29	0.64
1:A:1918:ASN:O	1:A:1946:TRP:NE1	2.30	0.64
1:A:2242:SER:HA	1:A:2245:MET:HE2	1.79	0.64
1:B:532:HIS:NE2	1:B:536:LEU:HD11	2.13	0.64
1:B:2118:LYS:HG2	1:B:2184:MET:HE1	1.80	0.64
1:A:858:ARG:HH22	1:A:1039:GLY:HA2	1.63	0.64
1:B:543:ASP:OD2	1:B:547:GLN:CD	2.41	0.63
1:B:2343:ILE:HG22	1:B:2354:ARG:HD3	1.79	0.63
1:A:1264:ILE:O	1:A:1268:TYR:CD2	2.51	0.63
1:B:737:MET:HE3	1:B:785:ILE:HD12	1.80	0.63
1:C:1588:ILE:HG21	1:C:1644:LEU:HD21	1.79	0.63
1:A:763:MET:HE1	1:A:804:LEU:HD22	1.79	0.63
1:B:543:ASP:CG	1:B:546:THR:HA	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1057:LEU:HD13	1:C:1079:LEU:HD13	1.80	0.63
1:C:2102:GLU:HA	1:C:2106:GLU:HB2	1.80	0.63
1:B:702:SER:O	1:B:742:ARG:NH1	2.31	0.63
1:C:567:ILE:HG13	1:C:653:GLU:HG2	1.79	0.63
1:C:780:GLN:OE1	1:C:849:ARG:NH2	2.27	0.63
1:A:1283:GLN:O	1:A:1286:CYS:N	2.31	0.63
1:A:2359:LEU:HD22	1:A:2391:MET:HE2	1.80	0.63
1:C:1687:LEU:HD11	1:C:1739:THR:HG21	1.81	0.63
1:C:2209:SER:O	1:C:2288:LYS:NZ	2.30	0.63
1:A:1917:LYS:HA	1:A:1921:PHE:HB2	1.81	0.63
1:C:1099:LEU:HD22	1:C:1114:GLN:HG3	1.82	0.62
1:C:1099:LEU:HD13	1:C:1157:LEU:HD11	1.81	0.62
1:C:1873:GLY:HA3	1:C:1878:GLY:HA2	1.81	0.62
1:A:662:ARG:HB2	1:A:700:TRP:HE1	1.64	0.62
1:B:536:LEU:HD13	1:B:548:LYS:HE3	1.80	0.62
1:A:1245:ILE:HD13	1:A:1257:VAL:HG21	1.82	0.62
1:B:2045:ILE:HG21	1:B:2084:VAL:HG13	1.82	0.62
1:A:1543:GLU:HB3	1:A:2060:LYS:HG2	1.82	0.62
1:C:1863:TYR:HE1	1:C:1955:ARG:HD3	1.64	0.62
1:A:1557:VAL:HB	1:A:1654:LEU:HG	1.81	0.61
1:A:609:ASN:OD1	1:A:610:HIS:ND1	2.32	0.61
1:A:764:ASP:HB2	1:A:803:ARG:HH21	1.65	0.61
1:B:805:GLN:O	1:B:808:GLN:NE2	2.33	0.61
1:A:2041:THR:HG22	1:A:2084:VAL:HG21	1.83	0.61
1:C:800:LEU:HD11	1:C:808:GLN:HG3	1.82	0.61
1:A:780:GLN:OE1	1:A:849:ARG:NH2	2.29	0.61
1:B:548:LYS:HZ3	1:B:580:PHE:HB2	1.65	0.61
1:B:1560:LYS:O	1:B:1569:ASN:ND2	2.32	0.61
1:A:1824:MET:HG3	1:A:1863:TYR:CE2	2.35	0.61
1:C:1363:SER:O	1:C:1366:ARG:N	2.30	0.61
1:C:1441:GLN:HB3	1:C:1445:LYS:HB2	1.82	0.61
1:B:1414:VAL:HG21	1:B:1491:VAL:HG22	1.83	0.61
1:A:418:ARG:NH1	1:A:459:ASP:OD2	2.33	0.61
1:B:1443:SER:O	1:B:1514:ARG:NH2	2.34	0.61
1:A:540:CYS:HA	1:A:544:ARG:HG3	1.83	0.61
1:A:1156:LYS:HE3	1:A:1287:GLU:HB2	1.83	0.61
1:B:2245:MET:HE1	1:B:2308:TRP:HD1	1.66	0.61
1:A:1467:ILE:HG21	1:A:1502:PHE:CE1	2.36	0.60
1:B:545:ASP:HB2	1:B:580:PHE:CD1	2.36	0.60
1:A:802:PRO:O	1:A:803:ARG:HD3	2.02	0.60
1:B:2168:VAL:HG13	1:B:2175:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:LYS:HG3	1:A:580:PHE:CG	2.36	0.60
1:B:1124:PRO:HG3	1:B:1233:MET:HE1	1.83	0.60
1:C:662:ARG:NH2	1:C:665:LEU:O	2.32	0.60
1:A:1824:MET:HG3	1:A:1863:TYR:HE2	1.66	0.60
1:C:1356:LEU:O	1:C:1359:THR:HB	2.01	0.60
1:A:523:ASP:OD1	1:A:524:ILE:HD12	2.01	0.60
1:A:2297:GLU:HG3	1:A:2301:LYS:HE3	1.84	0.60
1:A:2375:ARG:NH1	1:C:2364:ASP:OD2	2.35	0.60
1:B:545:ASP:HB2	1:B:580:PHE:HD1	1.67	0.60
1:B:1159:LEU:HA	1:B:1162:ILE:HG22	1.84	0.60
1:C:2406:GLN:OE1	1:C:2412:LYS:NZ	2.34	0.60
1:A:2209:SER:O	1:A:2288:LYS:NZ	2.33	0.60
1:B:542:GLN:H	1:B:542:GLN:CD	2.09	0.60
1:B:2013:MET:HE1	1:B:2047:LEU:HG	1.84	0.60
1:C:695:GLU:OE1	1:C:735:ASN:ND2	2.33	0.59
1:A:1264:ILE:O	1:A:1268:TYR:CE2	2.55	0.59
1:B:1333:GLN:NE2	1:B:1377:THR:HB	2.16	0.59
1:C:1701:LEU:O	1:C:1706:HIS:N	2.34	0.59
1:C:1999:MET:SD	1:C:2002:ARG:NH1	2.62	0.59
1:A:2355:ILE:HD13	1:A:2401:ALA:HB2	1.84	0.59
1:B:390:ILE:HG23	1:B:395:ILE:HB	1.83	0.59
1:C:1361:LEU:C	1:C:1363:SER:H	2.09	0.59
1:A:547:GLN:HB2	1:A:551:TRP:NE1	2.16	0.59
1:B:1885:ILE:O	1:B:1887:ARG:NH1	2.35	0.59
1:C:1707:PRO:HB3	1:C:1969:ILE:HD12	1.83	0.59
1:B:1498:ILE:HD12	1:B:2003:MET:HE1	1.83	0.59
1:C:1336:PHE:HA	1:C:1339:MET:HE2	1.83	0.59
1:C:1694:VAL:HA	1:C:1710:LEU:HD22	1.82	0.59
1:B:493:ARG:NH2	1:B:496:GLU:OE1	2.36	0.59
1:C:1333:GLN:HG3	1:C:1378:LEU:HD12	1.84	0.59
1:A:802:PRO:C	1:A:803:ARG:HD3	2.28	0.59
1:B:577:CYS:O	1:B:599:ARG:NE	2.35	0.59
1:C:741:GLU:HG2	1:C:792:LEU:HD11	1.84	0.58
1:C:1123:LEU:HD21	1:C:1234:PRO:HD3	1.83	0.58
1:B:2183:VAL:HG21	1:B:2227:LYS:HD2	1.85	0.58
1:B:2325:VAL:HA	1:B:2333:LEU:HD11	1.84	0.58
1:A:509:ASN:O	1:A:513:ASN:ND2	2.36	0.58
1:A:1123:LEU:HD23	1:A:1124:PRO:HD3	1.84	0.58
1:A:1592:GLY:HA2	1:A:1645:ARG:HD3	1.84	0.58
1:A:544:ARG:O	1:A:547:GLN:HG2	2.03	0.58
1:A:672:LEU:HB3	1:A:711:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG23	1:A:395:ILE:HB	1.84	0.58
1:B:543:ASP:OD2	1:B:547:GLN:N	2.37	0.58
1:B:1326:LYS:HG3	1:B:1329:ARG:HH22	1.68	0.58
1:B:541:SER:CA	1:B:544:ARG:HH21	2.16	0.58
1:B:1318:ASP:HA	1:B:1322:HIS:HB2	1.85	0.58
1:B:2351:GLN:NE2	1:B:2398:CYS:SG	2.77	0.58
1:B:1334:GLU:HA	1:B:1337:PHE:HD2	1.68	0.57
1:B:1437:LEU:HD12	1:B:1440:PHE:HD2	1.69	0.57
1:B:567:ILE:HG22	1:B:571:LYS:NZ	2.19	0.57
1:B:1323:CYS:O	1:B:1371:HIS:NE2	2.25	0.57
1:C:1653:HIS:CD2	1:C:1991:VAL:HG22	2.39	0.57
1:A:1824:MET:CG	1:A:1863:TYR:CE2	2.88	0.57
1:A:413:LEU:HD12	1:A:416:ILE:HD11	1.86	0.57
1:A:1034:PRO:HA	1:A:1037:ARG:HH12	1.68	0.57
1:A:1441:GLN:HB3	1:A:1445:LYS:HB2	1.86	0.57
1:A:1714:LEU:HD11	1:A:1794:ALA:HB2	1.86	0.57
1:B:345:ILE:HG22	1:B:347:SER:H	1.69	0.57
1:B:1664:PRO:HB2	1:B:1667:PHE:HB3	1.86	0.57
1:C:495:ALA:HB2	1:C:507:VAL:HG11	1.86	0.57
1:C:737:MET:HE3	1:C:785:ILE:HD12	1.85	0.57
1:A:405:HIS:HA	1:A:445:ILE:HG22	1.87	0.57
1:A:494:LEU:HB3	1:A:503:MET:HE2	1.86	0.57
1:B:2225:LEU:HD23	1:B:2228:LEU:HD13	1.87	0.57
1:C:1653:HIS:HD2	1:C:1991:VAL:HG22	1.68	0.57
1:C:1924:GLU:HG2	1:C:1943:LYS:HG2	1.87	0.57
1:A:1445:LYS:C	1:A:1447:PHE:H	2.12	0.57
1:A:1577:MET:HE2	1:A:1886:GLN:HA	1.87	0.57
1:A:1713:VAL:HA	1:A:1791:PRO:HD2	1.87	0.57
1:B:1369:ALA:HA	1:B:1426:ILE:HD11	1.87	0.57
1:B:1554:LYS:NZ	1:B:1898:TYR:OH	2.29	0.57
1:C:1585:ILE:O	1:C:1648:GLN:NE2	2.32	0.56
1:C:1813:ASN:HB2	1:C:1943:LYS:HE3	1.86	0.56
1:A:729:PRO:HG3	1:A:776:ARG:HG3	1.86	0.56
1:A:2447:GLN:HG3	1:A:2460:SER:HA	1.86	0.56
1:B:1446:LYS:HE3	1:B:1512:CYS:HB2	1.87	0.56
1:B:2052:LEU:HA	1:B:2056:GLY:HA3	1.88	0.56
1:B:2206:MET:HE2	1:B:2236:ILE:HD11	1.87	0.56
1:B:2381:GLN:HB2	1:B:2456:PHE:O	2.05	0.56
1:B:2410:ASP:OD1	1:B:2411:LEU:N	2.38	0.56
1:C:623:TYR:OH	1:C:653:GLU:OE1	2.24	0.56
1:A:1591:THR:O	1:A:1645:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:GLU:HA	1:B:725:LEU:HD12	1.87	0.56
1:B:1380:ARG:HH21	1:B:1429:GLY:HA2	1.71	0.56
1:A:345:ILE:HG22	1:A:347:SER:H	1.70	0.56
1:B:1520:VAL:HG22	1:B:2047:LEU:HD22	1.87	0.56
1:C:345:ILE:HG22	1:C:347:SER:H	1.71	0.56
1:C:2237:ARG:O	1:C:2261:ASP:HB2	2.05	0.56
1:C:845:GLN:OE1	1:C:849:ARG:NH1	2.38	0.56
1:C:2324:GLN:O	1:C:2328:SER:OG	2.21	0.56
1:B:1406:TRP:HE3	1:B:1407:LEU:HD22	1.70	0.56
1:B:1664:PRO:HG2	1:B:1668:TRP:CE2	2.41	0.56
1:B:2160:VAL:O	1:B:2178:TYR:OH	2.20	0.56
1:B:1141:MET:HE3	1:B:1145:ARG:HE	1.70	0.56
1:C:1462:LEU:HD21	1:C:1504:LEU:HD23	1.86	0.56
1:B:552:ILE:HD11	1:B:573:ILE:HG23	1.88	0.56
1:B:1037:ARG:NH1	1:B:1142:GLU:OE2	2.39	0.56
1:B:790:ILE:HA	1:B:793:LEU:HD12	1.87	0.55
1:C:2045:ILE:HG21	1:C:2084:VAL:HG13	1.87	0.55
1:B:1408:LYS:NZ	1:B:1461:GLU:OE2	2.40	0.55
1:C:1591:THR:O	1:C:1645:ARG:NH1	2.38	0.55
1:A:1824:MET:CG	1:A:1863:TYR:HE2	2.19	0.55
1:A:2348:ASP:OD2	1:A:2354:ARG:NH2	2.24	0.55
1:A:1470:ALA:HB1	1:A:1999:MET:HG3	1.89	0.55
1:C:505:HIS:O	1:C:509:ASN:ND2	2.38	0.55
1:A:754:LEU:HD22	1:A:763:MET:HA	1.88	0.55
1:B:1431:LEU:O	1:B:1435:LYS:HG3	2.07	0.55
1:B:1666:GLY:HA2	1:B:1669:LYS:HE3	1.88	0.55
1:A:1653:HIS:HD2	1:A:1991:VAL:HG22	1.72	0.55
1:B:1448:HIS:HA	1:B:1452:GLU:HG3	1.89	0.55
1:B:2366:ARG:HG3	1:C:2366:ARG:HH22	1.71	0.55
1:A:359:ASN:HD21	1:A:412:LYS:HB3	1.72	0.55
1:A:1813:ASN:HD22	1:A:1943:LYS:HE3	1.72	0.55
1:A:1871:HIS:HE2	1:A:1878:GLY:HA3	1.72	0.55
1:B:355:LEU:HD23	1:B:412:LYS:HE2	1.88	0.55
1:A:1400:LEU:O	1:A:1404:ILE:HG12	2.06	0.55
1:C:1502:PHE:CD2	1:C:2012:PHE:HB2	2.42	0.55
1:B:695:GLU:OE1	1:B:735:ASN:ND2	2.33	0.54
1:C:1369:ALA:HA	1:C:1426:ILE:HD11	1.87	0.54
1:C:1524:THR:HG23	1:C:1525:GLU:OE1	2.06	0.54
1:A:1427:LEU:HD21	1:A:1491:VAL:HG12	1.89	0.54
1:B:1653:HIS:CD2	1:B:1991:VAL:HG22	2.37	0.54
1:B:2409:GLY:O	1:B:2413:ARG:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LEU:HD12	1:A:548:LYS:NZ	2.21	0.54
1:C:559:LEU:HB2	1:C:566:VAL:HG22	1.87	0.54
1:C:1333:GLN:HG3	1:C:1378:LEU:HB2	1.89	0.54
1:C:1524:THR:HG23	1:C:1525:GLU:N	2.23	0.54
1:C:2409:GLY:O	1:C:2413:ARG:HG3	2.07	0.54
1:A:702:SER:HA	1:A:742:ARG:HH12	1.73	0.54
1:A:1820:ARG:NH2	1:A:1911:ASP:O	2.41	0.54
1:A:736:GLY:O	1:A:740:PHE:HB2	2.08	0.54
1:C:1247:TRP:O	1:C:1268:TYR:OH	2.21	0.54
1:C:1813:ASN:OD1	1:C:1947:ASN:ND2	2.41	0.54
1:C:2365:ASP:OD1	1:C:2366:ARG:N	2.36	0.54
1:B:2247:SER:HA	1:B:2309:GLU:OE1	2.08	0.54
1:C:1041:ARG:HH12	1:C:1143:THR:HG22	1.72	0.54
1:B:536:LEU:CD2	1:B:546:THR:HG21	2.37	0.54
1:A:438:GLN:HA	1:A:446:VAL:HG12	1.90	0.54
1:B:1247:TRP:O	1:B:1268:TYR:OH	2.24	0.54
1:C:2328:SER:O	1:C:2383:ARG:NH2	2.35	0.54
1:B:1357:LEU:HD22	1:B:1375:TYR:HE1	1.73	0.53
1:C:1309:GLU:O	1:C:1313:GLN:NE2	2.40	0.53
1:C:790:ILE:HA	1:C:793:LEU:HD12	1.91	0.53
1:A:2453:ASN:O	1:A:2455:TYR:N	2.41	0.53
1:B:1910:MET:HA	1:B:1915:GLU:HG2	1.90	0.53
1:C:1664:PRO:HG2	1:C:1668:TRP:CE2	2.43	0.53
1:C:2194:THR:HG22	1:C:2198:LYS:HZ2	1.72	0.53
1:C:2368:GLY:H	1:C:2371:ASP:HB2	1.73	0.53
1:C:1034:PRO:HA	1:C:1037:ARG:HH12	1.73	0.53
1:A:567:ILE:HB	1:A:568:PRO:HD3	1.90	0.53
1:A:1307:SER:O	1:A:1313:GLN:NE2	2.36	0.53
1:B:607:GLN:HA	1:B:611:ALA:HA	1.90	0.53
1:B:1441:GLN:OE1	1:B:1445:LYS:HB3	2.09	0.53
1:B:1924:GLU:HG2	1:B:1943:LYS:HG2	1.90	0.53
1:C:1521:ASP:O	1:C:1524:THR:CG2	2.33	0.53
1:C:1987:ILE:O	1:C:1988:GLU:HG3	2.07	0.53
1:A:1642:GLY:O	1:A:1646:HIS:ND1	2.30	0.53
1:B:1709:MET:SD	1:B:1965:LEU:HB3	2.49	0.53
1:B:1740:LEU:HD23	1:B:1795:ILE:HG12	1.90	0.53
1:C:1159:LEU:HA	1:C:1162:ILE:HG22	1.90	0.53
1:C:1376:PHE:HB3	1:C:1380:ARG:NH1	2.20	0.53
1:A:1883:TYR:CD2	1:A:1910:MET:HG2	2.44	0.53
1:B:545:ASP:CB	1:B:580:PHE:HD1	2.21	0.53
1:B:1320:LEU:HD21	1:B:1378:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2050:ARG:O	1:B:2054:THR:OG1	2.23	0.53
1:C:1445:LYS:C	1:C:1447:PHE:H	2.14	0.53
1:A:1435:LYS:HD2	1:A:1503:GLU:HG3	1.90	0.53
1:B:1561:ASN:ND2	1:B:1566:CYS:HB3	2.23	0.53
1:B:1873:GLY:HA3	1:B:1878:GLY:HA2	1.91	0.53
1:C:1709:MET:SD	1:C:1965:LEU:HB3	2.49	0.53
1:A:630:TYR:HD2	1:A:634:HIS:HB2	1.74	0.53
1:A:805:GLN:O	1:A:808:GLN:NE2	2.42	0.53
1:A:1235:ASP:OD1	1:A:1235:ASP:N	2.42	0.53
1:B:613:VAL:HG23	1:B:664:LEU:HD22	1.91	0.53
1:B:1447:PHE:CG	1:B:1514:ARG:HD2	2.44	0.53
1:C:1353:PHE:HA	1:C:1356:LEU:HB3	1.91	0.53
1:C:2013:MET:SD	1:C:2047:LEU:HD21	2.49	0.53
1:A:557:GLU:HA	1:A:560:ARG:HD2	1.90	0.52
1:A:1523:LEU:HD11	1:A:2012:PHE:HE2	1.74	0.52
1:B:1988:GLU:OE2	1:B:1989:ARG:NH2	2.40	0.52
1:C:1452:GLU:O	1:C:1457:ASN:ND2	2.38	0.52
1:A:1084:SER:HB3	1:A:1087:GLN:HG2	1.90	0.52
1:A:1987:ILE:O	1:A:1988:GLU:HG3	2.08	0.52
1:C:627:MET:HA	1:C:630:TYR:CE1	2.44	0.52
1:C:1948:ALA:HB1	1:C:1951:LEU:HD21	1.92	0.52
1:A:505:HIS:O	1:A:509:ASN:ND2	2.41	0.52
1:A:800:LEU:HD11	1:A:808:GLN:HG3	1.90	0.52
1:A:1326:LYS:H	1:A:1326:LYS:HD2	1.73	0.52
1:B:2328:SER:O	1:B:2383:ARG:NH2	2.36	0.52
1:C:542:GLN:O	1:C:544:ARG:HG3	2.09	0.52
1:C:1673:LEU:N	1:C:1676:GLU:O	2.43	0.52
1:C:2067:ALA:HA	1:C:2070:TRP:HD1	1.73	0.52
1:A:620:LEU:HD22	1:A:657:ARG:HD2	1.92	0.52
1:A:1707:PRO:HB3	1:A:1969:ILE:HD12	1.92	0.52
1:A:2079:ARG:HA	1:A:2085:ARG:HH21	1.73	0.52
1:B:754:LEU:HD22	1:B:763:MET:HA	1.91	0.52
1:B:1568:MET:HG3	1:B:1667:PHE:HE2	1.73	0.52
1:B:1643:VAL:HG13	1:B:1671:PHE:CZ	2.45	0.52
1:B:1697:LEU:HD23	1:B:1710:LEU:HD11	1.91	0.52
1:B:2408:ASN:O	1:B:2408:ASN:ND2	2.43	0.52
1:C:1329:ARG:NH2	1:C:1371:HIS:HD2	2.07	0.52
1:A:1653:HIS:CD2	1:A:1991:VAL:HG22	2.45	0.52
1:A:1871:HIS:NE2	1:A:1878:GLY:HA3	2.25	0.52
1:B:846:GLU:HA	1:B:849:ARG:HD3	1.90	0.52
1:C:508:LEU:HD23	1:C:511:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1684:HIS:HE1	1:C:1688:GLU:HB2	1.73	0.52
1:A:1380:ARG:HE	1:A:1432:GLY:HA3	1.75	0.52
1:A:1757:TYR:HD1	1:A:1784:LEU:HB2	1.74	0.52
1:B:1283:GLN:HA	1:B:1286:CYS:SG	2.49	0.52
1:A:544:ARG:HB3	1:A:544:ARG:HH11	1.75	0.52
1:B:1337:PHE:HE1	1:B:1381:HIS:HB2	1.75	0.52
1:C:1531:THR:HG21	1:C:1537:GLU:HG2	1.92	0.52
1:A:1246:ILE:HG21	1:A:1319:LEU:HD21	1.92	0.52
1:B:1713:VAL:HA	1:B:1791:PRO:HD2	1.92	0.52
1:C:2303:LEU:HD12	1:C:2339:LEU:HD21	1.91	0.52
1:A:418:ARG:NH2	1:A:455:LYS:O	2.42	0.51
1:A:735:ASN:OD1	1:A:738:LYS:NZ	2.43	0.51
1:B:1248:ALA:HB1	1:B:1254:LEU:HA	1.91	0.51
1:B:1567:TYR:CZ	1:B:1684:HIS:HB2	2.45	0.51
1:B:1673:LEU:HB2	1:B:1678:VAL:HG22	1.92	0.51
1:A:1326:LYS:HG3	1:A:1329:ARG:NH1	2.24	0.51
1:C:717:LYS:HZ3	1:C:751:GLU:HB2	1.74	0.51
1:C:2426:LEU:HD21	1:C:2463:ALA:HB3	1.92	0.51
1:A:1244:LYS:HG3	1:A:1261:ASN:HD21	1.74	0.51
1:A:1664:PRO:HB2	1:A:1667:PHE:HB3	1.92	0.51
1:A:2376:SER:HB2	1:A:2384:ALA:HB2	1.91	0.51
1:B:1913:ASP:HA	1:B:1916:MET:HE1	1.92	0.51
1:A:526:ASP:OD1	1:A:527:LEU:N	2.44	0.51
1:A:2206:MET:HE1	1:A:2279:LEU:HG	1.93	0.51
1:B:1041:ARG:HG3	1:B:1044:MET:HE2	1.92	0.51
1:C:563:ASP:HB3	1:C:565:TRP:NE1	2.26	0.51
1:C:1144:ARG:HB3	1:C:1145:ARG:HH12	1.75	0.51
1:C:1330:GLN:NE2	1:C:1374:ASP:OD2	2.44	0.51
1:B:413:LEU:HA	1:B:416:ILE:HD12	1.92	0.51
1:B:1444:GLU:OE2	1:B:1514:ARG:NH1	2.42	0.51
1:B:1694:VAL:HG12	1:B:1710:LEU:HD22	1.92	0.51
1:C:509:ASN:O	1:C:513:ASN:ND2	2.43	0.51
1:C:720:PHE:HA	1:C:724:VAL:HB	1.93	0.51
1:C:1283:GLN:O	1:C:1287:GLU:HG2	2.11	0.51
1:A:2045:ILE:HG21	1:A:2084:VAL:HG13	1.93	0.51
1:B:2162:ASN:OD1	1:B:2165:ARG:NH1	2.43	0.51
1:C:516:HIS:NE2	1:C:568:PRO:HB2	2.26	0.51
1:C:2307:CYS:O	1:C:2354:ARG:NH2	2.43	0.51
1:C:2416:THR:O	1:C:2419:VAL:HG22	2.10	0.51
1:B:1235:ASP:N	1:B:1235:ASP:OD1	2.42	0.51
1:A:337:LYS:O	1:A:341:ARG:HG2	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:GLU:OE1	1:A:735:ASN:ND2	2.39	0.51
1:A:696:ALA:HA	1:A:699:LYS:HE3	1.93	0.51
1:B:495:ALA:HB2	1:B:507:VAL:HG11	1.94	0.50
1:C:1560:LYS:HE3	1:C:1663:VAL:HG13	1.93	0.50
1:A:1750:LEU:N	1:A:1817:GLU:O	2.41	0.50
1:A:1886:GLN:N	1:A:1896:ARG:O	2.39	0.50
1:B:776:ARG:HA	1:B:779:ILE:HG22	1.94	0.50
1:B:1307:SER:O	1:B:1313:GLN:NE2	2.39	0.50
1:B:1536:CYS:HB2	1:B:2099:ARG:HH22	1.77	0.50
1:B:2133:CYS:HB3	1:B:2155:HIS:CE1	2.47	0.50
1:A:503:MET:HA	1:A:506:LYS:HE2	1.93	0.50
1:A:2052:LEU:HA	1:A:2056:GLY:HA3	1.93	0.50
1:A:2448:SER:O	1:A:2450:GLU:N	2.37	0.50
1:A:1763:LEU:HD12	1:A:1769:TYR:HB2	1.92	0.50
1:B:1268:TYR:HB3	1:B:1322:HIS:HB3	1.94	0.50
1:B:2102:GLU:HA	1:B:2106:GLU:HG3	1.94	0.50
1:C:1353:PHE:O	1:C:1354:ILE:C	2.54	0.50
1:C:1467:ILE:HG21	1:C:1502:PHE:CE1	2.46	0.50
1:C:2007:MET:HA	1:C:2063:VAL:HG13	1.92	0.50
1:A:2018:THR:HG22	1:A:2018:THR:O	2.12	0.50
1:B:1336:PHE:HD1	1:B:1339:MET:HE2	1.77	0.50
1:A:776:ARG:HA	1:A:779:ILE:HG22	1.92	0.50
1:A:1303:LEU:HD22	1:A:1339:MET:HE2	1.93	0.50
1:A:2062:VAL:HG23	1:A:2063:VAL:HG23	1.94	0.50
1:B:1576:TYR:HD2	1:B:1577:MET:HE2	1.77	0.50
1:C:716:ASN:HA	1:C:719:PHE:CE1	2.47	0.50
1:C:1354:ILE:HG22	1:C:1355:THR:N	2.26	0.50
1:A:1239:ILE:HD11	1:A:1295:CYS:SG	2.52	0.50
1:B:546:THR:O	1:B:548:LYS:HG2	2.12	0.50
1:A:790:ILE:HG12	1:A:856:VAL:HG22	1.94	0.49
1:A:1719:ALA:N	1:A:1785:LEU:O	2.33	0.49
1:A:1996:VAL:HA	1:A:1999:MET:HE2	1.93	0.49
1:C:1456:ALA:O	1:C:1458:LEU:N	2.45	0.49
1:C:1658:ARG:N	1:C:1995:ASN:OD1	2.29	0.49
1:C:1919:GLN:HA	1:C:1946:TRP:CD1	2.47	0.49
1:C:2052:LEU:HA	1:C:2056:GLY:HA3	1.94	0.49
1:A:1722:LYS:HB2	1:A:1731:TYR:HB2	1.94	0.49
1:A:435:TRP:CD1	1:A:471:CYS:HB3	2.47	0.49
1:A:540:CYS:HA	1:A:544:ARG:CG	2.42	0.49
1:A:563:ASP:HB3	1:A:565:TRP:NE1	2.26	0.49
1:B:553:ASP:HA	1:B:556:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1423:GLU:H	1:B:1426:ILE:HD12	1.75	0.49
1:C:1357:LEU:O	1:C:1360:VAL:N	2.45	0.49
1:A:2185:TYR:OH	1:A:2195:GLN:OE1	2.27	0.49
1:A:784:ASP:OD1	1:A:785:ILE:N	2.46	0.49
1:C:658:LEU:HD11	1:C:700:TRP:HB2	1.93	0.49
1:A:1573:GLN:HB3	1:A:1900:PHE:HD2	1.77	0.49
1:A:2416:THR:O	1:A:2419:VAL:HG22	2.12	0.49
1:B:784:ASP:N	1:B:784:ASP:OD1	2.45	0.49
1:A:1740:LEU:O	1:A:1796:GLN:N	2.34	0.49
1:A:2154:ASP:OD1	1:A:2195:GLN:NE2	2.40	0.49
1:C:2196:LEU:HD22	1:C:2201:VAL:HG21	1.94	0.49
1:A:1502:PHE:CD2	1:A:2012:PHE:HB2	2.48	0.49
1:A:2362:ILE:HG23	1:A:2365:ASP:HB2	1.95	0.49
1:B:563:ASP:HB3	1:B:565:TRP:CZ3	2.48	0.49
1:B:1701:LEU:O	1:B:1706:HIS:N	2.44	0.49
1:B:1945:TRP:H	1:B:1945:TRP:CD1	2.30	0.49
1:A:547:GLN:HB2	1:A:551:TRP:HE1	1.76	0.49
1:B:1588:ILE:HG21	1:B:1644:LEU:HD21	1.94	0.49
1:C:598:TYR:O	1:C:602:LEU:HG	2.13	0.49
1:C:1247:TRP:HE3	1:C:1264:ILE:HB	1.78	0.49
1:A:1710:LEU:HD21	1:A:1714:LEU:HD23	1.94	0.49
1:B:1041:ARG:HH12	1:B:1143:THR:HG22	1.77	0.49
1:C:1824:MET:HE2	1:C:1863:TYR:HD2	1.78	0.49
1:B:1031:LEU:HB3	1:B:1033:MET:HE1	1.93	0.48
1:B:1033:MET:HG3	1:B:1036:LEU:HD13	1.94	0.48
1:B:1348:ARG:HE	1:B:1351:LEU:HD22	1.78	0.48
1:B:1395:ASN:ND2	1:B:1399:LEU:HD21	2.28	0.48
1:C:498:ASP:OD2	1:C:504:ALA:N	2.46	0.48
1:C:1673:LEU:HD21	1:C:1684:HIS:CE1	2.48	0.48
1:C:1751:LEU:O	1:C:1755:GLU:HG2	2.12	0.48
1:B:1309:GLU:O	1:B:1313:GLN:NE2	2.46	0.48
1:C:2309:GLU:HA	1:C:2350:TRP:CD1	2.47	0.48
1:A:627:MET:HA	1:A:630:TYR:CE1	2.49	0.48
1:A:1709:MET:SD	1:A:1965:LEU:HB3	2.53	0.48
1:B:1558:GLY:HA3	1:B:1903:GLY:HA2	1.95	0.48
1:B:1559:LEU:H	1:B:1903:GLY:HA2	1.78	0.48
1:C:1520:VAL:HG13	1:C:2047:LEU:HD12	1.96	0.48
1:C:1642:GLY:O	1:C:1646:HIS:ND1	2.33	0.48
1:C:2309:GLU:HG3	1:C:2348:ASP:HB2	1.95	0.48
1:A:2248:SER:HB3	1:A:2350:TRP:CE2	2.48	0.48
1:B:1384:ASN:O	1:B:1388:ASN:N	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1731:TYR:HH	1:B:1771:CYS:HG	1.46	0.48
1:C:1323:CYS:SG	1:C:1324:HIS:N	2.87	0.48
1:A:1262:GLU:O	1:A:1265:THR:OG1	2.24	0.48
1:B:620:LEU:HD21	1:B:657:ARG:HB3	1.95	0.48
1:B:2245:MET:HE1	1:B:2308:TRP:CD1	2.48	0.48
1:C:1022:TRP:O	1:C:1086:SER:OG	2.24	0.48
1:C:1361:LEU:C	1:C:1363:SER:N	2.72	0.48
1:C:1474:TYR:CE1	1:C:1478:MET:HE3	2.49	0.48
1:C:1910:MET:HA	1:C:1915:GLU:HB3	1.95	0.48
1:C:2085:ARG:NH1	1:C:2130:ASP:OD2	2.46	0.48
1:B:543:ASP:OD2	1:B:547:GLN:NE2	2.46	0.48
1:B:720:PHE:HA	1:B:724:VAL:HB	1.95	0.48
1:B:1326:LYS:HG3	1:B:1329:ARG:HH12	1.78	0.48
1:C:662:ARG:NH1	1:C:704:LEU:HA	2.29	0.48
1:C:847:ALA:HA	1:C:850:MET:HE2	1.96	0.48
1:A:469:PHE:HE2	1:A:506:LYS:HE3	1.78	0.48
1:A:1742:VAL:HG23	1:A:1744:ILE:HD11	1.95	0.48
1:B:541:SER:HA	1:B:544:ARG:NH2	2.29	0.48
1:B:855:THR:HA	1:B:858:ARG:HG2	1.95	0.48
1:B:2248:SER:HB3	1:B:2350:TRP:CE2	2.48	0.48
1:B:2362:ILE:HG22	1:B:2363:PRO:HD2	1.95	0.48
1:C:1235:ASP:OD1	1:C:1235:ASP:N	2.44	0.48
1:B:540:CYS:O	1:B:543:ASP:N	2.47	0.48
1:B:1527:TYR:CE2	1:B:2004:GLN:HB2	2.49	0.48
1:C:1717:SER:HA	1:C:1736:SER:HA	1.95	0.48
1:C:1723:ILE:HG12	1:C:1730:ARG:HD2	1.96	0.48
1:C:2164:LEU:HD23	1:C:2168:VAL:HG21	1.95	0.48
1:B:498:ASP:OD2	1:B:504:ALA:N	2.45	0.48
1:B:729:PRO:HG3	1:B:776:ARG:HG3	1.95	0.48
1:B:2321:LEU:O	1:B:2325:VAL:HG23	2.14	0.48
1:C:1386:ALA:HA	1:C:1391:ILE:HB	1.94	0.48
1:C:1592:GLY:HA2	1:C:1645:ARG:HD3	1.95	0.48
1:A:1246:ILE:HD13	1:A:1289:LEU:HG	1.96	0.48
1:A:1442:THR:OG1	1:A:1443:SER:N	2.46	0.48
1:B:1412:ASP:HA	1:B:1415:LYS:HE3	1.96	0.48
1:C:790:ILE:HG12	1:C:856:VAL:HG22	1.96	0.48
1:A:1096:TYR:CZ	1:A:1153:LYS:HB3	2.50	0.47
1:A:1456:ALA:O	1:A:1458:LEU:N	2.47	0.47
1:A:1531:THR:HG21	1:A:1537:GLU:HG2	1.96	0.47
1:B:418:ARG:NH2	1:B:455:LYS:O	2.47	0.47
1:C:855:THR:HA	1:C:858:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1657:SER:HA	1:C:1995:ASN:HD21	1.78	0.47
1:C:1731:TYR:OH	1:C:1771:CYS:SG	2.66	0.47
1:C:1756:GLN:NE2	1:C:1760:GLY:O	2.46	0.47
1:A:625:GLU:O	1:A:629:LEU:HG	2.14	0.47
1:A:1545:LEU:HD23	1:A:2060:LYS:HD3	1.95	0.47
1:B:450:HIS:ND1	1:B:490:LEU:HD22	2.29	0.47
1:B:1896:ARG:HH21	1:B:1907:GLU:HG2	1.79	0.47
1:C:435:TRP:NE1	1:C:475:SER:OG	2.43	0.47
1:C:1526:MET:HE3	1:C:1527:TYR:HE1	1.79	0.47
1:A:536:LEU:HB3	1:A:548:LYS:HE3	1.96	0.47
1:B:1502:PHE:CD2	1:B:2012:PHE:HB2	2.50	0.47
1:C:762:MET:HE2	1:C:802:PRO:HD2	1.95	0.47
1:C:1254:LEU:HD23	1:C:1254:LEU:O	2.14	0.47
1:C:1520:VAL:HG22	1:C:2047:LEU:HD13	1.96	0.47
1:A:701:TYR:HB3	1:A:705:MET:HE1	1.97	0.47
1:A:705:MET:HE3	1:A:743:PHE:CZ	2.50	0.47
1:A:714:ASP:OD1	1:A:715:ILE:HG13	2.15	0.47
1:C:1362:GLY:HA2	1:C:1366:ARG:HB2	1.97	0.47
1:C:1380:ARG:HG3	1:C:1436:GLU:HG3	1.96	0.47
1:C:1566:CYS:HB2	1:C:1880:TYR:H	1.79	0.47
1:C:2176:GLN:HB2	1:C:2177:GLN:OE1	2.14	0.47
1:A:476:TRP:CD1	1:A:487:LEU:HD13	2.49	0.47
1:A:620:LEU:HD21	1:A:657:ARG:HB3	1.96	0.47
1:A:850:MET:HA	1:A:853:VAL:HG12	1.96	0.47
1:A:1397:GLU:OE2	1:A:1401:ASN:ND2	2.46	0.47
1:A:1576:TYR:HA	1:A:1651:PHE:HE1	1.79	0.47
1:B:658:LEU:HD21	1:B:700:TRP:HB2	1.96	0.47
1:C:1149:LEU:HA	1:C:1287:GLU:OE2	2.14	0.47
1:A:556:ILE:O	1:A:560:ARG:HG3	2.14	0.47
1:A:628:ARG:HH12	1:A:687:ASN:HB2	1.79	0.47
1:A:1356:LEU:O	1:A:1359:THR:HG22	2.15	0.47
1:B:1130:LEU:HD12	1:B:1131:THR:HG23	1.97	0.47
1:B:1282:GLU:HG2	1:B:1328:VAL:HG23	1.96	0.47
1:B:1333:GLN:NE2	1:B:1374:ASP:O	2.47	0.47
1:C:1084:SER:HB3	1:C:1087:GLN:HG2	1.96	0.47
1:A:2256:PRO:O	1:A:2258:PRO:HD3	2.15	0.47
1:B:1387:TYR:HB2	1:B:1440:PHE:CE1	2.49	0.47
1:B:1749:ASN:HA	1:B:1817:GLU:HB2	1.97	0.47
1:B:2202:PRO:O	1:B:2206:MET:HG3	2.14	0.47
1:C:404:LEU:HD13	1:C:449:VAL:HG22	1.97	0.47
1:C:1919:GLN:HG3	1:C:1920:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2194:THR:HG22	1:C:2198:LYS:NZ	2.29	0.47
1:A:662:ARG:HB2	1:A:700:TRP:NE1	2.29	0.47
1:A:1309:GLU:O	1:A:1313:GLN:NE2	2.48	0.47
1:C:1551:ARG:HB2	1:C:1659:LEU:C	2.38	0.47
1:A:2172:GLY:O	1:A:2173:ARG:HB2	2.14	0.47
1:B:1337:PHE:CE1	1:B:1381:HIS:HB2	2.49	0.47
1:B:1757:TYR:HD1	1:B:1784:LEU:HB2	1.80	0.47
1:B:1904:ASP:OD1	1:B:1905:VAL:N	2.48	0.47
1:C:672:LEU:HD23	1:C:711:LEU:HD11	1.96	0.47
1:C:1434:THR:O	1:C:1438:LEU:HB2	2.14	0.47
1:C:1920:CYS:HB3	1:C:1948:ALA:HB2	1.97	0.47
1:A:540:CYS:SG	1:A:541:SER:N	2.88	0.47
1:B:1559:LEU:N	1:B:1903:GLY:HA2	2.29	0.47
1:B:2172:GLY:O	1:B:2173:ARG:HB2	2.14	0.47
1:C:1412:ASP:HA	1:C:1415:LYS:HB3	1.96	0.47
1:A:827:TYR:OH	1:A:1023:GLN:HG2	2.14	0.46
1:A:1243:GLN:OE1	1:A:1247:TRP:NE1	2.48	0.46
1:A:2042:MET:O	1:A:2046:GLN:HG3	2.15	0.46
1:B:1380:ARG:NH2	1:B:1428:GLU:HG3	2.27	0.46
1:B:1512:CYS:SG	1:B:1515:ASN:ND2	2.86	0.46
1:B:1576:TYR:HD1	1:B:1651:PHE:CD1	2.33	0.46
1:C:1307:SER:O	1:C:1313:GLN:NE2	2.43	0.46
1:A:847:ALA:HA	1:A:850:MET:HE2	1.98	0.46
1:A:1325:SER:O	1:A:1328:VAL:HG12	2.14	0.46
1:C:1145:ARG:NH2	1:C:1254:LEU:HD22	2.30	0.46
1:C:1287:GLU:O	1:C:1291:VAL:HG23	2.14	0.46
1:C:1824:MET:SD	1:C:1824:MET:N	2.88	0.46
1:A:431:LEU:HD23	1:A:434:ILE:HD12	1.98	0.46
1:A:536:LEU:HD12	1:A:548:LYS:HZ2	1.79	0.46
1:A:1159:LEU:HA	1:A:1162:ILE:HG22	1.97	0.46
1:A:1647:LEU:HG	1:A:1651:PHE:CE2	2.49	0.46
1:B:337:LYS:O	1:B:341:ARG:HG2	2.15	0.46
1:B:457:ALA:HA	1:B:460:PHE:HD2	1.81	0.46
1:B:1742:VAL:HB	1:B:1753:SER:HB2	1.97	0.46
1:C:1500:ALA:HA	1:C:1503:GLU:OE2	2.14	0.46
1:C:2309:GLU:HA	1:C:2350:TRP:HD1	1.79	0.46
1:C:2385:TYR:CZ	1:C:2389:LYS:HD2	2.49	0.46
1:A:802:PRO:C	1:A:804:LEU:H	2.23	0.46
1:A:1963:ASP:HA	1:A:1966:ILE:HD12	1.96	0.46
1:B:1813:ASN:OD1	1:B:1947:ASN:ND2	2.48	0.46
1:C:536:LEU:HB3	1:C:548:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:776:ARG:HA	1:C:779:ILE:HG22	1.97	0.46
1:A:389:TRP:O	1:A:393:ASN:ND2	2.36	0.46
1:A:1319:LEU:O	1:A:1329:ARG:HG2	2.16	0.46
1:A:1551:ARG:HB2	1:A:1659:LEU:C	2.41	0.46
1:B:541:SER:N	1:B:544:ARG:HH21	2.12	0.46
1:B:1561:ASN:HD21	1:B:1566:CYS:HB3	1.81	0.46
1:B:1754:LEU:HD11	1:B:1822:LEU:HD21	1.96	0.46
1:C:858:ARG:HG3	1:C:859:GLU:OE1	2.15	0.46
1:C:1096:TYR:CZ	1:C:1153:LYS:HB3	2.51	0.46
1:C:1247:TRP:NE1	1:C:1315:PHE:HD1	2.14	0.46
1:C:1408:LYS:HZ1	1:C:1456:ALA:HB1	1.80	0.46
1:A:399:VAL:O	1:A:403:SER:OG	2.26	0.46
1:A:1740:LEU:HD12	1:A:1795:ILE:HG12	1.97	0.46
1:B:823:LEU:HD11	1:B:850:MET:HE2	1.97	0.46
1:B:1572:ILE:HD11	1:B:1667:PHE:CZ	2.51	0.46
1:C:1080:PHE:HZ	1:C:1095:VAL:HG21	1.80	0.46
1:B:1262:GLU:O	1:B:1265:THR:OG1	2.27	0.46
1:C:540:CYS:SG	1:C:541:SER:N	2.88	0.46
1:C:1141:MET:O	1:C:1145:ARG:HG2	2.16	0.46
1:C:1522:SER:O	1:C:1526:MET:HG3	2.16	0.46
1:A:553:ASP:HA	1:A:556:ILE:HD12	1.97	0.46
1:A:1586:LEU:HD21	1:A:1651:PHE:HB2	1.98	0.46
1:B:1786:ILE:HD12	1:B:1824:MET:HE2	1.97	0.46
1:C:749:CYS:SG	1:C:761:TYR:HD2	2.38	0.46
1:C:1144:ARG:HB3	1:C:1145:ARG:NH1	2.30	0.46
1:C:2322:LEU:HA	1:C:2325:VAL:HG12	1.98	0.46
1:A:1085:ALA:HB1	1:A:1136:LEU:HD21	1.97	0.46
1:A:1664:PRO:HG2	1:A:1668:TRP:CE2	2.51	0.46
1:A:2188:LEU:HB3	1:A:2192:GLU:OE1	2.16	0.46
1:A:2454:GLY:O	1:A:2455:TYR:HB2	2.15	0.46
1:B:1429:GLY:O	1:B:1433:VAL:N	2.37	0.46
1:B:1099:LEU:HD13	1:B:1157:LEU:HD11	1.97	0.46
1:B:2341:LEU:O	1:B:2345:LEU:HG	2.15	0.46
1:C:2079:ARG:HB3	1:C:2122:PHE:CZ	2.51	0.46
1:A:400:LEU:HG	1:A:404:LEU:HD11	1.97	0.45
1:A:578:SER:O	1:A:599:ARG:NH2	2.45	0.45
1:A:1896:ARG:HH21	1:A:1907:GLU:HG2	1.81	0.45
1:A:2160:VAL:O	1:A:2178:TYR:OH	2.26	0.45
1:B:542:GLN:HG2	1:B:543:ASP:N	2.31	0.45
1:B:665:LEU:HD23	1:B:704:LEU:HD11	1.98	0.45
1:B:1387:TYR:HB2	1:B:1440:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2049:ALA:HB1	1:B:2092:VAL:HG21	1.97	0.45
1:C:2033:LEU:HD12	1:C:2037:ALA:HB3	1.98	0.45
1:A:1014:HIS:HB3	1:A:1016:ARG:HG2	1.97	0.45
1:B:827:TYR:HE2	1:B:1024:VAL:HA	1.81	0.45
1:B:1815:TYR:HE1	1:B:1917:LYS:HG3	1.80	0.45
1:B:2034:LEU:HD12	1:B:2037:ALA:H	1.80	0.45
1:C:2333:LEU:HD21	1:C:2383:ARG:HG3	1.99	0.45
1:A:1536:CYS:HB2	1:A:2099:ARG:HH22	1.82	0.45
1:A:2247:SER:HA	1:A:2309:GLU:OE1	2.16	0.45
1:B:790:ILE:HG12	1:B:856:VAL:HG22	1.99	0.45
1:B:2133:CYS:HB3	1:B:2155:HIS:HE1	1.80	0.45
1:B:2426:LEU:HD12	1:B:2467:LEU:HD22	1.99	0.45
1:C:784:ASP:OD1	1:C:784:ASP:N	2.47	0.45
1:A:1241:ALA:O	1:A:1245:ILE:HG12	2.16	0.45
1:B:1139:ALA:HB1	1:B:1144:ARG:HB2	1.97	0.45
1:B:1536:CYS:HB2	1:B:2099:ARG:NH2	2.31	0.45
1:B:2303:LEU:HD12	1:B:2339:LEU:HD21	1.98	0.45
1:C:544:ARG:N	1:C:547:GLN:HE22	2.15	0.45
1:C:1325:SER:O	1:C:1328:VAL:HG12	2.15	0.45
1:C:1640:ASN:HB3	1:C:1700:ALA:HB2	1.97	0.45
1:B:797:TYR:HB3	1:B:860:TYR:HE1	1.81	0.45
1:B:1719:ALA:N	1:B:1785:LEU:O	2.40	0.45
1:A:1012:SER:OG	1:A:1013:LEU:N	2.48	0.45
1:B:1320:LEU:HD22	1:B:1375:TYR:HA	1.98	0.45
1:B:1357:LEU:HB3	1:B:1379:LEU:HD12	1.98	0.45
1:C:1380:ARG:HD2	1:C:1432:GLY:C	2.42	0.45
1:A:1380:ARG:NE	1:A:1432:GLY:HA3	2.32	0.45
1:A:2410:ASP:OD1	1:A:2411:LEU:N	2.49	0.45
1:C:705:MET:HB2	1:C:742:ARG:HH11	1.82	0.45
1:C:2271:ILE:HD13	1:C:2280:PHE:HE2	1.80	0.45
1:A:1762:LEU:HD13	1:A:1781:VAL:HG22	1.98	0.45
1:A:2220:TYR:CZ	1:A:2222:TYR:HB2	2.52	0.45
1:B:1557:VAL:HB	1:B:1654:LEU:HD13	1.99	0.45
1:B:2164:LEU:HD11	1:B:2208:VAL:HG21	1.99	0.45
1:A:341:ARG:O	1:A:345:ILE:HG12	2.17	0.45
1:A:544:ARG:CZ	1:A:548:LYS:HZ3	2.30	0.45
1:A:1567:TYR:CE2	1:A:1684:HIS:HB2	2.52	0.45
1:B:1493:GLY:N	1:B:1497:THR:OG1	2.49	0.45
1:C:558:GLU:HG3	1:C:565:TRP:HB3	1.99	0.45
1:C:567:ILE:HG22	1:C:571:LYS:NZ	2.32	0.45
1:A:623:TYR:OH	1:A:653:GLU:OE1	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:TYR:HB2	1:A:1154:ILE:HD11	1.99	0.45
1:A:1278:ASP:O	1:A:1282:GLU:HG2	2.17	0.45
1:A:1369:ALA:C	1:A:1370:LYS:HD3	2.42	0.45
1:A:1936:ARG:O	1:A:1937:MET:HE2	2.18	0.45
1:B:685:ALA:HB1	1:B:694:ARG:HG2	1.99	0.45
1:C:450:HIS:HB3	1:C:490:LEU:HD13	1.99	0.45
1:C:2088:PHE:O	1:C:2092:VAL:HG22	2.17	0.45
1:A:564:LYS:HE2	1:A:564:LYS:HB2	1.78	0.44
1:A:717:LYS:NZ	1:A:747:VAL:O	2.50	0.44
1:B:1318:ASP:O	1:B:1323:CYS:N	2.50	0.44
1:B:2375:ARG:HD2	1:C:2323:TRP:HH2	1.82	0.44
1:C:1357:LEU:C	1:C:1359:THR:N	2.73	0.44
1:C:1430:HIS:HA	1:C:1433:VAL:HG12	1.99	0.44
1:C:1672:ARG:HB2	1:C:1677:PRO:HA	1.98	0.44
1:C:1673:LEU:HB2	1:C:1678:VAL:HG22	1.97	0.44
1:C:1820:ARG:NH2	1:C:1911:ASP:O	2.50	0.44
1:C:2033:LEU:HD21	1:C:2080:HIS:HB3	1.98	0.44
1:A:1774:CYS:HB3	1:A:1776:LYS:HG2	1.99	0.44
1:B:736:GLY:O	1:B:740:PHE:HB2	2.18	0.44
1:B:1446:LYS:NZ	1:B:1510:VAL:O	2.22	0.44
1:C:736:GLY:O	1:C:740:PHE:HB2	2.17	0.44
1:C:1326:LYS:H	1:C:1326:LYS:HD2	1.82	0.44
1:C:1332:ALA:O	1:C:1335:GLN:HG3	2.17	0.44
1:A:355:LEU:HD22	1:A:409:TYR:CE1	2.53	0.44
1:B:435:TRP:NE1	1:B:475:SER:OG	2.40	0.44
1:B:1358:PHE:HD2	1:B:1361:LEU:HD21	1.82	0.44
1:C:1748:GLN:O	1:C:1816:PHE:HA	2.18	0.44
1:A:381:LEU:HD12	1:A:385:ARG:HB3	1.99	0.44
1:A:399:VAL:HG11	1:A:413:LEU:HD13	1.99	0.44
1:A:717:LYS:HZ3	1:A:751:GLU:HB2	1.83	0.44
1:B:1369:ALA:HB1	1:B:1423:GLU:CD	2.41	0.44
1:C:741:GLU:HG2	1:C:792:LEU:HD21	1.98	0.44
1:C:1330:GLN:HE21	1:C:1374:ASP:CG	2.25	0.44
1:C:2202:PRO:HD3	1:C:2235:LEU:HD13	1.99	0.44
1:A:753:LYS:O	1:A:754:LEU:HD23	2.17	0.44
1:A:1744:ILE:HG23	1:A:1816:PHE:CD1	2.53	0.44
1:B:1326:LYS:H	1:B:1326:LYS:HD2	1.82	0.44
1:B:1673:LEU:N	1:B:1676:GLU:O	2.51	0.44
1:C:400:LEU:HD23	1:C:404:LEU:HD21	1.98	0.44
1:C:567:ILE:HB	1:C:568:PRO:HD3	2.00	0.44
1:C:2406:GLN:HA	1:C:2412:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:THR:HG22	1:A:1318:ASP:OD2	2.17	0.44
1:A:1243:GLN:O	1:A:1247:TRP:HD1	2.01	0.44
1:A:1445:LYS:C	1:A:1447:PHE:N	2.76	0.44
1:B:559:LEU:O	1:B:619:ASN:ND2	2.51	0.44
1:C:2011:GLN:O	1:C:2015:LYS:HG2	2.18	0.44
1:C:2211:ASP:CG	1:C:2217:PRO:HB3	2.43	0.44
1:A:1588:ILE:O	1:A:1648:GLN:NE2	2.37	0.44
1:A:1793:LEU:HB3	1:A:1953:TYR:HB2	1.99	0.44
1:A:2277:ASP:HA	1:A:2281:VAL:HB	2.00	0.44
1:B:1337:PHE:CZ	1:B:1378:LEU:HD23	2.52	0.44
1:B:2165:ARG:O	1:B:2215:GLY:HA3	2.17	0.44
1:C:1562:ALA:HB2	1:C:1668:TRP:CH2	2.52	0.44
1:C:1866:VAL:HG12	1:C:1885:ILE:HD12	2.00	0.44
1:A:547:GLN:CB	1:A:551:TRP:CD1	2.97	0.44
1:A:552:ILE:HD11	1:A:573:ILE:HG23	2.00	0.44
1:A:672:LEU:HD23	1:A:711:LEU:HD11	2.00	0.44
1:B:396:LEU:HD11	1:B:430:ASP:HB3	2.00	0.44
1:B:2124:ALA:O	1:B:2153:SER:OG	2.33	0.44
1:C:337:LYS:O	1:C:341:ARG:HG2	2.18	0.44
1:C:630:TYR:CD2	1:C:634:HIS:HB2	2.44	0.44
1:C:827:TYR:CE2	1:C:1024:VAL:HA	2.52	0.44
1:C:2367:ASP:HB3	1:C:2371:ASP:HB2	2.00	0.44
1:A:1663:VAL:HG12	1:A:1665:ARG:HE	1.83	0.43
1:B:340:LEU:HD23	1:B:341:ARG:HH12	1.82	0.43
1:B:426:LEU:HB3	1:B:464:GLN:NE2	2.33	0.43
1:B:705:MET:HE1	1:B:743:PHE:CD2	2.53	0.43
1:B:1813:ASN:HB2	1:B:1943:LYS:HE3	2.00	0.43
1:C:703:LYS:HA	1:C:703:LYS:HD2	1.86	0.43
1:C:2046:GLN:O	1:C:2050:ARG:HD3	2.18	0.43
1:C:2409:GLY:O	1:C:2413:ARG:N	2.46	0.43
1:B:1774:CYS:HB3	1:B:1776:LYS:HG2	1.99	0.43
1:C:2208:VAL:C	1:C:2210:LEU:H	2.27	0.43
1:A:544:ARG:HB3	1:A:544:ARG:NH1	2.33	0.43
1:A:720:PHE:HA	1:A:724:VAL:HB	2.01	0.43
1:A:858:ARG:HG3	1:A:859:GLU:OE1	2.18	0.43
1:A:1076:LEU:HA	1:A:1079:LEU:HD12	2.01	0.43
1:B:534:LYS:NZ	1:B:538:TYR:HB2	2.33	0.43
1:B:540:CYS:HA	1:B:543:ASP:O	2.18	0.43
1:B:540:CYS:SG	1:B:541:SER:N	2.90	0.43
1:B:720:PHE:CD2	1:B:747:VAL:HG21	2.53	0.43
1:B:1993:LYS:O	1:B:1997:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2334:ARG:HB3	1:B:2335:PRO:HD3	2.00	0.43
1:B:2375:ARG:HE	1:C:2323:TRP:HZ3	1.66	0.43
1:C:479:ALA:O	1:C:484:ARG:NH1	2.52	0.43
1:C:758:ARG:H	1:C:758:ARG:HG2	1.61	0.43
1:A:2395:PHE:HD1	1:A:2401:ALA:O	2.02	0.43
1:A:2412:LYS:HB3	1:B:2221:GLN:HG2	1.99	0.43
1:B:1744:ILE:HD11	1:B:1797:LEU:HD22	2.00	0.43
1:B:1763:LEU:HD12	1:B:1769:TYR:HB2	2.00	0.43
1:C:1361:LEU:O	1:C:1363:SER:N	2.51	0.43
1:C:1963:ASP:HA	1:C:1966:ILE:HD12	2.01	0.43
1:C:2373:ILE:O	1:C:2377:LYS:HG3	2.18	0.43
1:A:1261:ASN:HD22	1:A:1264:ILE:HD12	1.83	0.43
1:A:1525:GLU:HA	1:A:1529:ILE:HB	2.01	0.43
1:A:2385:TYR:HB2	1:A:2457:LEU:HD11	1.99	0.43
1:B:1012:SER:OG	1:B:1013:LEU:N	2.52	0.43
1:B:1332:ALA:O	1:B:1335:GLN:NE2	2.50	0.43
1:B:1592:GLY:HA2	1:B:1645:ARG:HD3	2.00	0.43
1:C:404:LEU:O	1:C:448:ASN:ND2	2.49	0.43
1:C:602:LEU:HA	1:C:605:GLN:HB2	2.00	0.43
1:C:1317:ILE:HD11	1:C:1356:LEU:HD11	2.00	0.43
1:C:1824:MET:HE2	1:C:1863:TYR:CD2	2.54	0.43
1:A:2361:GLY:HA3	1:A:2367:ASP:O	2.18	0.43
1:B:665:LEU:HD21	1:B:710:ASP:HB3	1.99	0.43
1:B:1154:ILE:O	1:B:1158:LEU:HG	2.19	0.43
1:B:1240:ARG:O	1:B:1243:GLN:HG3	2.18	0.43
1:C:545:ASP:HA	1:C:580:PHE:CE1	2.53	0.43
1:C:1239:ILE:HD12	1:C:1292:MET:HG3	2.00	0.43
1:C:2057:PHE:HE1	1:C:2067:ALA:HB1	1.83	0.43
1:A:516:HIS:HB3	1:A:565:TRP:CZ3	2.54	0.43
1:A:1057:LEU:HD13	1:A:1079:LEU:HD13	1.99	0.43
1:A:1354:ILE:HD11	1:A:1382:LEU:HG	2.00	0.43
1:A:1559:LEU:N	1:A:1903:GLY:HA2	2.34	0.43
1:A:1763:LEU:HB3	1:A:1767:ASN:O	2.18	0.43
1:A:2334:ARG:HH21	1:A:2450:GLU:HB2	1.84	0.43
1:B:1466:PHE:HA	1:B:1491:VAL:HB	2.01	0.43
1:B:2042:MET:O	1:B:2046:GLN:HG3	2.18	0.43
1:B:2366:ARG:O	1:B:2375:ARG:NH2	2.52	0.43
1:C:574:ARG:HD2	1:C:660:PHE:CD1	2.53	0.43
1:C:738:LYS:HG3	1:C:742:ARG:HH21	1.83	0.43
1:C:2064:ARG:HD3	1:C:2067:ALA:HB2	2.00	0.43
1:A:1673:LEU:HG	1:A:1674:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2150:LEU:HD23	1:A:2150:LEU:HA	1.90	0.43
1:B:2136:PRO:HD2	1:B:2155:HIS:CE1	2.53	0.43
1:C:340:LEU:HD23	1:C:341:ARG:HH12	1.83	0.43
1:C:1750:LEU:HD23	1:C:1818:PHE:HB3	2.00	0.43
1:A:548:LYS:HB3	1:A:580:PHE:CE2	2.54	0.43
1:A:1265:THR:CA	1:A:1268:TYR:CD2	2.90	0.43
1:B:479:ALA:HB1	1:B:483:GLN:HB3	2.00	0.43
1:B:1280:GLU:HA	1:B:1283:GLN:OE1	2.19	0.43
1:B:1498:ILE:HD11	1:B:2008:GLU:OE2	2.17	0.43
1:B:2453:ASN:OD1	1:B:2454:GLY:N	2.43	0.43
1:C:1763:LEU:HD12	1:C:1769:TYR:HB2	2.00	0.43
1:C:2042:MET:O	1:C:2046:GLN:HG3	2.19	0.43
1:C:2473:LEU:HD23	1:C:2473:LEU:HA	1.89	0.43
1:A:1368:ARG:HD2	1:A:1371:HIS:ND1	2.33	0.43
1:A:1467:ILE:HD13	1:A:1502:PHE:CE1	2.54	0.43
1:A:1824:MET:HG2	1:A:1863:TYR:CE2	2.54	0.43
1:B:559:LEU:HB2	1:B:566:VAL:HG12	2.01	0.43
1:B:1233:MET:N	1:B:1234:PRO:HD2	2.34	0.43
1:B:1498:ILE:HD11	1:B:2008:GLU:CD	2.43	0.43
1:C:850:MET:HA	1:C:853:VAL:HG12	2.01	0.43
1:C:1329:ARG:NH1	1:C:1374:ASP:OD2	2.52	0.43
1:C:1408:LYS:NZ	1:C:1456:ALA:HB1	2.34	0.43
1:C:1885:ILE:O	1:C:1887:ARG:NH1	2.52	0.43
1:C:2277:ASP:HA	1:C:2281:VAL:HB	2.00	0.43
1:A:450:HIS:ND1	1:A:490:LEU:HD22	2.34	0.42
1:B:1456:ALA:O	1:B:1458:LEU:N	2.52	0.42
1:B:1463:ILE:HG13	1:B:1464:ASP:N	2.33	0.42
1:B:2256:PRO:O	1:B:2258:PRO:HD3	2.18	0.42
1:C:567:ILE:HD11	1:C:657:ARG:NH1	2.34	0.42
1:C:1061:CYS:HB3	1:C:1116:HIS:HB3	2.01	0.42
1:C:1559:LEU:N	1:C:1903:GLY:HA2	2.34	0.42
1:C:1989:ARG:O	1:C:1993:LYS:HG2	2.19	0.42
1:C:2348:ASP:OD1	1:C:2354:ARG:NH1	2.52	0.42
1:A:681:TRP:NE1	1:A:686:GLU:OE2	2.52	0.42
1:A:1647:LEU:HG	1:A:1651:PHE:HE2	1.83	0.42
1:A:1873:GLY:HA3	1:A:1878:GLY:HA2	2.00	0.42
1:A:2202:PRO:O	1:A:2206:MET:HG3	2.19	0.42
1:B:1691:ASN:HA	1:B:1694:VAL:HG22	2.01	0.42
1:C:511:LEU:HD13	1:C:532:HIS:HA	2.00	0.42
1:C:542:GLN:HE22	1:C:544:ARG:CD	2.32	0.42
1:C:576:ILE:O	1:C:580:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:TRP:NE1	1:A:475:SER:OG	2.43	0.42
1:A:1544:TYR:O	1:A:1545:LEU:HD22	2.19	0.42
1:A:1672:ARG:HH21	1:A:1677:PRO:HD3	1.85	0.42
1:A:2165:ARG:O	1:A:2215:GLY:HA3	2.20	0.42
1:B:1096:TYR:CZ	1:B:1153:LYS:HB3	2.53	0.42
1:B:1149:LEU:HB3	1:B:1284:VAL:HG22	2.01	0.42
1:C:546:THR:O	1:C:549:ILE:N	2.52	0.42
1:C:702:SER:HA	1:C:742:ARG:HH12	1.84	0.42
1:A:1129:MET:HE3	1:A:1135:PHE:CE1	2.54	0.42
1:B:672:LEU:HB3	1:B:711:LEU:HG	2.02	0.42
1:B:1145:ARG:NH2	1:B:1254:LEU:H	2.17	0.42
1:B:1556:PHE:HD2	1:B:1905:VAL:HG11	1.84	0.42
1:B:2208:VAL:O	1:B:2209:SER:OG	2.21	0.42
1:C:540:CYS:O	1:C:543:ASP:HB2	2.19	0.42
1:C:1864:ARG:O	1:C:1954:GLU:N	2.38	0.42
1:C:1915:GLU:O	1:C:1919:GLN:HG2	2.19	0.42
1:C:2079:ARG:HB3	1:C:2122:PHE:HZ	1.84	0.42
1:A:358:VAL:O	1:A:362:ILE:HG12	2.19	0.42
1:A:1306:LEU:HB3	1:A:1312:TRP:CG	2.55	0.42
1:B:542:GLN:CD	1:B:542:GLN:N	2.77	0.42
1:B:1762:LEU:HD13	1:B:1781:VAL:HG22	2.01	0.42
1:B:2010:PHE:CD2	1:B:2064:ARG:HA	2.53	0.42
1:C:1357:LEU:O	1:C:1358:PHE:C	2.62	0.42
1:C:1386:ALA:O	1:C:1391:ILE:N	2.48	0.42
1:C:2062:VAL:HG23	1:C:2063:VAL:HG23	2.01	0.42
1:A:1149:LEU:O	1:A:1153:LYS:HG3	2.19	0.42
1:A:2309:GLU:OE2	1:A:2348:ASP:HB2	2.20	0.42
1:B:1084:SER:HB3	1:B:1087:GLN:HG2	2.01	0.42
1:B:1435:LYS:CE	1:B:1503:GLU:HB3	2.50	0.42
1:B:1579:PRO:HD3	1:B:1887:ARG:HE	1.85	0.42
1:B:1673:LEU:HG	1:B:1674:TRP:CD1	2.54	0.42
1:C:1243:GLN:O	1:C:1247:TRP:HD1	2.03	0.42
1:C:2017:LEU:HD21	1:C:2047:LEU:HD22	2.01	0.42
1:A:1033:MET:HB3	1:A:1036:LEU:HD13	2.01	0.42
1:A:1045:LYS:HA	1:A:1045:LYS:HD2	1.86	0.42
1:A:1060:ILE:HG13	1:A:1079:LEU:HD11	2.01	0.42
1:A:1447:PHE:O	1:A:1452:GLU:HB2	2.20	0.42
1:A:2421:TRP:CE2	1:A:2425:GLU:HG3	2.55	0.42
1:B:1395:ASN:HB3	1:B:1399:LEU:HD11	2.00	0.42
1:B:1532:ALA:HB1	1:B:2050:ARG:HG3	2.01	0.42
1:B:1690:PHE:O	1:B:1694:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:MET:SD	1:C:763:MET:N	2.92	0.42
1:B:1459:ILE:O	1:B:1463:ILE:HG12	2.20	0.42
1:C:1244:LYS:HE2	1:C:1261:ASN:OD1	2.19	0.42
1:C:1498:ILE:HG22	1:C:2008:GLU:HG3	2.02	0.42
1:A:548:LYS:HA	1:A:548:LYS:HD3	1.64	0.42
1:A:711:LEU:HD22	1:A:719:PHE:CE1	2.55	0.42
1:A:758:ARG:H	1:A:758:ARG:HG2	1.64	0.42
1:A:1099:LEU:O	1:A:1114:GLN:NE2	2.53	0.42
1:A:2057:PHE:HE1	1:A:2067:ALA:HB1	1.85	0.42
1:A:2355:ILE:O	1:A:2359:LEU:HG	2.20	0.42
1:C:335:ARG:HA	1:C:338:MET:HE2	2.02	0.42
1:C:1358:PHE:HZ	1:C:1383:LEU:HD11	1.85	0.42
1:C:1388:ASN:OD1	1:C:1389:SER:N	2.53	0.42
1:C:1539:LEU:C	1:C:1541:GLU:H	2.27	0.42
1:C:2154:ASP:OD1	1:C:2195:GLN:NE2	2.53	0.42
1:A:2331:TYR:HB3	1:A:2452:SER:OG	2.19	0.42
1:B:711:LEU:O	1:B:715:ILE:HB	2.20	0.42
1:B:1095:VAL:O	1:B:1099:LEU:HG	2.20	0.42
1:B:1406:TRP:O	1:B:1410:ILE:HG12	2.20	0.42
1:B:1790:PRO:O	1:B:1863:TYR:OH	2.21	0.42
1:A:613:VAL:HG23	1:A:664:LEU:HD22	2.01	0.41
1:A:762:MET:SD	1:A:801:GLY:N	2.93	0.41
1:A:1527:TYR:HE1	1:A:2004:GLN:HB2	1.84	0.41
1:A:1749:ASN:HA	1:A:1817:GLU:HB2	2.02	0.41
1:B:543:ASP:OD2	1:B:547:GLN:OE1	2.37	0.41
1:B:1045:LYS:HA	1:B:1045:LYS:HD2	1.85	0.41
1:B:1333:GLN:HG2	1:B:1337:PHE:HE2	1.85	0.41
1:C:1740:LEU:N	1:C:1794:ALA:O	2.41	0.41
1:A:628:ARG:HA	1:A:631:ALA:HB3	2.02	0.41
1:A:1048:PRO:HA	1:A:1049:PRO:HD3	1.97	0.41
1:A:1141:MET:SD	1:A:1255:GLN:HB3	2.60	0.41
1:B:1259:SER:HB3	1:B:1264:ILE:HD11	2.01	0.41
1:B:2322:LEU:HD23	1:B:2322:LEU:HA	1.92	0.41
1:C:549:ILE:HA	1:C:552:ILE:HG22	2.02	0.41
1:C:1292:MET:HB3	1:C:1296:PHE:CD2	2.54	0.41
1:C:1664:PRO:HB2	1:C:1667:PHE:HB3	2.02	0.41
1:C:2368:GLY:O	1:C:2372:THR:HG23	2.21	0.41
1:C:2402:TYR:CZ	1:C:2406:GLN:HG3	2.55	0.41
1:A:1152:LEU:HD23	1:A:1288:ALA:HA	2.01	0.41
1:A:1263:GLU:O	1:A:1267:ILE:HD12	2.20	0.41
1:B:400:LEU:HD23	1:B:404:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:SER:O	1:B:544:ARG:NH2	2.51	0.41
1:B:672:LEU:HD23	1:B:711:LEU:HD11	2.02	0.41
1:B:1446:LYS:O	1:B:1515:ASN:ND2	2.46	0.41
1:B:1469:PRO:HG3	1:B:1490:PRO:CA	2.50	0.41
1:B:2398:CYS:HB3	1:B:2401:ALA:HB3	2.03	0.41
1:C:574:ARG:HD3	1:C:663:PHE:HD2	1.85	0.41
1:C:1588:ILE:O	1:C:1648:GLN:NE2	2.39	0.41
1:A:1560:LYS:HB2	1:A:1663:VAL:HG22	2.03	0.41
1:B:1247:TRP:HE3	1:B:1264:ILE:HB	1.85	0.41
1:B:2027:PRO:HA	1:B:2028:PRO:HD3	1.96	0.41
1:C:399:VAL:HG11	1:C:413:LEU:HD13	2.02	0.41
1:C:711:LEU:O	1:C:715:ILE:HB	2.20	0.41
1:C:1154:ILE:O	1:C:1158:LEU:HG	2.20	0.41
1:C:2168:VAL:HG13	1:C:2175:LEU:HD21	2.02	0.41
1:A:508:LEU:HD22	1:A:532:HIS:ND1	2.36	0.41
1:C:546:THR:O	1:C:549:ILE:HB	2.21	0.41
1:C:1447:PHE:O	1:C:1452:GLU:HB2	2.20	0.41
1:A:653:GLU:HB3	1:A:657:ARG:HH12	1.85	0.41
1:A:742:ARG:HA	1:A:745:LYS:HD2	2.02	0.41
1:B:458:TRP:CE2	1:B:499:LYS:HD2	2.56	0.41
1:B:1031:LEU:HB3	1:B:1033:MET:CE	2.51	0.41
1:B:2253:PRO:HA	1:B:2254:PRO:HD3	1.97	0.41
1:C:479:ALA:HB1	1:C:483:GLN:HB3	2.02	0.41
1:C:672:LEU:HB3	1:C:711:LEU:HG	2.02	0.41
1:C:1548:VAL:O	1:C:1660:GLN:HB3	2.21	0.41
1:A:450:HIS:HB3	1:A:490:LEU:HD13	2.03	0.41
1:A:1452:GLU:HG3	1:A:1455:GLY:H	1.85	0.41
1:B:720:PHE:CE1	1:B:743:PHE:HB3	2.55	0.41
1:B:1683:GLN:HG2	1:B:1877:GLY:HA2	2.01	0.41
1:C:1045:LYS:HA	1:C:1045:LYS:HD2	1.88	0.41
1:A:544:ARG:HH22	1:A:580:PHE:HD1	1.62	0.41
1:A:732:LEU:HD11	1:A:736:GLY:HA3	2.02	0.41
1:B:540:CYS:O	1:B:543:ASP:C	2.64	0.41
1:B:541:SER:HA	1:B:544:ARG:HH21	1.86	0.41
1:B:2008:GLU:H	1:B:2008:GLU:HG2	1.63	0.41
1:C:652:GLN:HG3	1:C:653:GLU:N	2.35	0.41
1:C:1524:THR:CG2	1:C:1525:GLU:N	2.83	0.41
1:C:2406:GLN:HA	1:C:2412:LYS:HZ3	1.86	0.41
1:A:1119:LYS:HA	1:A:1119:LYS:HD3	1.91	0.41
1:A:1264:ILE:C	1:A:1268:TYR:CE2	2.99	0.41
1:A:1316:ILE:HG13	1:A:1336:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1536:CYS:HB2	1:A:2099:ARG:NH2	2.35	0.41
1:B:542:GLN:HG2	1:B:543:ASP:H	1.85	0.41
1:B:549:ILE:HA	1:B:552:ILE:HG22	2.02	0.41
1:B:672:LEU:N	1:B:710:ASP:O	2.39	0.41
1:B:717:LYS:HE3	1:B:747:VAL:HA	2.02	0.41
1:B:1386:ALA:O	1:B:1390:ASN:N	2.54	0.41
1:B:2067:ALA:HA	1:B:2070:TRP:HD1	1.85	0.41
1:B:2366:ARG:HH12	1:C:2323:TRP:CD1	2.39	0.41
1:C:639:PRO:HG3	1:C:690:TYR:CD2	2.56	0.41
1:C:802:PRO:C	1:C:804:LEU:H	2.29	0.41
1:C:854:LEU:HA	1:C:857:LEU:HD12	2.03	0.41
1:C:1427:LEU:HD21	1:C:1491:VAL:HG12	2.03	0.41
1:C:1739:THR:HA	1:C:1794:ALA:HB3	2.03	0.41
1:C:2024:LEU:O	1:C:2033:LEU:HD11	2.21	0.41
1:A:390:ILE:HG12	1:A:395:ILE:HD12	2.03	0.41
1:B:1588:ILE:HB	1:B:1648:GLN:NE2	2.36	0.41
1:C:1414:VAL:HG11	1:C:1491:VAL:HG22	2.03	0.41
1:C:2020:ASN:O	1:C:2024:LEU:HG	2.21	0.41
1:A:662:ARG:O	1:A:666:LYS:HG2	2.21	0.40
1:A:845:GLN:OE1	1:A:849:ARG:NH1	2.54	0.40
1:A:1495:PRO:N	1:A:1496:PRO:HD2	2.35	0.40
1:A:1824:MET:HG2	1:A:1863:TYR:CD2	2.56	0.40
1:B:1723:ILE:HG12	1:B:1730:ARG:HD2	2.03	0.40
1:C:630:TYR:HB2	1:C:634:HIS:ND1	2.36	0.40
1:C:1825:GLU:HB3	1:C:1826:PRO:HD3	2.01	0.40
1:A:1701:LEU:O	1:A:1706:HIS:N	2.51	0.40
1:B:512:TRP:CD1	1:B:554:ARG:HH12	2.39	0.40
1:B:1121:GLY:C	1:B:1124:PRO:HD2	2.47	0.40
1:B:1887:ARG:H	1:B:1887:ARG:HG2	1.74	0.40
1:B:2081:SER:OG	1:B:2084:VAL:HB	2.21	0.40
1:C:1041:ARG:HH22	1:C:1143:THR:HG22	1.86	0.40
1:C:1265:THR:O	1:C:1269:GLU:HG3	2.22	0.40
1:C:1319:LEU:O	1:C:1329:ARG:HG2	2.21	0.40
1:C:1404:ILE:HD12	1:C:1404:ILE:H	1.85	0.40
1:C:1445:LYS:C	1:C:1447:PHE:N	2.77	0.40
1:C:1710:LEU:O	1:C:1714:LEU:HG	2.20	0.40
1:C:1744:ILE:HG13	1:C:1798:LYS:N	2.36	0.40
1:C:2242:SER:HA	1:C:2245:MET:CE	2.51	0.40
1:C:2283:THR:HG23	1:C:2287:LYS:NZ	2.37	0.40
1:C:536:LEU:HB3	1:C:548:LYS:HZ2	1.86	0.40
1:C:536:LEU:O	1:C:548:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:GLU:HA	1:C:849:ARG:HD3	2.01	0.40
1:C:1357:LEU:O	1:C:1360:VAL:HG22	2.21	0.40
1:C:1814:ASP:HB2	1:C:1816:PHE:CZ	2.57	0.40
1:C:2200:SER:HB3	1:C:2203:ALA:HB3	2.03	0.40
1:C:2290:ILE:O	1:C:2294:SER:HB3	2.21	0.40
1:A:1026:ASP:OD2	1:A:1084:SER:OG	2.33	0.40
1:A:1513:VAL:HG21	1:A:2039:GLU:HB2	2.02	0.40
1:B:548:LYS:HE2	1:B:576:ILE:HG23	2.04	0.40
1:B:753:LYS:O	1:B:754:LEU:HD23	2.21	0.40
1:B:1560:LYS:HD2	1:B:1661:TYR:CE2	2.56	0.40
1:B:2364:ASP:HB2	1:C:2283:THR:HG22	2.04	0.40
1:C:827:TYR:HE2	1:C:1024:VAL:HA	1.86	0.40
1:C:1095:VAL:O	1:C:1099:LEU:HG	2.21	0.40
1:C:1567:TYR:HB2	1:C:1686:ALA:HB2	2.02	0.40
1:C:1672:ARG:HA	1:C:1678:VAL:HG23	2.03	0.40
1:C:2240:ASN:HB3	1:C:2270:PRO:HA	2.04	0.40
1:A:494:LEU:HD22	1:A:503:MET:HE1	2.04	0.40
1:A:536:LEU:HD12	1:A:548:LYS:CE	2.50	0.40
1:A:680:ILE:HD12	1:A:700:TRP:CZ3	2.56	0.40
1:A:778:VAL:HG21	1:A:790:ILE:HG13	2.04	0.40
1:A:1585:ILE:HG22	1:A:1648:GLN:HG2	2.03	0.40
1:A:1682:GLU:HB3	1:A:1684:HIS:CE1	2.57	0.40
1:A:1687:LEU:HA	1:A:1690:PHE:HB3	2.04	0.40
1:A:1694:VAL:HG12	1:A:1710:LEU:HD13	2.02	0.40
1:A:1869:LEU:HD23	1:A:1950:ILE:HD12	2.02	0.40
1:A:2229:TYR:CD2	1:A:2293:CYS:HB2	2.56	0.40
1:B:526:ASP:HA	1:B:529:LEU:HD12	2.03	0.40
1:B:711:LEU:O	1:B:712:ASP:HB2	2.21	0.40
1:B:1028:GLY:O	1:B:1037:ARG:NH2	2.55	0.40
1:B:1462:LEU:O	1:B:1467:ILE:HD12	2.21	0.40
1:B:1539:LEU:C	1:B:1541:GLU:H	2.30	0.40
1:C:2172:GLY:C	1:C:2174:HIS:H	2.29	0.40
1:C:2180:ASN:HA	1:C:2183:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1721/2579 (67%)	1631 (95%)	86 (5%)	4 (0%)	43	71
1	B	1721/2579 (67%)	1631 (95%)	90 (5%)	0	100	100
1	C	1708/2579 (66%)	1614 (94%)	88 (5%)	6 (0%)	30	60
All	All	5150/7737 (67%)	4876 (95%)	264 (5%)	10 (0%)	44	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	ARG
1	A	2454	GLY
1	C	2365	ASP
1	C	546	THR
1	C	1348	ARG
1	C	2248	SER
1	A	541	SER
1	C	1362	GLY
1	C	712	ASP
1	A	712	ASP

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	1544/2286 (68%)	1539 (100%)	5 (0%)	86	86
1	B	1544/2286 (68%)	1542 (100%)	2 (0%)	88	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1532/2286 (67%)	1527 (100%)	5 (0%)	86	86
All	All	4620/6858 (67%)	4608 (100%)	12 (0%)	84	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	542	GLN
1	A	544	ARG
1	A	545	ASP
1	A	547	GLN
1	A	548	LYS
1	B	545	ASP
1	B	547	GLN
1	C	542	GLN
1	C	545	ASP
1	C	1354	ILE
1	C	1356	LEU
1	C	1357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	A	408	GLN
1	A	716	ASN
1	A	807	ASN
1	A	817	GLN
1	A	1032	ASN
1	A	1064	HIS
1	A	1392	ASN
1	A	1402	ASN
1	A	2004	GLN
1	A	2011	GLN
1	A	2046	GLN
1	A	2177	GLN
1	A	2357	ASN
1	A	2374	GLN
1	B	344	GLN
1	B	356	ASN
1	B	406	GLN
1	B	478	ASN

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Mol	Chain	Res	Type
1	B	516	HIS
1	B	610	HIS
1	B	655	GLN
1	B	716	ASN
1	B	799	ASN
1	B	807	ASN
1	B	1064	HIS
1	B	1333	GLN
1	B	1472	ASN
1	B	1640	ASN
1	B	1729	HIS
1	B	1741	ASN
1	B	1746	ASN
1	B	2011	GLN
1	B	2155	HIS
1	B	2177	GLN
1	B	2221	GLN
1	B	2234	GLN
1	C	408	GLN
1	C	478	ASN
1	C	532	HIS
1	C	542	GLN
1	C	610	HIS
1	C	655	GLN
1	C	676	GLN
1	C	799	ASN
1	C	1032	ASN
1	C	1392	ASN
1	C	1402	ASN
1	C	2046	GLN
1	C	2180	ASN
1	C	2257	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

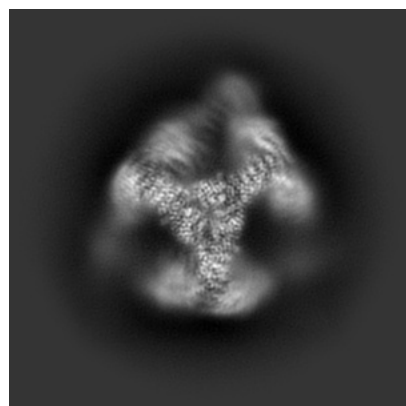
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14368. These allow visual inspection of the internal detail of the map and identification of artifacts.

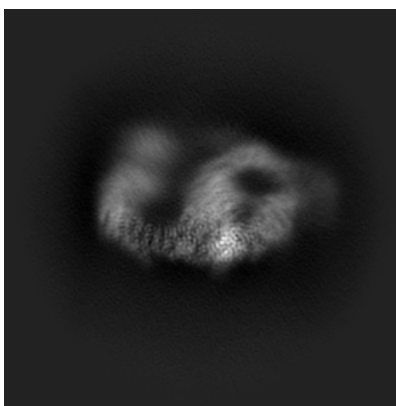
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

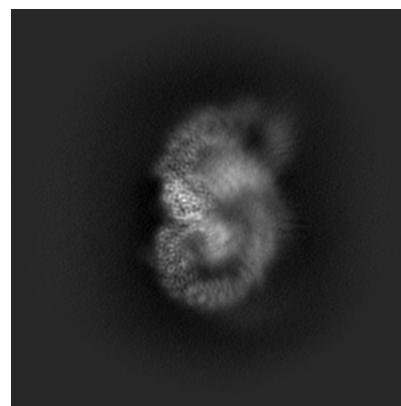
6.1.1 Primary map



X

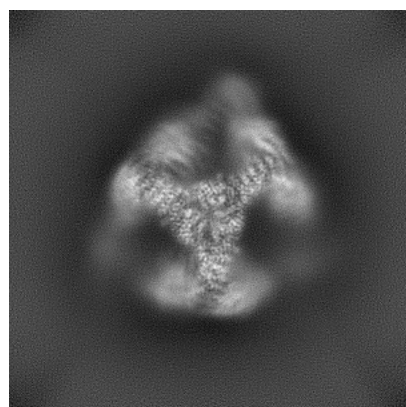


Y

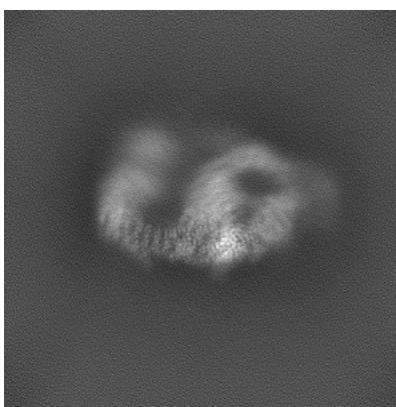


Z

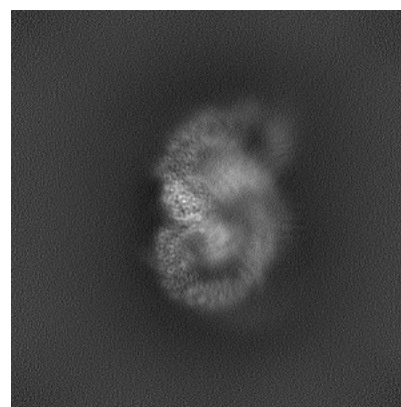
6.1.2 Raw map



X



Y

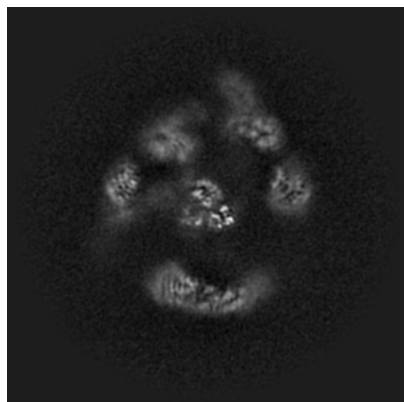


Z

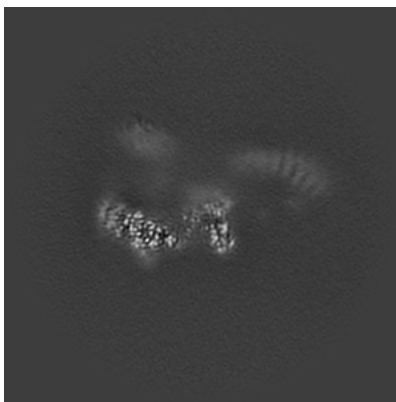
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

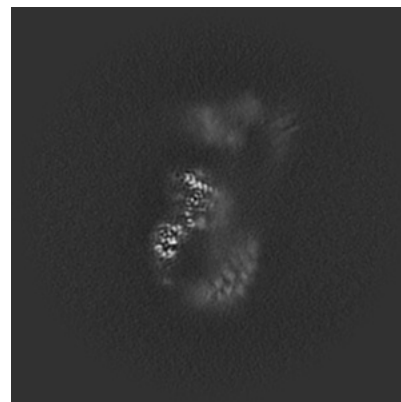
6.2.1 Primary map



X Index: 224

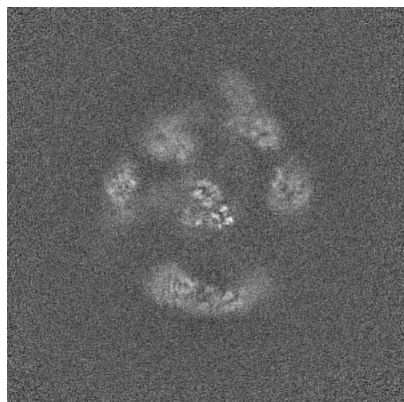


Y Index: 224

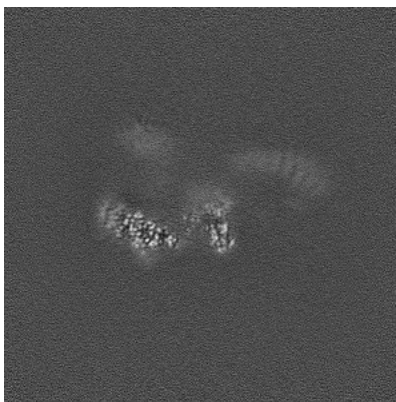


Z Index: 224

6.2.2 Raw map



X Index: 224



Y Index: 224

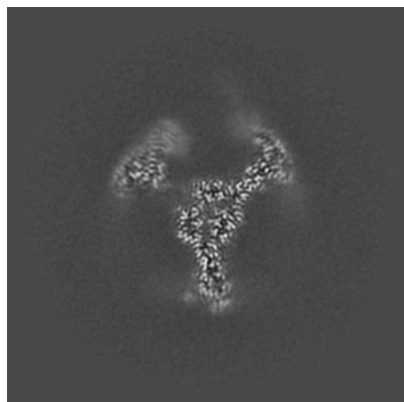


Z Index: 224

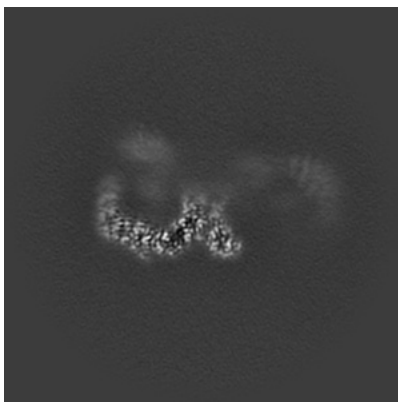
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

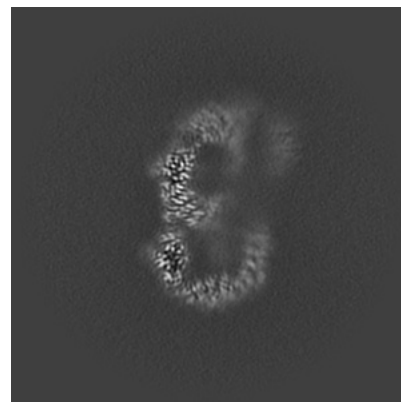
6.3.1 Primary map



X Index: 196

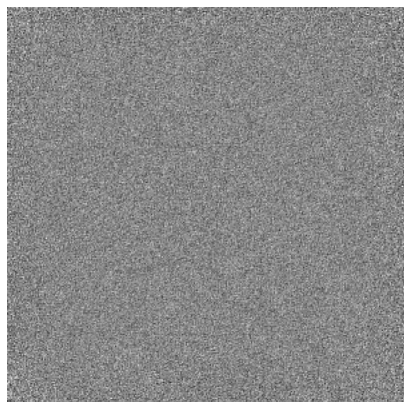


Y Index: 237

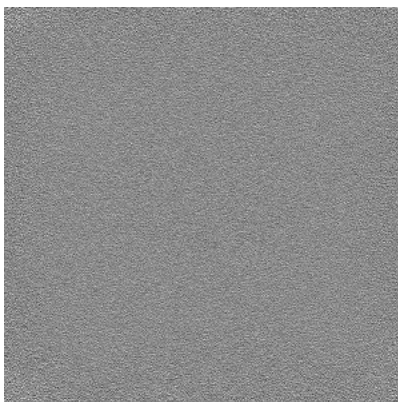


Z Index: 248

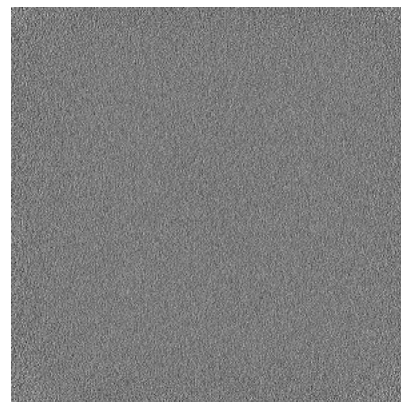
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

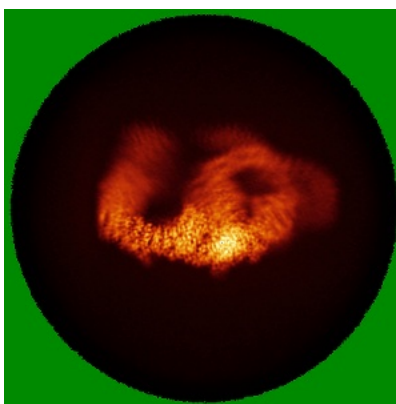
The images above show the largest variance slices of the map in three orthogonal directions.

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

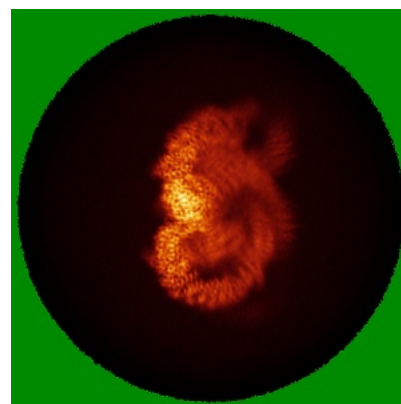
6.4.1 Primary map



X

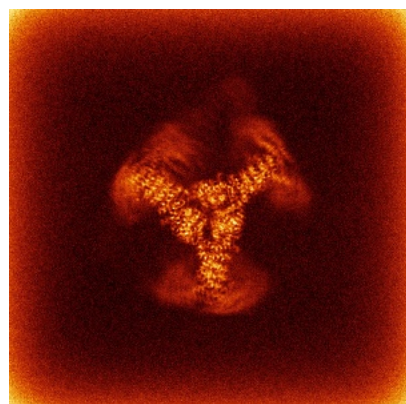


Y



Z

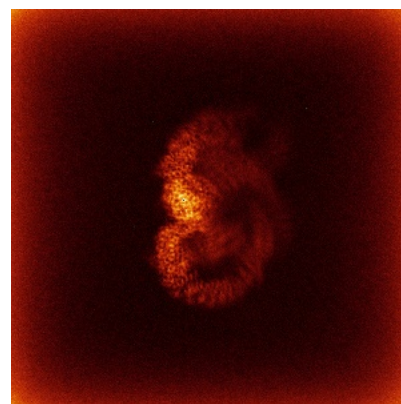
6.4.2 Raw map



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.

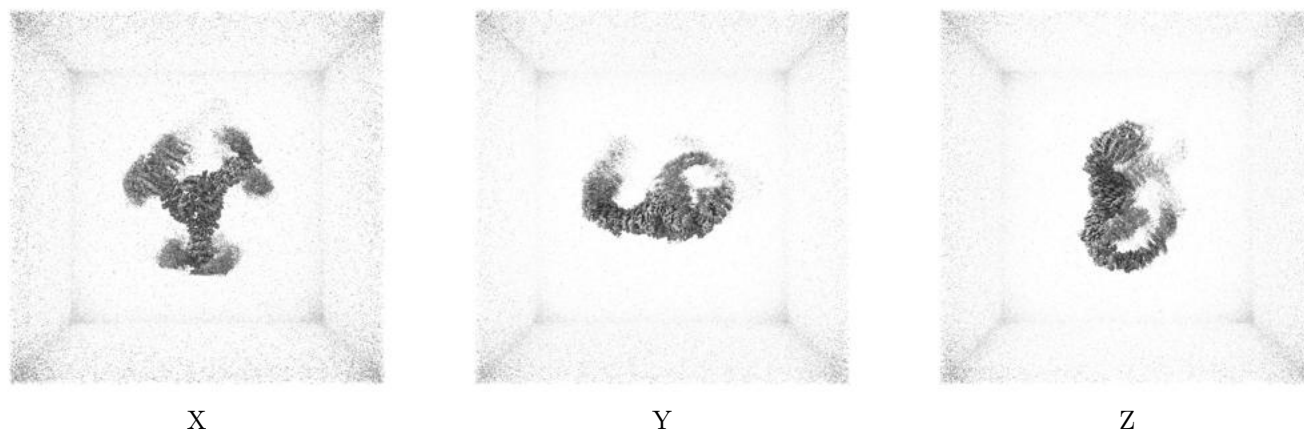
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.221. 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.

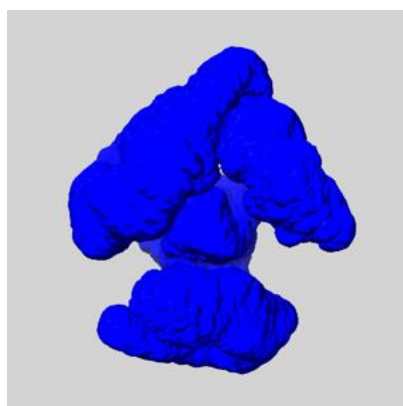
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

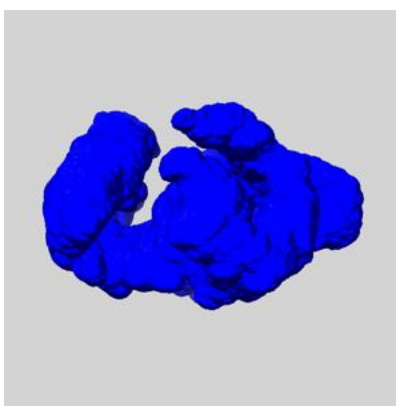
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

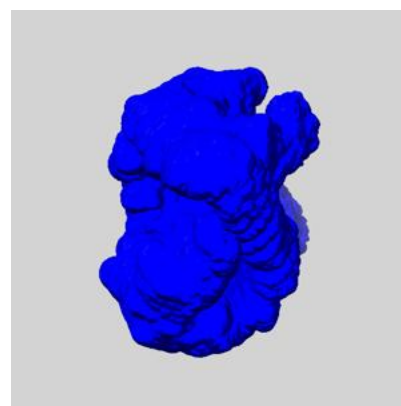
6.6.1 emd_14368_msk_1.map [i](#)



X



Y

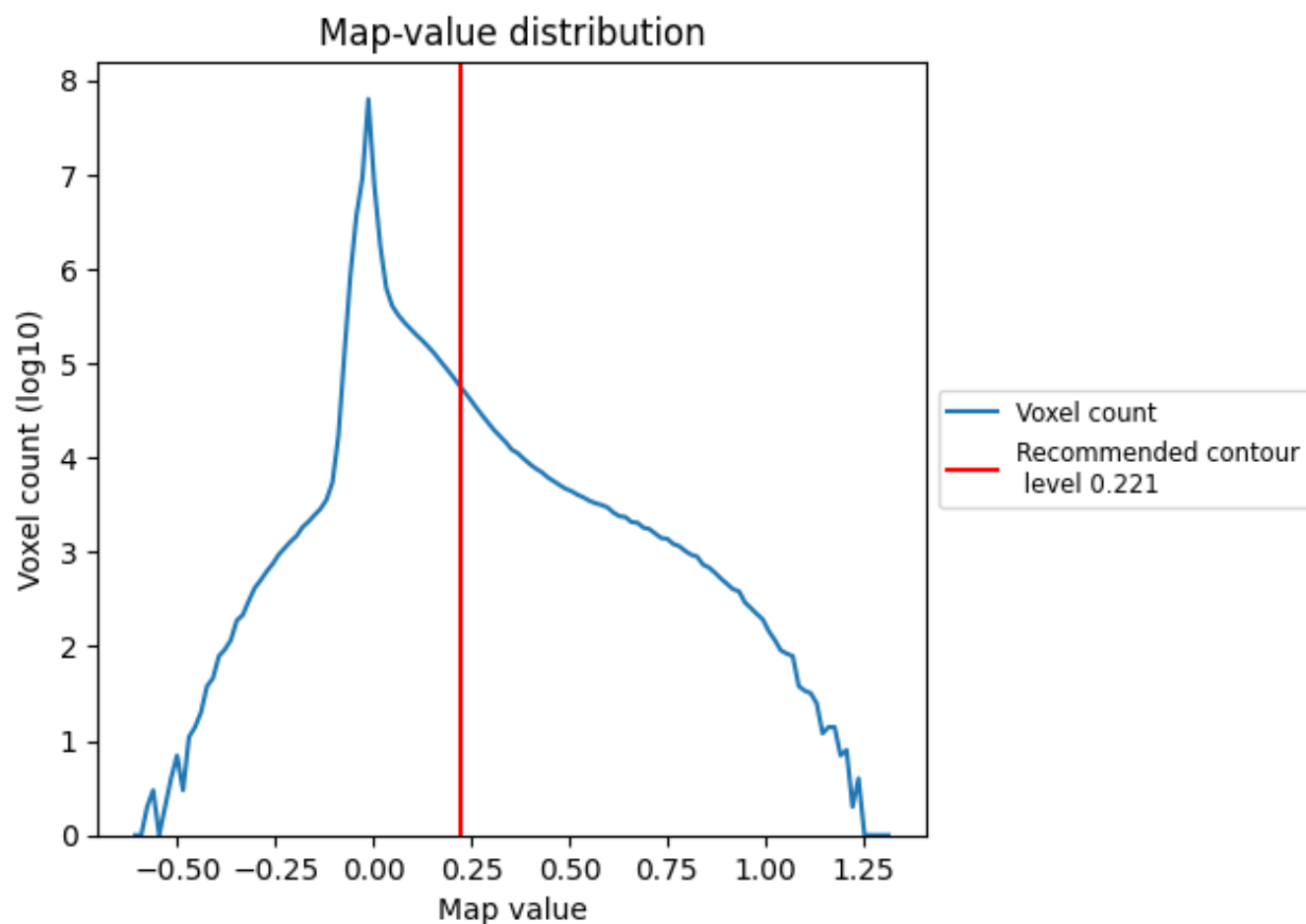


Z

7 Map analysis [i](#)

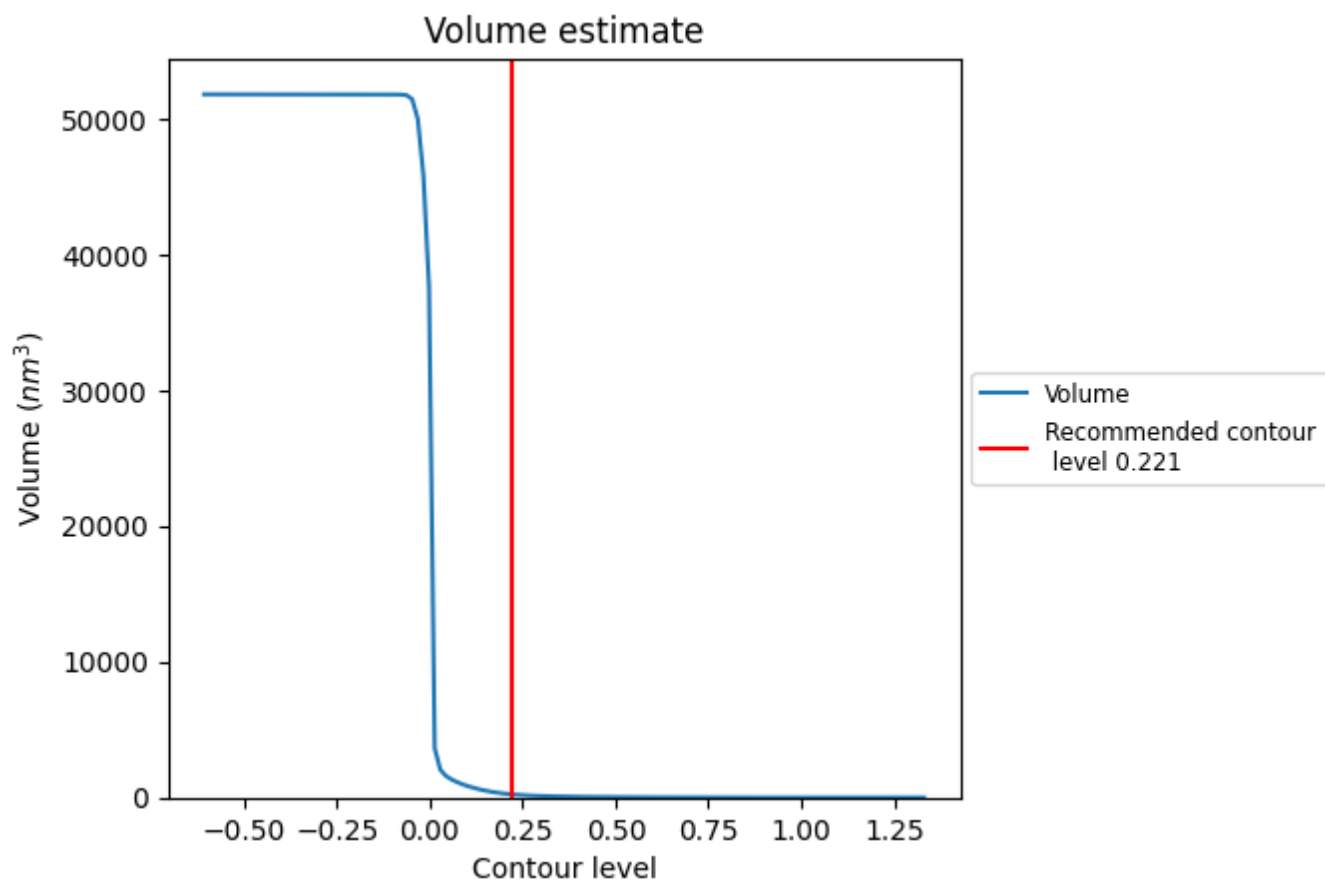
This section contains the results of statistical analysis of the map.

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.

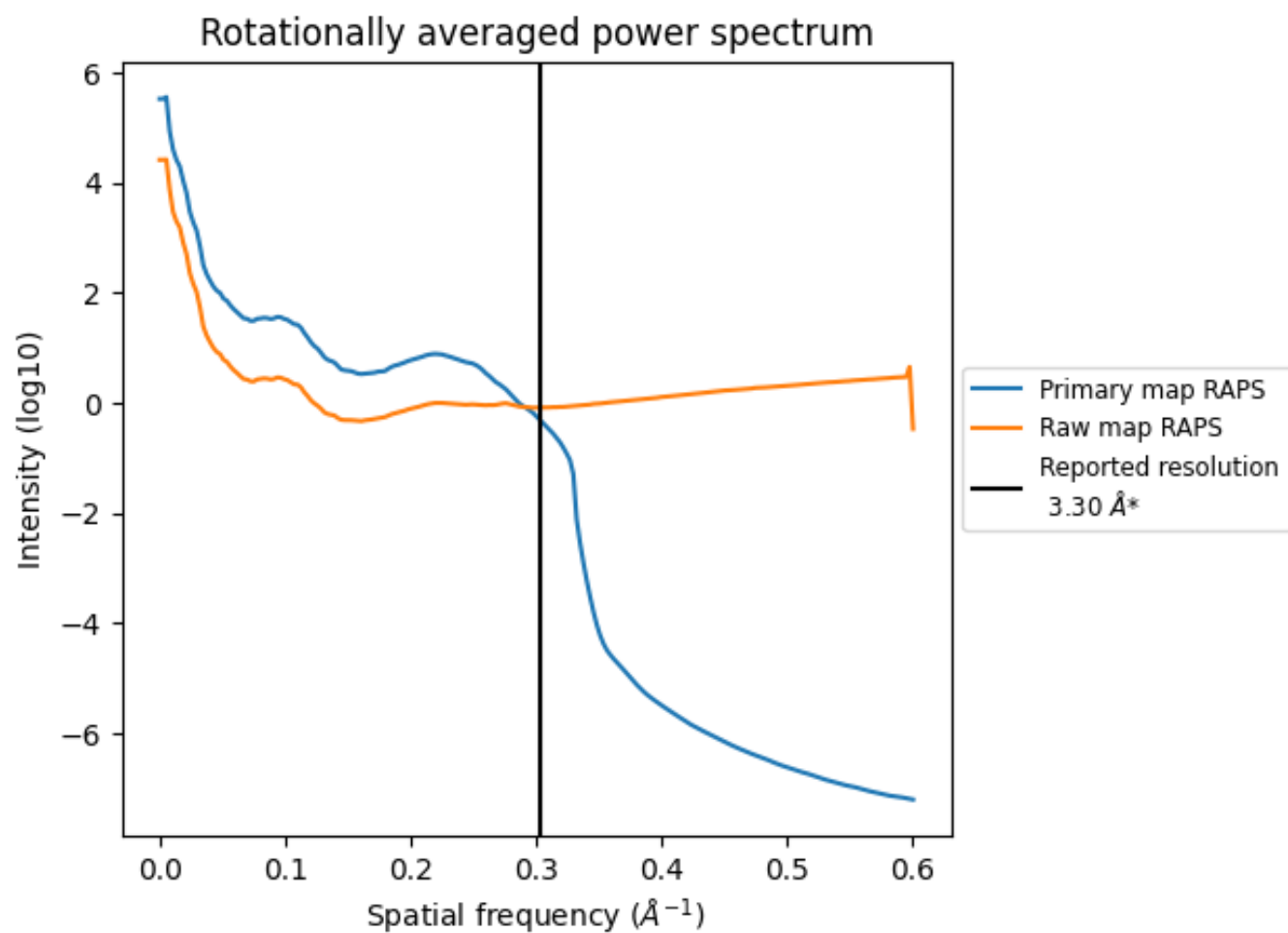
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm³; this corresponds to an approximate mass of 212 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 ⓘ

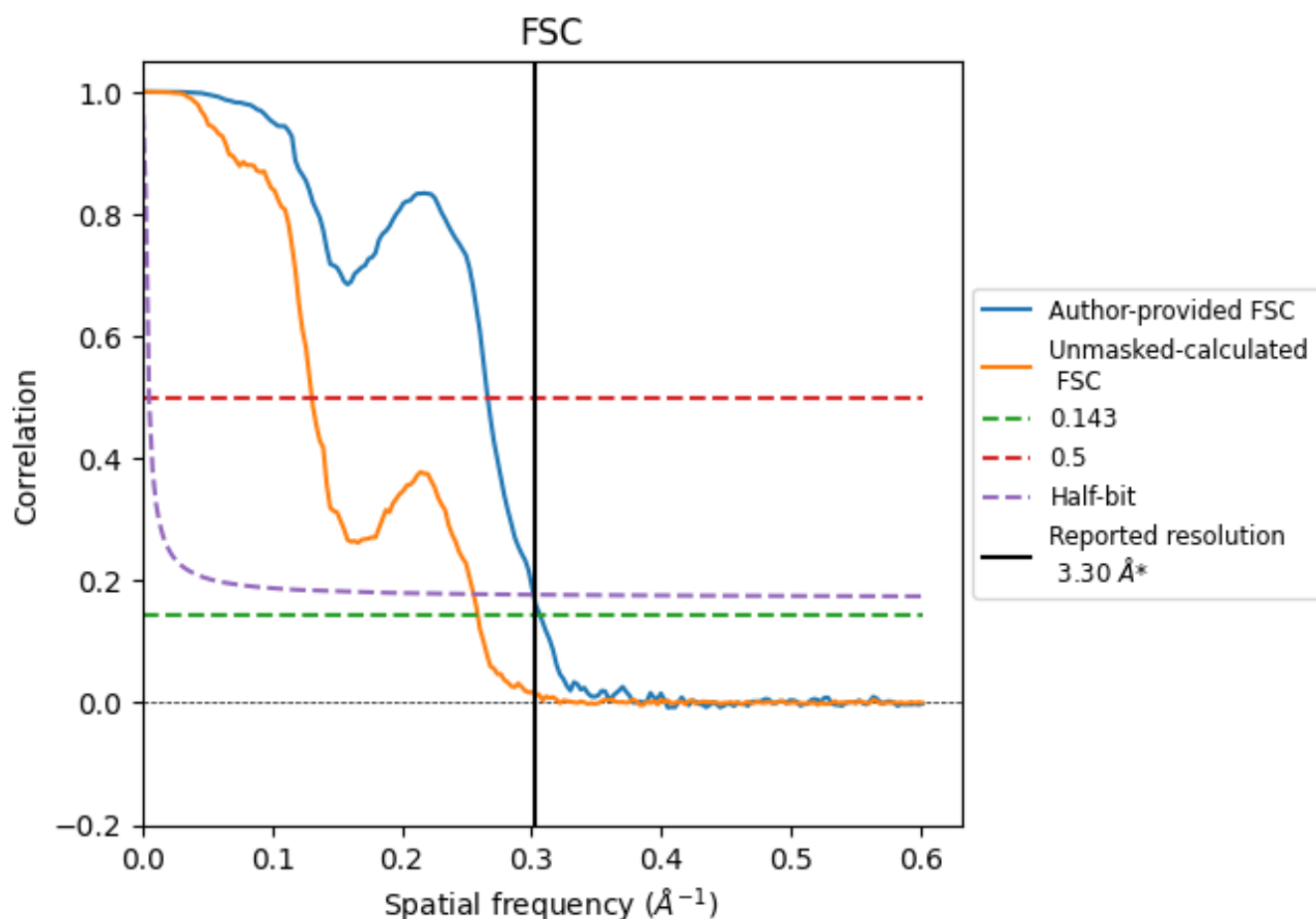


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 Å⁻¹

8.2 Resolution estimates

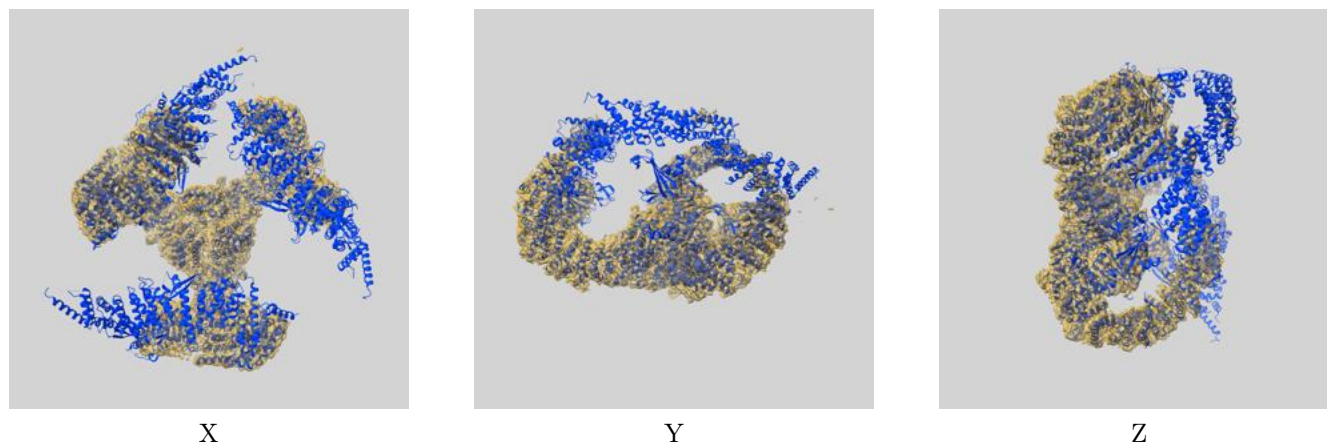
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.76	3.32
Unmasked-calculated*	3.87	7.65	3.92

*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 3.87 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

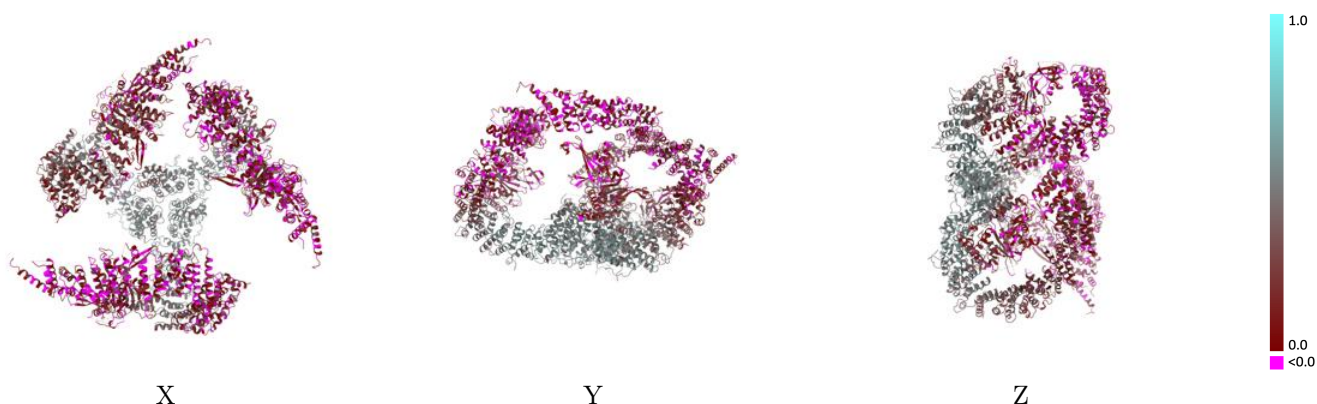
This section contains information regarding the fit between EMDB map EMD-14368 and PDB model 7YXX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



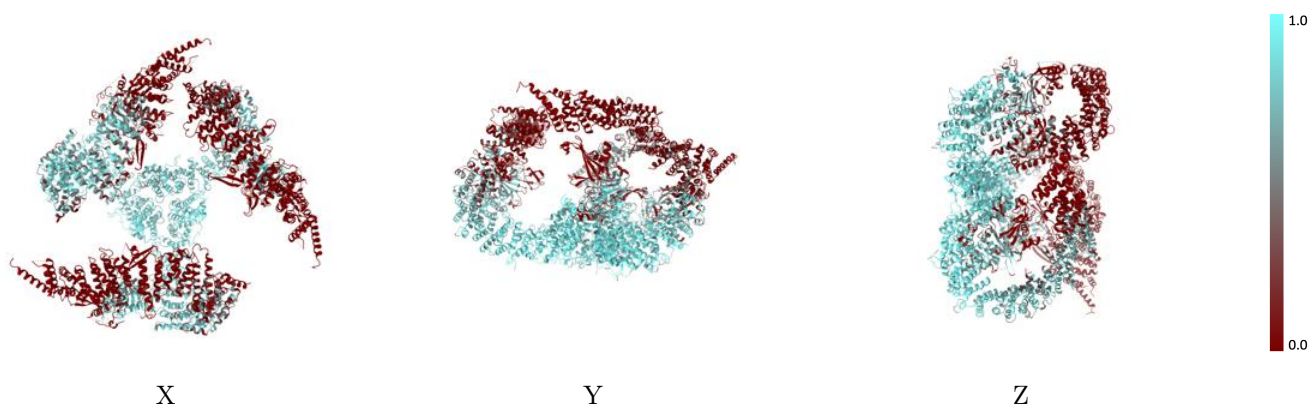
The images above show the 3D surface view of the map at the recommended contour level 0.221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



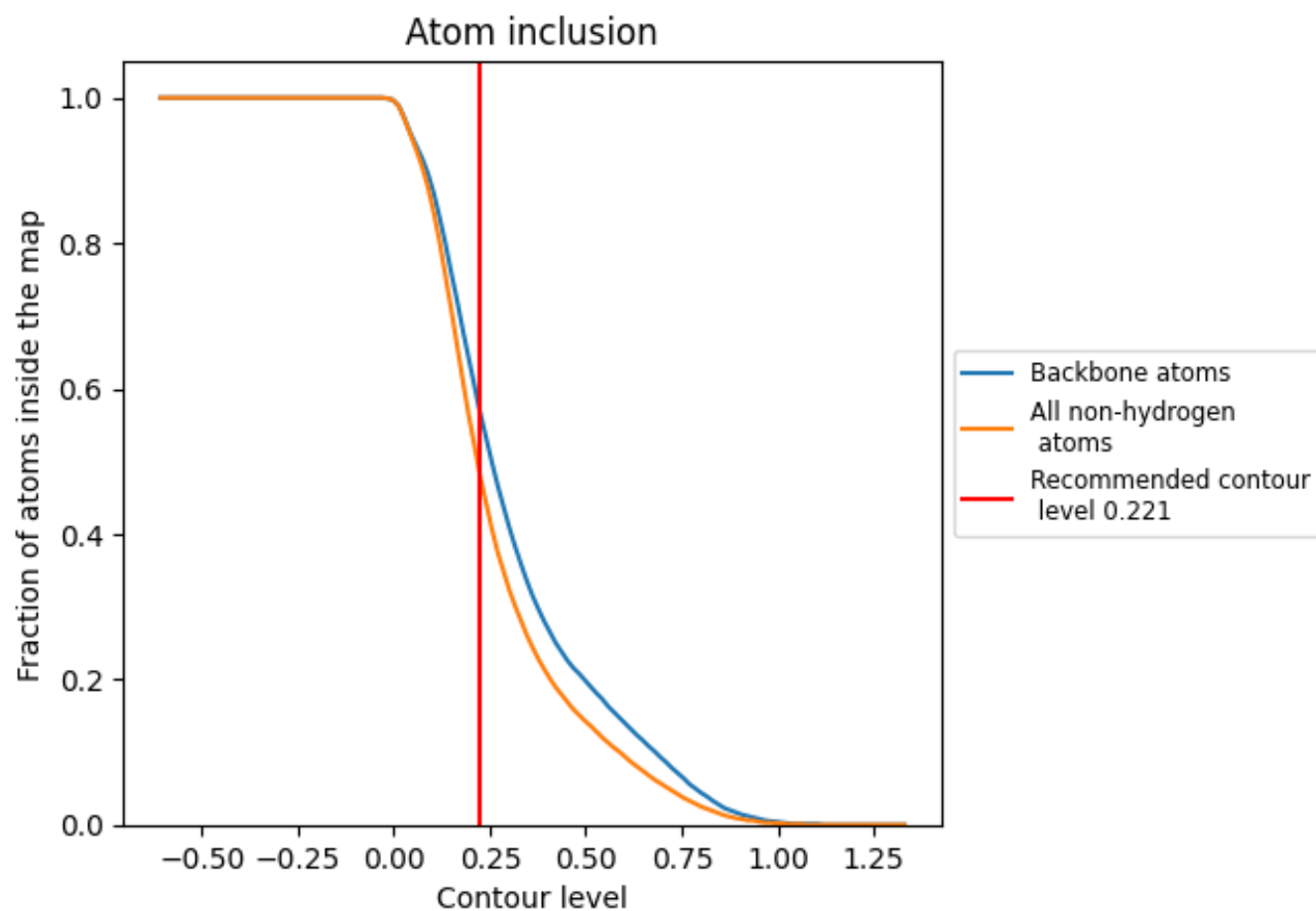
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.221).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 49% 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 (0.221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4900	0.2580
A	0.5790	0.3010
B	0.4570	0.2330
C	0.4330	0.2400

