



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:20 AM UTC

PDB ID : 6JI8 / pdb_00006ji8
EMDB ID : EMD-9833
Title : Structure of RyR2 (F/apoCaM dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-20
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

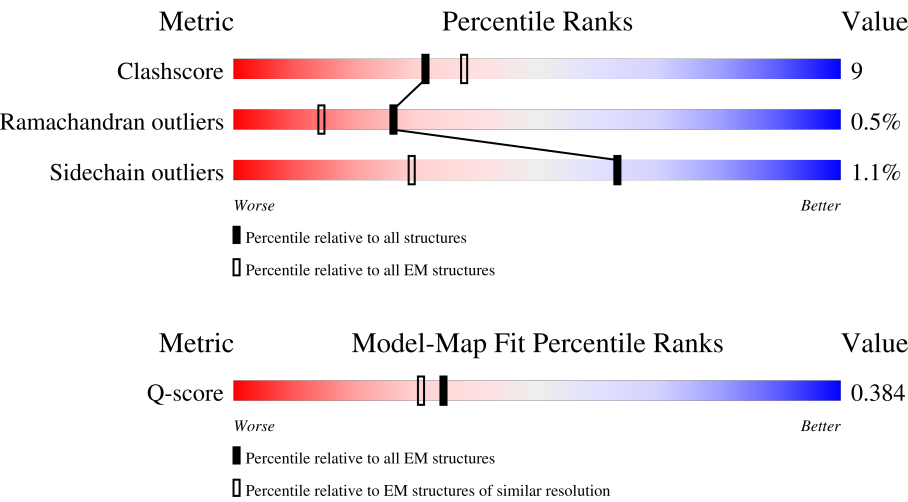
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	4968	11% 57% 13% 29%
1	D	4968	11% 57% 13% 29%
1	G	4968	11% 57% 13% 29%
1	J	4968	11% 57% 13% 29%

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Mol	Chain	Length	Quality of chain
2	B	108	 81%17%..
2	E	108	 81%17%..
2	H	108	 84%14%..
2	K	108	 81%17%..
3	C	149	 45%72%19%•7%
3	F	149	 44%72%20%•7%
3	I	149	 46%72%19%•7%
3	L	149	 45%73%19%•7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 115060 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		
1	D	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		
1	G	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		
1	J	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		
3	F	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		
3	I	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		
3	L	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		

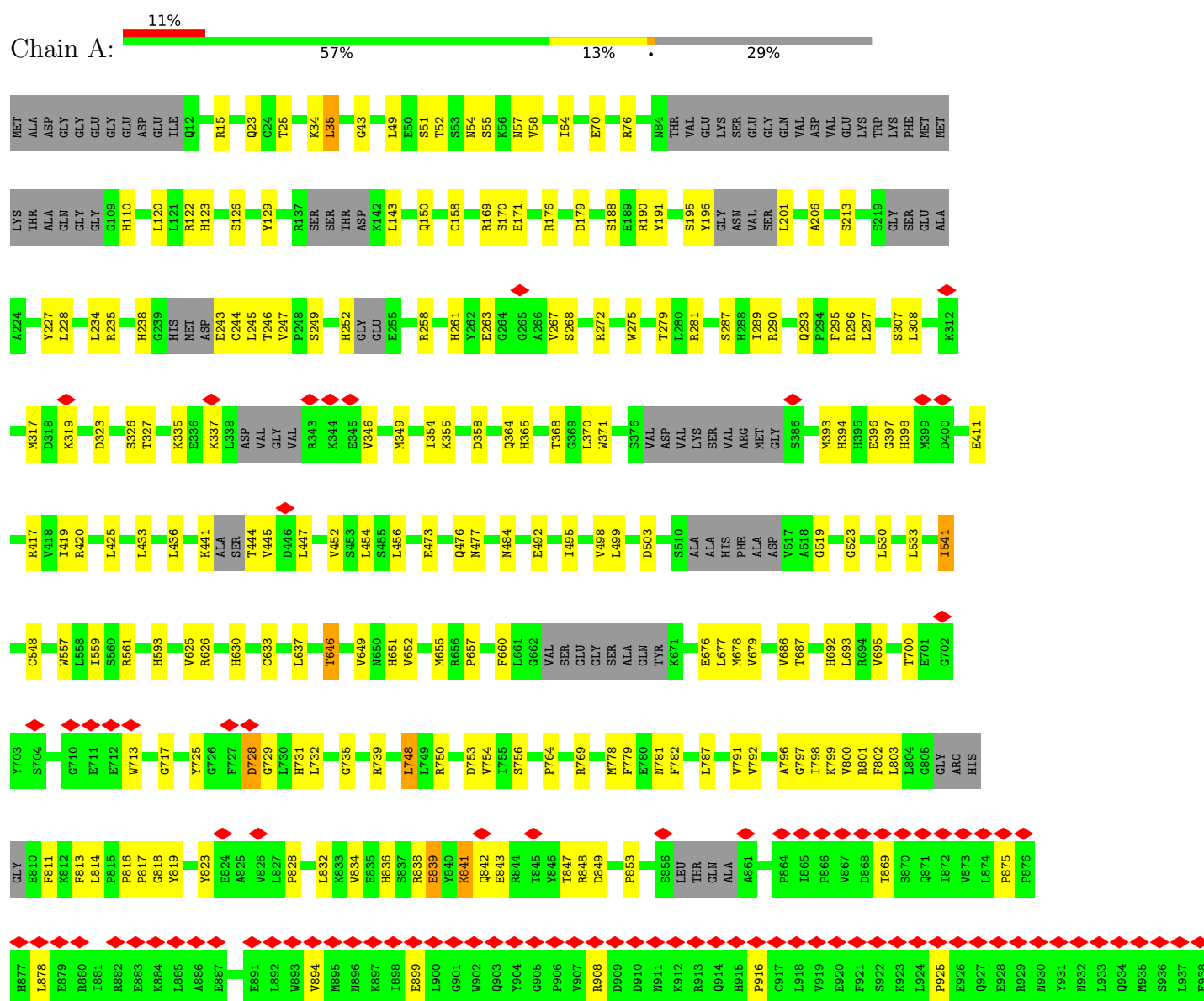
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	J	1	Total 1	Zn 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RyR2



T2088	A2071	V2075	L2076	L2081	V2082	R2083	L2088	T2106	T2117	L2120	L2124	G2125	Q2126	T2127	V2133	ARG	MET	GLY	LYS	E2138	L2142	V2155	N2161	L2162	N2163	R2164	N2168	N2173	G2181	GLY	GLY	GLY	GLY	GLY	GLY	ASN	G2343	I2354	ALA	GLU	ASP	PRO	SER	ARG	ASP															
ASP	THR	LEU	GLU	LYS	PRO	CYS	ALA	ASN	ALA	SER	GLY	ASP	GLY	GLY	ALA	GLU	GLY	GLY	LYS	GLY	LEU	ASP	ASN	K1904	M1907	L1894	K1904	M1907	L1824	F1825	Y1826	I1830	I1830	Y1945	R1944	V2037	T2038	Y2039	LEU	LYS	LYS	LYS	GLN	ALA	ALA	SER	PHE	SER												
ARG	SER	PRO	GLN	GLU	ILE	ASN	MET	LEU	LEU	LEU	ASN	PHE	LYS	ASP	SER	E1986	P1990	I1993	R1994	D2013	ASP	GLY	ASN	SER	ASP	L2024	V2037	T2038	Y2039	LEU	LYS	LYS	LYS	GLN	ALA	GLU	GLU	LYS	LEU	VAL	GLU	THR	ALA	ASP	SER	LYS	LYS	SER												
L2941	E2260	P2261	E2264	V2267	L2275	GLN	SER	CYS	GLN	MET	LEU	VAL	SER	LYS	GLY	TYR	PRO	ASP	ILE	TRP	ASN	P2293	R2298	R2304	E2316	L2324	E2330	CYS	PHE	GLY	PRO	ALA	LEU	ARG	GLY	GLY	GLY	ASN	G2343	I2354	ALA	GLU	ASP	PRO	SER	ARG	ASP													
L999	A1000	E1001	M1002	Q1014	GLY	TRP	THR	GLY	ILE	GLN	ASP	VAL	LYS	ASN	R1027	R1028	Y1035	A1036	L1037	L1038	D1039	D1040	R1041	T1042	K1043	L1044	S1045	M1046	K1047	D1048	S1049	L1050	R1051	E1052	A1053	V1054	R1055	T1056	L1057	L1058	G1059	Y1060	G1061	Y1062	M1063	L1064	E1065	A1066	PRO	ASP	GLN	ASP	HIS	ALA	ALA					
ARG	ALA	GLU	VAL	CYS	SER	GLY	THR	GLY	F1084	R1086	R1089	A1090	E1091	K1092	T1093	Y1094	E1104	F1105	A1106	V1108	T1109	V1115	R1119	E1127	L1128	K1044	G1129	F1135	A1136	W1145	H1146	Q1147	GLY	V1161	V1162	G1163	V1166	E1170	H1171	T1172	M1173	L1183	D1184	D1185	G1186	S1187	S1188													
D1196	V1209	A1210	Q1211	R1214	M1215	N1216	F1217	G1218	S1222	T1228	L1232	A1240	N1242	T1248	M1249	W1250	L1251	P1256	V1261	E1266	H1267	R1272	I1273	D1274	GLY	THR	ILE	ASP	SER	VAL	PRO	CYS	LEU	LYS	V1285	T1286	Q1287	K1288	S1289	F1290	Q1293	L1294	S1295	S1296	T1297															
D1298	R1303	L1304	C1310	ALA	GLU	ASN	ASN	GLN	GLU	VAL	PRO	THR	LYS	THR	GLN	GLY	ILE	ARG	LEU	LYS	GLN	ARG	PHE	LEU	LEU	ARG	THR	ASP	ASP	PHE	ALA	VAL	THR	LEU	HIS	ASP	GLY	HIS	VAL	ASP	PRO	TYR	ASP	ARG	VAL	ASP	TYR	LEU	ASP	MET	GLN	THR	SER							
ALA	THR	LYS	PRO	PHE	ASN	ASN	HIS	LYS	PRO	ASP	TYR	ALA	GLN	GLU	LYS	PRO	SER	ILE	ARG	LEU	LYS	GLN	ARG	PHE	LEU	LEU	ARG	THR	ALA	ALA	HIS	ASP	VAL	ARG	ASP	VAL	ARG	ASP	ASP	ASP	ASP	ASP	TYR	LEU	ASP	MET	GLN	THR	SER											
T1425	Y1426	R1431	P1434	GLY	GLN	GLU	ALA	N1440	V1441	W1442	V1443	W1445	D1449	F1450	H1451	L1459	ASP	ARG	VAL	ARG	THR	T1466	V1467	T1468	D1471	E1472	K1475	V1476	H1477	E1478	S1479	R1482	S1483	N1484	CYS	Y1486	M1487	A1490	GLY	GLU	SER	MET	SER	PRO	GLY	GLN	GLY	ARG												
N1501	L1505	V1510	V1511	ASP	ALA	ALA	SER	G1516	L1517	L1518	G1524	K1525	S1528	Y1531	P1535	P1541	A1542	F1543	F1544	Q1554	F1555	E1556	LEU	GLY	ARG	ILE	LYS	ASN	VAL	PRO	LEU	SER	A1568	G1569	L1570	E1574	M1577	P1578	V1579	P1580	Q1581	H1587	V1588	Q1589	F1590	V1594														
L1595	R1598	M1601	Q1602	F1603	L1604	R1610	I1611	W1617	L1618	V1619	Q1620	C1621	L1622	M1628	S1629	L1630	E1634	E1635	D1640	I1641	T1645	Y1655	R1659	V1664	R1671	S1678	H1679	V1680	D1681	E1682	P1683	Q1684	L1685	I1689	E1690	P1695	Y1703	D1704	L1705	L1706	Y1714																			
R1718	I1726	M1729	K1734	L1748	G1752	S1756	L1757	M1761	F1768	V1769	S1770	L1787	K1790	R1807	D1808	P1809	V1810	G1811	F1816	L1817	L1821	L1824	F1825	Y1826	I1830	I1830	Y1945	R1944	V2037	T2038	Y2039	LEU	LYS	LYS	LYS	GLN	ALA	ALA	SER	PHE	LYS	GLU	ALA	THR	ALA	ASP	ARG	LYS	THR	LYS	GLU	GLU	SER							
ASP	THR	LEU	GLU	LYS	PRO	CYS	ALA	ASN	ALA	SER	GLY	ASP	GLY	GLY	ALA	GLU	GLY	GLY	LYS	GLY	LEU	ASP	ASN	K1904	M1907	L1894	K1904	M1907	L1824	F1825	Y1826	I1830	I1830	Y1945	R1944	V2037	T2038	Y2039	LEU	LYS	LYS	LYS	GLN	ALA	ALA	SER	PHE	LYS	GLU	ALA	THR	ALA	ASP	ARG	LYS	THR	LYS	GLU	GLU	SER
ARG	SER	PRO	GLN	GLU	ILE	ASN	MET	LEU	LEU	LEU	ASN	PHE	LYS	ASP	SER	E1986	P1990	I1993	R1994	D2013	ASP	GLY	ASN	SER	ASP	L2024	V2037	T2038	Y2039	LEU	LYS	LYS	LYS	GLN	ALA	GLU	GLU	LYS	LEU	VAL	GLU	THR	ALA	ASP	SER	LYS	LYS	LYS	LYS	SER	LYS	LYS	GLU	GLU	SER					
T2088	A2071	V2075	L2076	L2081	V2082	R2083	L2088	T2106	T2117	L2120	L2124	G2125	Q2126	T2127	V2133	ARG	MET	GLY	LYS	E2138	L2142	V2155	N2161	L2162	N2163	R2164	N2168	N2173	G2181	GLY	GLY	GLY	GLY	GLY	GLY	ASN	G2343	I2354	ALA	GLU	ASP	PRO	SER	ARG	ASP															

GLN	LEU	LEU	LEU	LYS	THR	HIS	PHE	LEU	PRO	ALA	VAL	GLY	PRO	GLY	GLN	SER	GLY	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GL
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T2511	R2402	E2138	GLY	LYS	R1807	L1822	Y1531	V1443	ALA
L2521	L2409	L2142	SER	ARG	D1808	M1628	Y1531	G1444	GLY
L2528	L2409	L2142	LEU	PRO	P1809	P1628	P1535	T1223	ILE
L2529	E2416	V2155	ASP	LYS	G1810	S1629	Y1535	T1228	PRO
T2537	E2316	N2161	ASN	G1893	G1811	L1630	L1459	GLY	ALA
S2548	L2394	L2163	SER	K1904	F1816	E1634	P1541	LEU	LEU
L2550	L2394	L2163	ASP	K1904	L1817	E1635	V1543	SER	ALA
H2551	E2330	R2168	L2024	D1931	L1821	D1640	Q1554	VAL	LEU
V2553	E2330	M2168	V2037	R1944	L1824	I1641	F1544	ARG	GLN
A2537	E2330	M2173	V2039	Y1945	F1825	T1645	T1465	PHE	GLY
S2548	GLY	M2173	LEU	M1949	Y1826	V1664	T1468	LEU	LEU
L2549	PRO	G2181	LYS	Q1950	I1830	R1671	D1471	THR	ASP
L2550	ALA	GLY	LYS	A1951	I1842	R1671	E1472	GLU	GLU
H2551	ARG	GLY	GLN	M1954	I1842	S1678	R1475	ASP	TYR
V2553	GLY	GLY	ALA	SER	E1847	V1680	V1476	ASP	ALA
A2537	GLY	SER	LYS	ALA	P1848	E1681	H1477	SER	ALA
S2548	GLY	GLU	LEU	LEU	S1849	E1682	E1478	SER	ALA
L2549	ASN	G2343	VAL	VAL	VAL	P1683	S1479	ASP	ASP
H2551	THR	L2354	GLY	THR	PHE	Q1684	R1482	PHE	PHE
V2553	THR	ALA	SER	ALA	GLY	L1685	S1483	GLU	GLU
A2537	ASP	GLU	LYS	THR	ALA	L1689	R1482	VAL	VAL
S2548	GLY	GLU	LYS	LYS	GLY	E1574	S1483	LEU	LEU
L2549	GLY	ASP	SER	GLY	PRO	P1695	N1484	MET	LEU
H2551	ASN	M2215	SER	PHE	GLU	Y1703	F1486	THR	THR
V2553	VAL	M2235	SER	ARG	GLU	L1706	M1487	SER	SER
A2537	VAL	L2241	T2058	SER	GLY	L1706	A1490	GLY	GLY
S2548	GLU	L2241	A2071	PRO	SER	Y1714	GLY	ASP	ASP
H2551	PRO	E2260	Q2072	PRO	THR	R1718	H1587	SER	LEU
L2549	SER	P2261	E2073	GLN	LEU	L1718	V1588	VAL	VAL
GLY	ALA	E2264	S2074	GLN	GLU	L1726	Q1589	ASP	PRO
R2582	GLY	E2267	V2075	ILE	LYS	I1726	F1590	ARG	ARG
Q2587	GLY	V2267	L2076	ASN	GLY	M1729	GLY	VAL	VAL
P2598	SER	L2275	L2081	MET	PRO	H1593	GLN	ASP	ASP
N2601	LYS	L2275	R2082	LEU	CYS	V1594	GLY	LYS	LYS
G2607	GLY	GLN	R2083	LEU	ALA	L1595	GLY	ASP	ASP
N2701	GLY	SER	T2106	ASN	SER	K1734	ARG	LYS	LYS
F2702	ILE	GLY	T2117	PHE	GLU	L1748	M1501	THR	ALA
L2489	GLY	GLY	T2117	LYS	ASP	G1752	L1505	SER	ALA
M2606	VAL	VAL	L2120	ASP	ARG	S1756	V1510	THR	LYS
P2607	ASP	LYS	G2125	SER	GLY	L1757	V1511	PRO	GLY
Y2622	ASP	GLY	L2124	E1986	PRO	M1761	ASP	PHE	PHE
G2627	THR	THR	Q2126	P1990	ALA	F1768	V1610	ASN	ASN
T2709	ILE	GLY	12127	I1993	GLU	S1770	I1611	GLN	GLU
S2710	ALA	ASP	V2133	R1994	GLU	L1787	G1516	HIS	HIS
N2711	ALA	ILE	ARG	GLY	GLY	L1787	L1517	LYS	VAL
L2712	LEU	GLY	MET	LYS	SER	L1787	L1518	ASP	PHE
L2713	SER	TRP	GLY	GLY	GLY	L1787	N1440	THR	THR
L2714	ALA	ASN	LYS	GLU	GLY	L1787	V1441	ALA	ALA
P2715	SER	GLY	LYS	ASP	GLY	L1787	W1442	GLN	SER
E2716	THR	PHE	LYS	THR	GLY	L1787	S1524	THR	THR
L2717	ALA	GLY	LYS	ASP	GLY	L1787	K1525	LYS	LYS
L2718	ALA	ALA	LYS	GLY	GLY	L1787	S1528	THR	THR

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E2766	K2767	E2768	K2769	E2770	L2771	E2772	K2773	E2774	E2775	E2776	K2777	E2778	E2779	L2780	K2781	E2782	E2783	E2784	E2785	E2786	E2787	E2788	E2789	L2790	E2791	E2792	E2793	E2794	E2795	E2796	D2797	SER	MET	ALA	LEU	LEU	TYR	ASN	ASN	ARG	THR	ARG	ARG	ILE	SER	SER	GLN	THR	SER	GLN	VAL	SER	E2816	D2817	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825
P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	T2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	I2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	H2730	D2731	K2732	E2733	S2734	N2735	D2736	K2737	L2738	A2739	N2740	G2741	N2742	I2743	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	N2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765			
L2489	GLU	VAL	G2492	L2503	ASP	THR	ALA	ALA	LEU	SER	ALA	T2511	L2521	L2528	L2529	THR	ARG	CYS	ALA	PRO	LEU	PHE	A2537	S2548	L2549	L2550	H2551	T2552	V2553	TYR	ARG	THR	PRO	THR	ILE	LYS	ALA	LYS	ASP	ASN	VAL	VAL	GLU	PRO	ASP	MET	GLY	GLN	LYS	SER	SER	MET	ASP	SER	GLY	N2601	HIS	ALA				
K2605	M2606	P2607	Y2622	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	A2652	L2653	SER	GLN	LYS	Y2658	L2665	C2669	A2672	V2673	A2674	P2678	A2679	ASP	TYR	MET	GLU	SER	ASN	VAL	VAL	GLU	PRO	ASP	MET	GLY	GLN	LYS	SER	SER	MET	ASP	SER	GLY	N2701	F2702	N2703	P2704	Q2705											
P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	T2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	I2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	H2730	D2731	K2732	E2733	S2734	N2735	D2736	K2737	L2738	A2739	N2740	G2741	N2742	I2743	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	N2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765			
E2766	K2767	E2768	K2769	E2770	L2771	E2772	K2773	E2774	E2775	E2776	K2777	E2778	E2779	L2780	K2781	E2782	E2783	E2784	E2785	E2786	E2787	E2788	E2789	L2790	E2791	E2792	E2793	E2794	E2795	E2796	D2797	SER	MET	ALA	LEU	LEU	TYR	ASN	ASN	ARG	THR	ARG	ARG	ILE	SER	SER	GLN	THR	SER	GLN	VAL	SER	E2816	D2817	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825
V1441	W1442	V1443	G1444	W1445	L1459	ASP	ARG	VAL	ARG	THR	V1465	T1466	V1467	D1471	E1472	A1475	V1476	H1477	E1478	S1479	R1482	S1483	N1484	CYS	Y1486	M1487	A1490	GLY	GLU	SER	MET	SER	PRO	GLY	GLN	ARG	N1501	L1505	V1510	V1511	ASP	ALA	ALA	SER	G1516	L1517	L1518	G1524	K1525													
S1528	Y1531	P1536	P1541	P1542	V1543	F1544	Q1554	F1555	E1556	LEU	GLY	ARG	ILE	LYS	ASN	VAL	MET	PRO	LEU	SER	A1568	G1569	L1570	E1574	N1577	P1578	V1579	P1580	Q1581	H1587	V1588	Q1589	F1590	V1594	L1595	R1598	N1601	Q1602	F1603	L1604	R1610	I1611	W1617	L1618	V1619	Q1620	C1621															
L1622	M1628	S1629	L1630	H1631	I1632	P1633	E1634	E1635	N1636	R1637	D1640	I1641	T1645	Y1655	R1659	V1664	R1671	S1678	H1679	V1680	D1681	E1682	P1683	Q1684	L1685	I1689	E1690	P1695	Y1703	D1704	L1705	L1706	Y1714	R1718	I1726	M1729	K1734	L1748	G1752	S1756																						
L1757	M1761	F1768	V1769	S1770	L1787	P1788	K1790	R1807	D1808	P1809	V1810	G1811	F1816	L1821	L1824	F1825	Y1826	T1830	I1846	V1847	E1848	S1849	VAL	PHE	GLY	GLU	ALA	ALA	GLY	PRO	GLU	GLU	SER	THR	GLU	PRO	PRO	GLN	GLN	ILE	ASN	MET	SER	GLY	LEU	ASP	SER	ASN	PHE	LYS	LEU	GLU	ASP									
GLY	PRO	ALA	GLU	GLU	SER	LYS	GLY	ARG	PRO	LYS	G1893	L1894	K1904	M1907	D1931	R1944	Y1945	M1949	L1950	A1951	H1954	SER	ALA	ALA	GLY	LEU	THR	ALA	ARG	LYS	THR	LYS	GLU	PHE	ARG	SER	PRO	PRO	GLN	GLN	ILE	ASN	MET	SER	GLY	LEU	LEU	ASN	PHE	LYS	ASP											
ASP	LYS	SER	E1986	P1990	T1993	R1994	D2013	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	SER	L2024	T2025	V2037	T2038	Y2039	LYS	LYS	LYS	GLN	ALA	GLY	LYS	LEU	VAL	GLU	SER	ASP	SER	SER	T2068	L2069	Q2060	A2071	Q2072	E2073	S2074	V2075	I2076	L2081	V2082	R2083															
L2088	Q2092	T2106	T2117	L2120	L2124	G2125	Q2126	T2127	V2133	ARG	MET	GLY	LYS	E2138	L2142	V2155	N2161	L2162	R2163	R2164	M2173	G2181	GLY	GLU	GLY	VAL	GLU	SER	LYS	ILE	THR	PHE	P2191	N2211	M2215	M2235	L2241	E2264	V2267	L2275	GLN	SER																				
CYS	GLN	MET	LEU	VAL	SER	LYS	GLY	TYR	PRO	ASP	ILE	TRP	ASN	P2293	R2298	R2304	E2316	L2324	E2330	CYS	PHE	GLY	PRO	ALA	LEU	ARG	GLY	GLY	GLY	ASN	G2343	I2354	ALA	ASP	PRO	SER	ARG	ASP	GLY	PRO	SER	THR	GLY	SER	SER	MET	PRO															
ASP	THR	GLU	GLY	GLU	GLU	ASP	ASP	THR	ILE	HIS	MET	G2386	D2398	R2402	L2409	T2420	R2421	R2426	S2426	L2427	L2433	T2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	SER	ALA	GLY	F2461	Y2477	GLY	ILE	GLU	GLY	Y2481	L2488											
L2489	GLU	VAL	G2492	L2503	ASP	THR	ALA	ALA	LEU	SER	ALA	T2511	L2521	L2528	L2529	THR	ARG	CYS	ALA	PRO	LEU	PHE	A2537	S2548	L2549	L2550	H2551	T2552	V2553	TYR	ARG	THR	PRO	THR	ILE	LYS	ALA	LYS	ASP	ASN	VAL	VAL	GLU	PRO	ASP	MET	GLY	GLN	LYS	SER	SER	MET	ASP	SER	GLY	N2601	HIS	ALA				
K2605	M2606	P2607	Y2622	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	A2652	L2653	SER	GLN	LYS	Y2658	L2665	C2669	A2672	V2673	A2674	P2678	A2679	ASP	TYR	MET	GLU	SER	ASN	VAL	VAL	GLU	PRO	ASP	MET	GLY	GLN	LYS	SER	SER	MET	ASP	SER	GLY	N2701	F2702	N2703	P2704	Q2705											
P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	T2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	I2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	H2730	D2731	K2732	E2733	S2734	N2735	D2736	K2737	L2738	A2739	N2740	G2741	N2742	I2743	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	N2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765			
E2766	K2767	E2768	K2769	E2770	L2771	E2772	K2773	E2774	E2775	E2776	K2777	E2778	E2779	L2780	K2781	E2782	E2783	E2784	E2785	E2786	E2787	E2788	E2789	L2790	E2791	E2792	E2793	E2794	E2795	E2796	D2797	SER	MET	ALA	LEU	LEU	TYR	ASN	ASN	ARG	THR	ARG	ARG	ILE	SER	SER	GLN	THR	SER	GLN	VAL	SER	E2816	D2817	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825





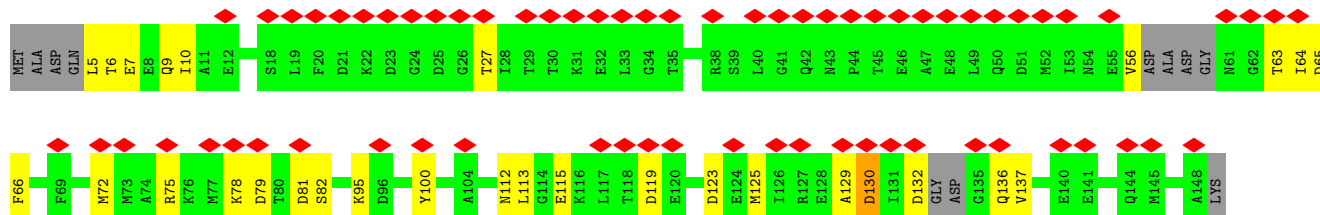
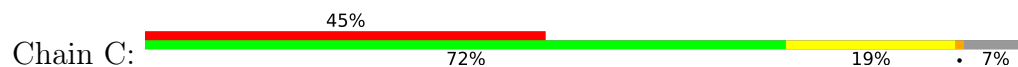




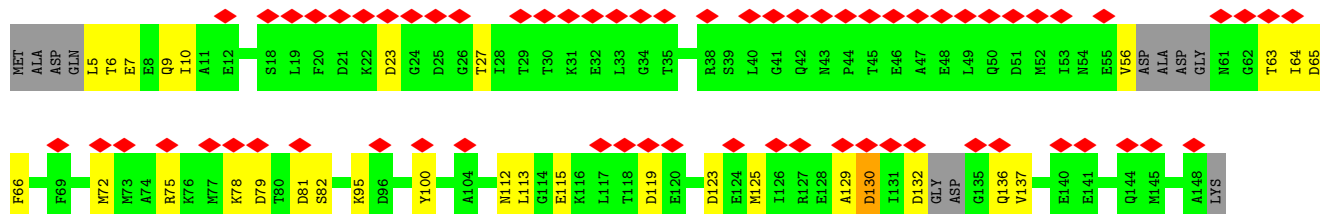
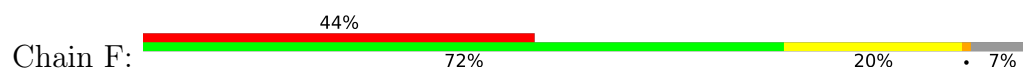
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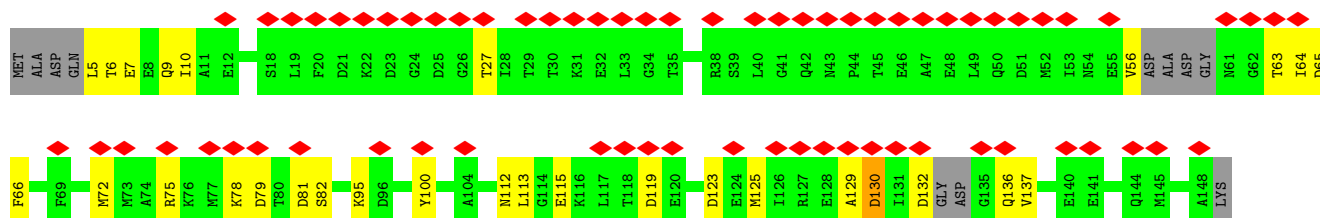
- Molecule 3: Calmodulin-1



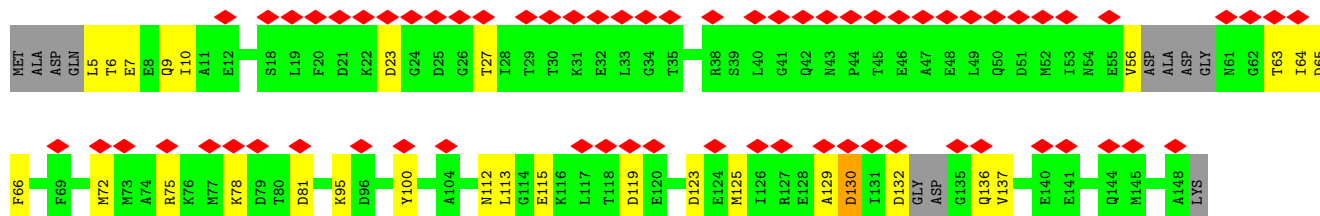
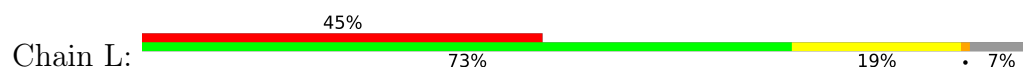
- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	208715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.43	1/27354 (0.0%)	0.73	16/36987 (0.0%)
1	D	0.43	1/27354 (0.0%)	0.73	16/36987 (0.0%)
1	G	0.43	1/27354 (0.0%)	0.73	16/36987 (0.0%)
1	J	0.43	1/27354 (0.0%)	0.73	16/36987 (0.0%)
2	B	0.36	0/835	0.62	0/1123
2	E	0.36	0/835	0.62	0/1123
2	H	0.36	0/835	0.62	0/1123
2	K	0.36	0/835	0.62	0/1123
3	C	0.29	0/1104	0.67	2/1479 (0.1%)
3	F	0.29	0/1104	0.67	2/1479 (0.1%)
3	I	0.29	0/1104	0.67	2/1479 (0.1%)
3	L	0.29	0/1104	0.67	2/1479 (0.1%)
All	All	0.43	4/117172 (0.0%)	0.73	72/158356 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	32
1	D	0	32
1	G	0	32
1	J	0	32
All	All	0	128

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1577	ASN	C-N	5.81	1.39	1.33
1	D	1577	ASN	C-N	5.81	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1577	ASN	C-N	5.81	1.39	1.33
1	J	1577	ASN	C-N	5.77	1.39	1.33

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	687	THR	N-CA-C	-5.71	98.63	110.80
1	A	687	THR	N-CA-C	-5.71	98.64	110.80
1	D	687	THR	N-CA-C	-5.71	98.64	110.80
1	G	687	THR	N-CA-C	-5.69	98.67	110.80
1	J	1163	GLY	N-CA-C	5.66	119.32	112.48
3	L	115	GLU	CA-C-O	-5.66	114.88	120.82
1	A	816	PRO	N-CA-C	5.64	117.58	110.70
1	J	816	PRO	N-CA-C	5.64	117.58	110.70
1	D	816	PRO	N-CA-C	5.63	117.57	110.70
3	C	115	GLU	CA-C-O	-5.63	114.91	120.82
3	I	115	GLU	CA-C-O	-5.63	114.91	120.82
1	A	1163	GLY	N-CA-C	5.62	119.28	112.48
1	D	1163	GLY	N-CA-C	5.62	119.28	112.48
1	G	1163	GLY	N-CA-C	5.62	119.28	112.48
1	G	816	PRO	N-CA-C	5.62	117.55	110.70
3	F	115	GLU	CA-C-O	-5.60	114.94	120.82
1	G	1471	ASP	CA-C-N	5.53	132.10	121.54
1	G	1471	ASP	C-N-CA	5.53	132.10	121.54
1	A	1471	ASP	CA-C-N	5.52	132.08	121.54
1	A	1471	ASP	C-N-CA	5.52	132.08	121.54
1	D	1471	ASP	CA-C-N	5.52	132.08	121.54
1	D	1471	ASP	C-N-CA	5.52	132.08	121.54
1	J	1471	ASP	CA-C-N	5.52	132.08	121.54
1	J	1471	ASP	C-N-CA	5.52	132.08	121.54
1	D	3606	MET	CA-C-N	5.49	126.96	120.09
1	D	3606	MET	C-N-CA	5.49	126.96	120.09
1	D	1290	PHE	N-CA-C	5.47	115.62	108.07
1	G	1290	PHE	N-CA-C	5.47	115.62	108.07
1	A	3606	MET	CA-C-N	5.46	126.91	120.09
1	A	3606	MET	C-N-CA	5.46	126.91	120.09
1	A	1290	PHE	N-CA-C	5.45	115.58	108.07
1	G	3606	MET	CA-C-N	5.45	126.90	120.09
1	G	3606	MET	C-N-CA	5.45	126.90	120.09
1	J	1290	PHE	N-CA-C	5.45	115.58	108.07
1	J	3606	MET	CA-C-N	5.44	126.89	120.09
1	J	3606	MET	C-N-CA	5.44	126.89	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	66	PHE	N-CA-CB	-5.35	104.11	110.42
3	C	66	PHE	N-CA-CB	-5.33	104.13	110.42
3	I	66	PHE	N-CA-CB	-5.33	104.13	110.42
3	F	66	PHE	N-CA-CB	-5.30	104.16	110.42
1	D	3803	VAL	N-CA-C	-5.30	98.32	109.34
1	A	3803	VAL	N-CA-C	-5.29	98.35	109.34
1	G	3803	VAL	N-CA-C	-5.29	98.35	109.34
1	J	3803	VAL	N-CA-C	-5.29	98.35	109.34
1	J	839	GLU	N-CA-C	5.27	122.03	110.80
1	G	686	VAL	CA-C-N	5.26	131.59	121.54
1	G	686	VAL	C-N-CA	5.26	131.59	121.54
1	G	1580	PRO	CA-C-N	5.26	131.59	121.54
1	G	1580	PRO	C-N-CA	5.26	131.59	121.54
1	A	839	GLU	N-CA-C	5.26	122.00	110.80
1	A	1580	PRO	CA-C-N	5.26	131.58	121.54
1	A	1580	PRO	C-N-CA	5.26	131.58	121.54
1	D	839	GLU	N-CA-C	5.26	122.00	110.80
1	D	1580	PRO	CA-C-N	5.26	131.58	121.54
1	D	1580	PRO	C-N-CA	5.26	131.58	121.54
1	G	839	GLU	N-CA-C	5.26	122.00	110.80
1	J	1580	PRO	CA-C-N	5.25	131.57	121.54
1	J	1580	PRO	C-N-CA	5.25	131.57	121.54
1	J	686	VAL	CA-C-N	5.25	131.57	121.54
1	J	686	VAL	C-N-CA	5.25	131.57	121.54
1	A	686	VAL	CA-C-N	5.25	131.56	121.54
1	A	686	VAL	C-N-CA	5.25	131.56	121.54
1	D	686	VAL	CA-C-N	5.25	131.56	121.54
1	D	686	VAL	C-N-CA	5.25	131.56	121.54
1	G	1682	GLU	N-CA-C	5.21	121.33	109.81
1	A	1682	GLU	N-CA-C	5.21	121.32	109.81
1	D	1682	GLU	N-CA-C	5.21	121.33	109.81
1	J	1682	GLU	N-CA-C	5.21	121.32	109.81
1	D	731	HIS	N-CA-C	5.19	116.99	110.24
1	G	731	HIS	N-CA-C	5.17	116.97	110.24
1	J	731	HIS	N-CA-C	5.17	116.97	110.24
1	A	731	HIS	N-CA-C	5.17	116.96	110.24

There are no chirality outliers.

All (128) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1266	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	1476	VAL	Peptide
1	A	1482	ARG	Peptide
1	A	1570	LEU	Peptide
1	A	1579	VAL	Peptide
1	A	1587	HIS	Peptide
1	A	1635	GLU	Peptide
1	A	1680	VAL	Peptide
1	A	1748	LEU	Peptide
1	A	1808	ASP	Peptide
1	A	1809	PRO	Peptide
1	A	1847	GLU	Peptide
1	A	2037	VAL	Peptide
1	A	2075	VAL	Peptide
1	A	261	HIS	Peptide
1	A	3611	ASN	Peptide
1	A	3612	LEU	Peptide
1	A	3634	GLU	Peptide
1	A	3802	SER	Peptide
1	A	3805	ASP	Peptide
1	A	3925	ILE	Peptide
1	A	4162	GLU	Peptide
1	A	4163	LYS	Peptide
1	A	4164	PRO	Peptide
1	A	729	GLY	Peptide
1	A	748	LEU	Peptide
1	A	791	VAL	Peptide
1	A	817	PRO	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	A	841	LYS	Peptide
1	D	1266	GLU	Peptide
1	D	1476	VAL	Peptide
1	D	1482	ARG	Peptide
1	D	1570	LEU	Peptide
1	D	1579	VAL	Peptide
1	D	1587	HIS	Peptide
1	D	1635	GLU	Peptide
1	D	1680	VAL	Peptide
1	D	1748	LEU	Peptide
1	D	1808	ASP	Peptide
1	D	1809	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	D	1847	GLU	Peptide
1	D	2037	VAL	Peptide
1	D	2075	VAL	Peptide
1	D	261	HIS	Peptide
1	D	3611	ASN	Peptide
1	D	3612	LEU	Peptide
1	D	3634	GLU	Peptide
1	D	3802	SER	Peptide
1	D	3805	ASP	Peptide
1	D	3925	ILE	Peptide
1	D	4162	GLU	Peptide
1	D	4163	LYS	Peptide
1	D	4164	PRO	Peptide
1	D	729	GLY	Peptide
1	D	748	LEU	Peptide
1	D	791	VAL	Peptide
1	D	817	PRO	Peptide
1	D	818	GLY	Peptide
1	D	819	TYR	Peptide
1	D	838	ARG	Peptide
1	D	841	LYS	Peptide
1	G	1266	GLU	Peptide
1	G	1476	VAL	Peptide
1	G	1482	ARG	Peptide
1	G	1570	LEU	Peptide
1	G	1579	VAL	Peptide
1	G	1587	HIS	Peptide
1	G	1635	GLU	Peptide
1	G	1680	VAL	Peptide
1	G	1748	LEU	Peptide
1	G	1808	ASP	Peptide
1	G	1809	PRO	Peptide
1	G	1847	GLU	Peptide
1	G	2037	VAL	Peptide
1	G	2075	VAL	Peptide
1	G	261	HIS	Peptide
1	G	3611	ASN	Peptide
1	G	3612	LEU	Peptide
1	G	3634	GLU	Peptide
1	G	3802	SER	Peptide
1	G	3805	ASP	Peptide
1	G	3925	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	G	4162	GLU	Peptide
1	G	4163	LYS	Peptide
1	G	4164	PRO	Peptide
1	G	729	GLY	Peptide
1	G	748	LEU	Peptide
1	G	791	VAL	Peptide
1	G	817	PRO	Peptide
1	G	818	GLY	Peptide
1	G	819	TYR	Peptide
1	G	838	ARG	Peptide
1	G	841	LYS	Peptide
1	J	1266	GLU	Peptide
1	J	1476	VAL	Peptide
1	J	1482	ARG	Peptide
1	J	1570	LEU	Peptide
1	J	1579	VAL	Peptide
1	J	1587	HIS	Peptide
1	J	1635	GLU	Peptide
1	J	1680	VAL	Peptide
1	J	1748	LEU	Peptide
1	J	1808	ASP	Peptide
1	J	1809	PRO	Peptide
1	J	1847	GLU	Peptide
1	J	2037	VAL	Peptide
1	J	2075	VAL	Peptide
1	J	261	HIS	Peptide
1	J	3611	ASN	Peptide
1	J	3612	LEU	Peptide
1	J	3634	GLU	Peptide
1	J	3802	SER	Peptide
1	J	3805	ASP	Peptide
1	J	3925	ILE	Peptide
1	J	4162	GLU	Peptide
1	J	4163	LYS	Peptide
1	J	4164	PRO	Peptide
1	J	729	GLY	Peptide
1	J	748	LEU	Peptide
1	J	791	VAL	Peptide
1	J	817	PRO	Peptide
1	J	818	GLY	Peptide
1	J	819	TYR	Peptide
1	J	838	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	J	841	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26851	0	25388	521	0
1	D	26851	0	25388	518	0
1	G	26851	0	25388	517	0
1	J	26851	0	25388	526	0
2	B	819	0	824	10	0
2	E	819	0	824	10	0
2	H	819	0	824	8	0
2	K	819	0	824	10	0
3	C	1094	0	1036	17	0
3	F	1094	0	1036	18	0
3	I	1094	0	1036	17	0
3	L	1094	0	1036	17	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
All	All	115060	0	108992	1951	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 9.

All (1951) 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:G:4518:LEU:HD21	1:G:4738:PHE:CE1	1.58	1.39
1:D:4518:LEU:HD21	1:D:4738:PHE:CE1	1.58	1.38
1:A:4518:LEU:HD21	1:A:4738:PHE:CE1	1.58	1.37
1:J:4518:LEU:HD21	1:J:4738:PHE:CE1	1.58	1.36
1:D:4733:GLY:HA3	1:D:4740:PHE:CE1	1.68	1.28
1:J:4097:PHE:HE2	1:J:4152:GLU:CG	1.46	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4097:PHE:HE2	1:D:4152:GLU:CG	1.46	1.26
1:A:4097:PHE:HE2	1:A:4152:GLU:CG	1.46	1.26
1:G:4097:PHE:HE2	1:G:4152:GLU:CG	1.46	1.26
1:J:4733:GLY:HA3	1:J:4740:PHE:CE1	1.68	1.26
1:A:4733:GLY:HA3	1:A:4740:PHE:CE1	1.68	1.26
1:G:4733:GLY:HA3	1:G:4740:PHE:CE1	1.68	1.25
1:D:4020:MET:HE3	1:D:4067:LEU:CD1	1.70	1.22
1:J:4020:MET:HE3	1:J:4067:LEU:CD1	1.70	1.21
1:A:4020:MET:HE3	1:A:4067:LEU:CD1	1.70	1.21
1:G:4020:MET:HE3	1:G:4067:LEU:CD1	1.70	1.20
1:D:4020:MET:HE1	1:D:4066:PHE:CD2	1.77	1.19
1:A:4753:THR:HG23	1:J:4770:LEU:HD13	1.22	1.19
1:G:4020:MET:HE1	1:G:4066:PHE:CD2	1.77	1.19
1:A:4753:THR:CG2	1:J:4770:LEU:CD1	2.20	1.18
1:A:4020:MET:HE1	1:A:4066:PHE:CD2	1.77	1.18
1:D:4770:LEU:CD1	1:G:4753:THR:CG2	2.22	1.18
1:J:4020:MET:HE1	1:J:4066:PHE:CD2	1.77	1.17
1:A:4753:THR:HG21	1:J:4770:LEU:CD1	1.74	1.17
1:A:4770:LEU:CD1	1:D:4753:THR:CG2	2.23	1.17
1:A:4097:PHE:CE2	1:A:4152:GLU:CG	2.28	1.17
1:G:4770:LEU:CD1	1:J:4753:THR:CG2	2.23	1.16
1:G:4097:PHE:CE2	1:G:4152:GLU:CG	2.28	1.16
1:A:4903:PRO:HB3	1:J:4955:ALA:CB	1.75	1.16
1:G:4770:LEU:HD13	1:J:4753:THR:HG23	1.26	1.16
1:J:4097:PHE:CE2	1:J:4152:GLU:CG	2.28	1.16
1:D:4097:PHE:CE2	1:D:4152:GLU:CG	2.28	1.15
1:G:4733:GLY:HA3	1:G:4740:PHE:CD1	1.82	1.14
1:G:4770:LEU:CD1	1:J:4753:THR:HG21	1.77	1.14
1:J:4733:GLY:HA3	1:J:4740:PHE:CD1	1.82	1.14
1:A:4733:GLY:HA3	1:A:4740:PHE:CD1	1.82	1.13
1:A:4955:ALA:CB	1:D:4903:PRO:HB3	1.78	1.13
1:D:4955:ALA:CB	1:G:4903:PRO:HB3	1.78	1.13
1:D:4733:GLY:HA3	1:D:4740:PHE:CD1	1.82	1.13
1:A:2427:LEU:HD11	1:J:143:LEU:HD13	1.25	1.12
1:A:4770:LEU:CD1	1:D:4753:THR:HG21	1.77	1.12
1:D:4770:LEU:CD1	1:G:4753:THR:HG21	1.77	1.12
1:G:4955:ALA:CB	1:J:4903:PRO:HB3	1.78	1.12
1:A:4753:THR:HG21	1:J:4770:LEU:HD11	1.29	1.11
1:A:4518:LEU:CD2	1:A:4738:PHE:HE1	1.63	1.11
1:D:4518:LEU:CD2	1:D:4738:PHE:HE1	1.63	1.11
1:J:4518:LEU:CD2	1:J:4738:PHE:HE1	1.63	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:HD13	1:G:2427:LEU:HD11	1.27	1.10
1:G:4020:MET:HE3	1:G:4067:LEU:HD11	1.29	1.10
1:A:143:LEU:HD13	1:D:2427:LEU:HD11	1.27	1.10
1:J:4573:LEU:HD21	1:J:4737:ASN:HD21	1.14	1.10
1:A:4770:LEU:HD13	1:D:4753:THR:HG23	1.25	1.10
1:D:4090:GLU:HB2	1:D:4091:PRO:HD3	1.19	1.10
1:G:4090:GLU:HB2	1:G:4091:PRO:HD3	1.26	1.10
1:G:4518:LEU:CD2	1:G:4738:PHE:HE1	1.63	1.10
1:D:4770:LEU:HD13	1:G:4753:THR:HG23	1.25	1.09
1:D:4573:LEU:HD21	1:D:4737:ASN:HD21	1.14	1.09
1:J:4020:MET:HE3	1:J:4067:LEU:HD11	1.29	1.08
1:G:4770:LEU:HD11	1:J:4753:THR:HG21	1.33	1.08
1:J:4090:GLU:HB2	1:J:4091:PRO:HD3	1.30	1.08
1:G:4573:LEU:HD21	1:G:4737:ASN:HD21	1.14	1.07
1:A:4020:MET:HE3	1:A:4067:LEU:HD11	1.29	1.07
1:A:4573:LEU:HD21	1:A:4737:ASN:HD21	1.14	1.07
1:A:4770:LEU:HD11	1:D:4753:THR:HG21	1.32	1.07
1:G:143:LEU:HD13	1:J:2427:LEU:HD11	1.26	1.07
1:D:4770:LEU:HD11	1:G:4753:THR:HG21	1.32	1.07
1:A:4090:GLU:HB2	1:A:4091:PRO:HD3	1.19	1.06
1:D:4020:MET:HE3	1:D:4067:LEU:HD11	1.29	1.06
1:A:4515:ASN:HD22	1:A:4744:LEU:CD2	1.69	1.05
1:D:4515:ASN:HD22	1:D:4744:LEU:CD2	1.69	1.05
1:G:143:LEU:CD1	1:J:2427:LEU:HD11	1.87	1.05
1:D:4573:LEU:CD2	1:D:4737:ASN:HD21	1.70	1.05
1:A:4573:LEU:CD2	1:A:4737:ASN:HD21	1.70	1.05
1:A:4519:LEU:HD21	1:J:4811:LEU:CD2	1.87	1.04
1:G:4573:LEU:CD2	1:G:4737:ASN:HD21	1.70	1.04
1:A:143:LEU:CD1	1:D:2427:LEU:HD11	1.86	1.04
1:A:2427:LEU:HD11	1:J:143:LEU:CD1	1.87	1.04
1:G:4515:ASN:ND2	1:G:4744:LEU:HD23	1.74	1.03
1:J:4515:ASN:HD22	1:J:4744:LEU:CD2	1.69	1.03
1:J:4573:LEU:CD2	1:J:4737:ASN:HD21	1.70	1.03
1:D:143:LEU:CD1	1:G:2427:LEU:HD11	1.87	1.03
1:D:4097:PHE:CE2	1:D:4152:GLU:HG2	1.93	1.03
1:G:4515:ASN:HD22	1:G:4744:LEU:CD2	1.69	1.03
1:A:4515:ASN:ND2	1:A:4744:LEU:HD23	1.74	1.03
1:G:4097:PHE:CE2	1:G:4152:GLU:HG2	1.93	1.02
1:J:4515:ASN:ND2	1:J:4744:LEU:HD23	1.74	1.02
1:A:4811:LEU:CD2	1:D:4519:LEU:HD21	1.90	1.01
1:D:4515:ASN:ND2	1:D:4744:LEU:HD23	1.74	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4811:LEU:CD2	1:G:4519:LEU:HD21	1.89	1.01
1:G:4733:GLY:CA	1:G:4740:PHE:CE1	2.43	1.01
1:G:4811:LEU:CD2	1:J:4519:LEU:HD21	1.90	1.00
1:A:4733:GLY:CA	1:A:4740:PHE:CE1	2.43	1.00
1:D:4733:GLY:CA	1:D:4740:PHE:CE1	2.43	1.00
1:J:4097:PHE:CE2	1:J:4152:GLU:HG2	1.93	1.00
1:J:4733:GLY:CA	1:J:4740:PHE:CE1	2.43	0.99
1:D:4021:PHE:CE2	1:D:4088:PHE:HD1	1.82	0.98
1:A:4753:THR:CG2	1:J:4770:LEU:HD13	1.87	0.98
1:A:4097:PHE:CE2	1:A:4152:GLU:HG2	1.93	0.97
1:D:4770:LEU:CD1	1:G:4753:THR:HG23	1.91	0.97
1:G:4518:LEU:CD2	1:G:4738:PHE:CE1	2.44	0.97
1:A:4770:LEU:HD13	1:D:4753:THR:CG2	1.90	0.97
1:J:4518:LEU:HD21	1:J:4738:PHE:CD1	1.99	0.97
1:A:4518:LEU:HD21	1:A:4738:PHE:CD1	1.99	0.97
1:A:4021:PHE:CZ	1:A:4088:PHE:CD1	2.53	0.96
1:A:4518:LEU:CD2	1:A:4738:PHE:CE1	2.44	0.96
1:A:4021:PHE:CE2	1:A:4088:PHE:HD1	1.83	0.96
1:A:4770:LEU:CD1	1:D:4753:THR:HG23	1.92	0.96
1:D:4021:PHE:CZ	1:D:4088:PHE:CD1	2.53	0.96
1:G:4518:LEU:HD21	1:G:4738:PHE:CD1	1.99	0.95
1:D:4518:LEU:HD21	1:D:4738:PHE:CD1	1.99	0.95
1:G:4770:LEU:HD13	1:J:4753:THR:CG2	1.90	0.95
1:G:4823:ARG:HB2	1:G:4823:ARG:NH2	1.82	0.95
1:D:4823:ARG:HB2	1:D:4823:ARG:NH2	1.82	0.95
1:D:4770:LEU:HD13	1:G:4753:THR:CG2	1.89	0.95
1:J:4823:ARG:NH2	1:J:4823:ARG:HB2	1.82	0.95
1:A:4823:ARG:HB2	1:A:4823:ARG:NH2	1.82	0.95
1:D:4873:GLU:HB2	1:G:4875:ARG:HH12	1.30	0.94
1:A:143:LEU:HD22	1:D:2427:LEU:HD13	1.47	0.94
1:A:4873:GLU:HB2	1:D:4875:ARG:HH12	1.30	0.94
1:D:4020:MET:HE1	1:D:4066:PHE:CE2	2.02	0.94
1:A:4020:MET:HE3	1:A:4067:LEU:HD12	1.48	0.94
1:A:2427:LEU:HD13	1:J:143:LEU:HD22	1.47	0.94
1:A:4753:THR:HG23	1:J:4770:LEU:CD1	1.89	0.94
1:G:4020:MET:HE1	1:G:4066:PHE:CE2	2.02	0.94
1:J:4020:MET:HE3	1:J:4067:LEU:HD12	1.48	0.94
1:A:4097:PHE:HE2	1:A:4152:GLU:CB	1.81	0.94
1:J:4020:MET:HE1	1:J:4066:PHE:CE2	2.02	0.94
1:A:4020:MET:HE1	1:A:4066:PHE:CE2	2.02	0.93
1:A:4875:ARG:NH1	1:J:4873:GLU:HB2	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4733:GLY:CA	1:D:4740:PHE:HE1	1.82	0.93
1:D:4873:GLU:HB2	1:G:4875:ARG:NH1	1.82	0.93
1:D:4097:PHE:HE2	1:D:4152:GLU:CB	1.80	0.93
1:G:4873:GLU:HB2	1:J:4875:ARG:HH12	1.31	0.93
1:D:4090:GLU:HB2	1:D:4091:PRO:CD	1.98	0.93
1:A:4903:PRO:HB3	1:J:4955:ALA:HB2	1.49	0.93
1:J:4515:ASN:HD22	1:J:4744:LEU:HD23	1.31	0.93
1:D:4518:LEU:CD2	1:D:4738:PHE:CE1	2.44	0.93
1:G:4097:PHE:HE2	1:G:4152:GLU:CB	1.81	0.93
1:D:4733:GLY:C	1:D:4740:PHE:HE1	1.77	0.92
1:A:4873:GLU:HB2	1:D:4875:ARG:NH1	1.83	0.92
1:G:143:LEU:HD22	1:J:2427:LEU:HD13	1.50	0.92
1:G:4770:LEU:CD1	1:J:4753:THR:HG23	1.93	0.92
1:A:4519:LEU:HD21	1:J:4811:LEU:HD23	1.49	0.92
1:A:4733:GLY:CA	1:A:4740:PHE:HE1	1.82	0.92
1:A:4875:ARG:HH12	1:J:4873:GLU:HB2	1.31	0.92
1:A:4090:GLU:HB2	1:A:4091:PRO:CD	1.98	0.92
1:J:4733:GLY:CA	1:J:4740:PHE:HE1	1.82	0.92
1:D:4020:MET:HE3	1:D:4067:LEU:HD12	1.48	0.91
1:A:4733:GLY:C	1:A:4740:PHE:HE1	1.78	0.91
1:G:4020:MET:HE3	1:G:4067:LEU:HD12	1.48	0.91
1:D:4097:PHE:CE2	1:D:4152:GLU:HG3	2.06	0.91
1:G:4733:GLY:HA3	1:G:4740:PHE:HE1	1.35	0.91
1:G:4873:GLU:HB2	1:J:4875:ARG:NH1	1.84	0.91
1:J:4097:PHE:HE2	1:J:4152:GLU:CB	1.82	0.91
1:J:4097:PHE:CE2	1:J:4152:GLU:HG3	2.05	0.91
1:A:4955:ALA:HB2	1:D:4903:PRO:HB3	1.52	0.91
1:G:4515:ASN:HD22	1:G:4744:LEU:HD23	1.31	0.91
1:G:4733:GLY:C	1:G:4740:PHE:HE1	1.78	0.91
1:D:4811:LEU:HD23	1:G:4519:LEU:HD21	1.52	0.90
1:J:4733:GLY:C	1:J:4740:PHE:HE1	1.78	0.90
1:J:4020:MET:HE1	1:J:4066:PHE:HD2	1.31	0.90
1:G:4020:MET:HE1	1:G:4066:PHE:HD2	1.31	0.90
1:G:4097:PHE:CE2	1:G:4152:GLU:HG3	2.05	0.90
1:D:143:LEU:HD22	1:G:2427:LEU:HD13	1.51	0.90
1:A:4811:LEU:HD23	1:D:4519:LEU:HD21	1.52	0.90
1:G:4955:ALA:HB2	1:J:4903:PRO:HB3	1.53	0.90
1:J:4733:GLY:HA3	1:J:4740:PHE:HE1	1.35	0.90
1:A:4020:MET:HE1	1:A:4066:PHE:HD2	1.31	0.89
1:A:4097:PHE:CE2	1:A:4152:GLU:HG3	2.05	0.89
1:D:4020:MET:HE1	1:D:4066:PHE:HD2	1.31	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4955:ALA:HB2	1:G:4903:PRO:HB3	1.52	0.89
1:G:4811:LEU:HD23	1:J:4519:LEU:HD21	1.52	0.89
1:D:4573:LEU:HD21	1:D:4737:ASN:ND2	1.88	0.88
1:J:4087:ARG:HG2	1:J:4087:ARG:HH11	1.36	0.88
1:G:4573:LEU:HD21	1:G:4737:ASN:ND2	1.88	0.88
1:D:4515:ASN:HD22	1:D:4744:LEU:HD23	1.31	0.88
1:D:4021:PHE:CE2	1:D:4088:PHE:CD1	2.61	0.87
1:A:143:LEU:CD2	1:D:2427:LEU:HD13	2.04	0.87
1:J:4573:LEU:HD21	1:J:4737:ASN:ND2	1.88	0.87
1:G:4090:GLU:HB2	1:G:4091:PRO:CD	2.04	0.87
1:A:4573:LEU:HD21	1:A:4737:ASN:ND2	1.88	0.86
1:D:4733:GLY:HA3	1:D:4740:PHE:HE1	1.35	0.86
1:A:2427:LEU:HD13	1:J:143:LEU:CD2	2.05	0.86
1:A:4021:PHE:CE2	1:A:4088:PHE:CD1	2.63	0.86
1:A:4903:PRO:CB	1:J:4955:ALA:CB	2.53	0.85
1:D:143:LEU:CD2	1:G:2427:LEU:HD13	2.07	0.85
1:G:4020:MET:CE	1:G:4067:LEU:HD12	2.07	0.85
1:A:4020:MET:CE	1:A:4067:LEU:HD12	2.07	0.85
1:G:143:LEU:CD2	1:J:2427:LEU:HD13	2.06	0.85
1:J:4020:MET:CE	1:J:4067:LEU:HD12	2.07	0.85
1:D:4020:MET:CE	1:D:4067:LEU:HD12	2.07	0.84
1:D:4811:LEU:HD21	1:G:4519:LEU:HD21	1.60	0.84
1:A:4515:ASN:HD22	1:A:4744:LEU:HD23	1.31	0.84
1:D:4020:MET:CE	1:D:4066:PHE:CD2	2.61	0.84
1:G:4733:GLY:CA	1:G:4740:PHE:HE1	1.82	0.84
1:A:4519:LEU:CD2	1:J:4811:LEU:CD2	2.55	0.84
1:G:4020:MET:CE	1:G:4066:PHE:CD2	2.61	0.84
1:A:4020:MET:CE	1:A:4066:PHE:CD2	2.61	0.84
1:J:4020:MET:CE	1:J:4067:LEU:CD1	2.56	0.83
1:A:143:LEU:CD2	1:D:2427:LEU:CD1	2.55	0.83
1:A:4955:ALA:CB	1:D:4903:PRO:CB	2.56	0.83
1:A:2427:LEU:CD1	1:J:143:LEU:CD2	2.57	0.83
1:D:4955:ALA:CB	1:G:4903:PRO:CB	2.57	0.83
1:G:4955:ALA:CB	1:J:4903:PRO:CB	2.57	0.83
1:D:4811:LEU:CD2	1:G:4519:LEU:CD2	2.57	0.83
1:A:4733:GLY:CA	1:A:4740:PHE:CD1	2.61	0.82
1:G:4087:ARG:HG2	1:G:4087:ARG:HH11	1.44	0.82
1:A:4907:GLU:OE2	1:J:4184:LYS:HD3	1.80	0.82
1:A:4519:LEU:HD21	1:J:4811:LEU:HD21	1.58	0.82
1:A:4519:LEU:CD2	1:J:4811:LEU:HD21	2.09	0.82
1:A:4811:LEU:HD21	1:D:4519:LEU:HD21	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4020:MET:CE	1:J:4066:PHE:CD2	2.61	0.82
1:A:4733:GLY:C	1:A:4740:PHE:CE1	2.58	0.82
1:A:4903:PRO:HB3	1:J:4955:ALA:HB3	1.62	0.82
1:D:4184:LYS:HD3	1:G:4907:GLU:OE2	1.79	0.81
1:G:4811:LEU:CD2	1:J:4519:LEU:CD2	2.58	0.81
1:D:4020:MET:CE	1:D:4067:LEU:CD1	2.56	0.81
1:A:4020:MET:CE	1:A:4067:LEU:CD1	2.56	0.81
1:A:4811:LEU:CD2	1:D:4519:LEU:CD2	2.58	0.81
1:A:4907:GLU:OE1	1:J:4184:LYS:HB2	1.80	0.81
1:D:4733:GLY:C	1:D:4740:PHE:CE1	2.58	0.81
1:J:4090:GLU:HB2	1:J:4091:PRO:CD	2.09	0.81
1:J:4733:GLY:CA	1:J:4740:PHE:CD1	2.61	0.81
1:G:4184:LYS:HD3	1:J:4907:GLU:OE2	1.81	0.81
1:A:4184:LYS:HD3	1:D:4907:GLU:OE2	1.79	0.81
1:G:4811:LEU:HD21	1:J:4519:LEU:HD21	1.61	0.81
1:D:4518:LEU:HD21	1:D:4738:PHE:HE1	1.00	0.81
1:J:4020:MET:CE	1:J:4066:PHE:CE2	2.63	0.81
1:D:4020:MET:CE	1:D:4066:PHE:CE2	2.63	0.81
1:G:4020:MET:CE	1:G:4066:PHE:CE2	2.63	0.81
1:G:4733:GLY:CA	1:G:4740:PHE:CD1	2.61	0.81
1:D:143:LEU:CD2	1:G:2427:LEU:CD1	2.59	0.81
1:A:4020:MET:CE	1:A:4066:PHE:CE2	2.63	0.80
1:G:4733:GLY:C	1:G:4740:PHE:CE1	2.58	0.80
1:J:4733:GLY:C	1:J:4740:PHE:CE1	2.58	0.80
1:A:4184:LYS:HB2	1:D:4907:GLU:OE1	1.81	0.80
1:G:143:LEU:CD2	1:J:2427:LEU:CD1	2.58	0.80
1:D:4184:LYS:HB2	1:G:4907:GLU:OE1	1.81	0.80
1:G:4184:LYS:HB2	1:J:4907:GLU:OE1	1.82	0.80
1:A:4515:ASN:HD22	1:A:4744:LEU:HD21	1.47	0.80
1:A:4811:LEU:HD21	1:D:4519:LEU:CD2	2.11	0.80
1:A:4086:LYS:NZ	1:A:4086:LYS:HB3	1.97	0.79
1:D:4515:ASN:HD22	1:D:4744:LEU:HD21	1.47	0.79
1:D:4811:LEU:HD21	1:G:4519:LEU:CD2	2.11	0.79
1:D:4733:GLY:CA	1:D:4740:PHE:CD1	2.61	0.79
1:D:4090:GLU:CB	1:D:4091:PRO:HD3	2.10	0.79
1:G:4811:LEU:HD21	1:J:4519:LEU:CD2	2.12	0.79
1:J:4020:MET:SD	1:J:4066:PHE:CE2	2.76	0.79
1:J:4518:LEU:HD21	1:J:4738:PHE:HE1	1.00	0.79
1:A:4955:ALA:HB3	1:D:4903:PRO:HB3	1.64	0.79
1:D:4020:MET:SD	1:D:4066:PHE:CE2	2.76	0.79
1:D:4086:LYS:NZ	1:D:4086:LYS:HB3	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4020:MET:CE	1:G:4067:LEU:CD1	2.56	0.79
1:G:4020:MET:SD	1:G:4066:PHE:CE2	2.76	0.79
1:A:4090:GLU:CB	1:A:4091:PRO:HD3	2.10	0.79
1:J:4518:LEU:CD2	1:J:4738:PHE:CE1	2.44	0.79
1:A:2427:LEU:CD1	1:J:143:LEU:HD22	2.13	0.78
1:A:4020:MET:SD	1:A:4066:PHE:CE2	2.76	0.78
1:A:4744:LEU:HD12	1:J:4777:VAL:HG13	1.64	0.78
1:G:4955:ALA:HB3	1:J:4903:PRO:HB3	1.65	0.78
1:A:143:LEU:HD22	1:D:2427:LEU:CD1	2.13	0.78
1:A:4903:PRO:HA	1:J:4955:ALA:HB1	1.65	0.78
1:J:4085:VAL:O	1:J:4089:HIS:HB3	1.84	0.78
1:A:4518:LEU:HD21	1:A:4738:PHE:HE1	1.00	0.77
1:D:4865:GLY:CA	1:G:4868:ILE:HG12	2.14	0.77
1:J:4087:ARG:HG2	1:J:4087:ARG:NH1	1.98	0.77
1:A:4865:GLY:CA	1:D:4868:ILE:HG12	2.15	0.76
1:A:4955:ALA:HB1	1:D:4903:PRO:HA	1.67	0.76
1:A:4868:ILE:HG12	1:J:4865:GLY:CA	2.15	0.76
1:A:4777:VAL:HG13	1:D:4744:LEU:HD12	1.67	0.76
1:D:4955:ALA:HB3	1:G:4903:PRO:HB3	1.65	0.76
1:D:4955:ALA:HB1	1:G:4903:PRO:HA	1.67	0.76
1:J:4515:ASN:HD22	1:J:4744:LEU:HD21	1.47	0.76
1:D:4777:VAL:HG13	1:G:4744:LEU:HD12	1.66	0.76
1:G:4955:ALA:HB1	1:J:4903:PRO:HA	1.68	0.76
1:G:143:LEU:HD22	1:J:2427:LEU:CD1	2.16	0.75
1:G:4777:VAL:HG13	1:J:4744:LEU:HD12	1.67	0.75
1:G:4865:GLY:CA	1:J:4868:ILE:HG12	2.16	0.75
1:G:4515:ASN:HD22	1:G:4744:LEU:HD21	1.47	0.75
1:A:2427:LEU:CD1	1:J:143:LEU:CD1	2.65	0.74
1:G:4070:CYS:SG	1:G:4088:PHE:CZ	2.81	0.74
1:A:2426:SER:OG	1:J:190:ARG:NH1	2.20	0.74
1:D:143:LEU:CD1	1:G:2427:LEU:CD1	2.66	0.73
1:D:4087:ARG:HG2	1:D:4087:ARG:HH11	1.54	0.73
1:A:143:LEU:CD1	1:D:2427:LEU:CD1	2.66	0.73
1:A:4087:ARG:HG2	1:A:4087:ARG:HH11	1.54	0.73
1:D:143:LEU:HD22	1:G:2427:LEU:CD1	2.17	0.73
1:D:4087:ARG:HG2	1:D:4087:ARG:NH1	2.04	0.73
1:G:190:ARG:NH1	1:J:2426:SER:OG	2.22	0.72
3:F:72:MET:HG2	3:F:75:ARG:HH21	1.55	0.72
1:G:4087:ARG:HG2	1:G:4087:ARG:NH1	2.00	0.72
3:I:72:MET:HG2	3:I:75:ARG:HH21	1.55	0.72
1:D:190:ARG:NH1	1:G:2426:SER:OG	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:394:HIS:HD2	1:J:397:GLY:H	1.38	0.71
1:A:4087:ARG:HG2	1:A:4087:ARG:NH1	2.04	0.71
1:G:4810:MET:HB3	1:J:4519:LEU:O	1.91	0.71
1:A:190:ARG:NH1	1:D:2426:SER:OG	2.24	0.70
1:A:394:HIS:HD2	1:A:397:GLY:H	1.38	0.70
1:D:3960:SER:HB2	1:D:4088:PHE:HE1	1.56	0.70
3:L:72:MET:HG2	3:L:75:ARG:HH21	1.55	0.70
1:A:3960:SER:HB2	1:A:4088:PHE:HE1	1.56	0.70
1:G:4020:MET:SD	1:G:4066:PHE:HE2	2.15	0.70
1:G:4021:PHE:CZ	1:G:4088:PHE:CD1	2.78	0.70
3:C:72:MET:HG2	3:C:75:ARG:HH21	1.55	0.70
1:A:4519:LEU:O	1:J:4810:MET:HB3	1.90	0.70
1:A:4810:MET:HB3	1:D:4519:LEU:O	1.92	0.70
1:G:143:LEU:CD1	1:J:2427:LEU:CD1	2.66	0.70
1:G:394:HIS:HD2	1:G:397:GLY:H	1.38	0.70
1:G:4097:PHE:HE2	1:G:4152:GLU:HG3	1.43	0.70
1:J:797:GLY:HA2	1:J:1622:LEU:HA	1.74	0.70
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.57	0.70
1:D:394:HIS:HD2	1:D:397:GLY:H	1.38	0.70
1:J:4796:LYS:NZ	1:J:4807:CYS:SG	2.65	0.70
1:A:797:GLY:HA2	1:A:1622:LEU:HA	1.74	0.69
1:G:4796:LYS:NZ	1:G:4807:CYS:SG	2.65	0.69
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.57	0.69
1:A:4744:LEU:HD12	1:J:4777:VAL:CG1	2.22	0.69
1:D:4810:MET:HB3	1:G:4519:LEU:O	1.92	0.69
1:D:4865:GLY:HA3	1:G:4868:ILE:HG12	1.74	0.69
1:J:4020:MET:SD	1:J:4066:PHE:HE2	2.15	0.69
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.65	0.69
1:A:4865:GLY:HA3	1:D:4868:ILE:HG12	1.75	0.69
1:D:4770:LEU:HD11	1:G:4753:THR:CG2	2.08	0.69
1:G:797:GLY:HA2	1:G:1622:LEU:HA	1.74	0.69
1:G:4515:ASN:ND2	1:G:4744:LEU:CD2	2.41	0.69
1:J:188:SER:HB2	1:J:190:ARG:HH21	1.57	0.69
1:A:4020:MET:SD	1:A:4066:PHE:HE2	2.15	0.69
1:A:4868:ILE:HG12	1:J:4865:GLY:HA3	1.75	0.69
1:A:4777:VAL:CG1	1:D:4744:LEU:HD12	2.23	0.68
1:D:4573:LEU:CD2	1:D:4737:ASN:ND2	2.52	0.68
1:D:4777:VAL:CG1	1:G:4744:LEU:HD12	2.23	0.68
1:G:188:SER:HB2	1:G:190:ARG:HH21	1.57	0.68
1:D:797:GLY:HA2	1:D:1622:LEU:HA	1.74	0.68
1:D:4823:ARG:HB2	1:D:4823:ARG:HH21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4156:SER:O	1:J:4160:GLN:HB2	1.94	0.68
1:D:4796:LYS:NZ	1:D:4807:CYS:SG	2.65	0.68
1:G:3845:GLN:HG3	1:G:3923:GLU:HG3	1.76	0.68
1:G:4777:VAL:CG1	1:J:4744:LEU:HD12	2.23	0.68
1:A:4156:SER:O	1:A:4160:GLN:HB2	1.94	0.68
1:D:4020:MET:SD	1:D:4066:PHE:HE2	2.15	0.68
1:G:4823:ARG:HB2	1:G:4823:ARG:HH21	1.59	0.68
1:J:1135:PHE:HB3	1:J:1173:MET:HE1	1.76	0.68
1:A:4823:ARG:HB2	1:A:4823:ARG:CZ	2.24	0.68
1:G:4865:GLY:HA3	1:J:4868:ILE:HG12	1.75	0.68
1:A:4823:ARG:HB2	1:A:4823:ARG:HH21	1.59	0.67
1:A:4086:LYS:HB3	1:A:4086:LYS:HZ3	1.58	0.67
1:A:4868:ILE:HG12	1:J:4865:GLY:HA2	1.76	0.67
1:J:4823:ARG:HB2	1:J:4823:ARG:HH21	1.59	0.67
1:D:4156:SER:O	1:D:4160:GLN:HB2	1.94	0.67
1:J:4097:PHE:CE2	1:J:4152:GLU:CB	2.72	0.67
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.68	0.67
1:G:4156:SER:O	1:G:4160:GLN:HB2	1.94	0.67
1:J:4823:ARG:HB2	1:J:4823:ARG:CZ	2.25	0.67
1:A:1135:PHE:HB3	1:A:1173:MET:HE1	1.76	0.67
1:D:1135:PHE:HB3	1:D:1173:MET:HE1	1.76	0.67
1:G:4823:ARG:HB2	1:G:4823:ARG:CZ	2.24	0.67
1:J:3845:GLN:HG3	1:J:3923:GLU:HG3	1.76	0.67
1:J:1303:ARG:HH12	1:J:1595:LEU:HB2	1.60	0.67
1:A:4097:PHE:CE2	1:A:4152:GLU:CB	2.71	0.66
1:D:4823:ARG:HB2	1:D:4823:ARG:CZ	2.24	0.66
1:A:1303:ARG:HH12	1:A:1595:LEU:HB2	1.60	0.66
1:D:3845:GLN:HG3	1:D:3923:GLU:HG3	1.76	0.66
1:D:4865:GLY:HA2	1:G:4868:ILE:HG12	1.76	0.66
1:G:150:GLN:NE2	1:G:158:CYS:SG	2.68	0.66
1:A:3845:GLN:HG3	1:A:3923:GLU:HG3	1.76	0.66
1:G:1135:PHE:HB3	1:G:1173:MET:HE1	1.76	0.66
1:G:4097:PHE:CE2	1:G:4152:GLU:CB	2.71	0.66
1:J:4021:PHE:CZ	1:J:4088:PHE:CD1	2.83	0.66
1:D:4097:PHE:CD2	1:D:4152:GLU:HG3	2.31	0.65
1:G:1303:ARG:HH12	1:G:1595:LEU:HB2	1.60	0.65
1:D:739:ARG:HH21	1:D:1535:PRO:HG3	1.62	0.65
1:G:4865:GLY:HA2	1:J:4868:ILE:HG12	1.78	0.65
1:A:4865:GLY:HA2	1:D:4868:ILE:HG12	1.77	0.65
1:J:150:GLN:NE2	1:J:158:CYS:SG	2.68	0.65
1:J:4020:MET:CE	1:J:4066:PHE:HD2	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ARG:HH21	1:A:1535:PRO:HG3	1.62	0.65
1:J:739:ARG:HH21	1:J:1535:PRO:HG3	1.62	0.65
1:D:4515:ASN:ND2	1:D:4744:LEU:CD2	2.41	0.65
1:G:4020:MET:CE	1:G:4066:PHE:HD2	2.06	0.65
1:J:649:VAL:HG11	1:J:713:TRP:HB3	1.79	0.65
1:D:1303:ARG:HH12	1:D:1595:LEU:HB2	1.60	0.65
1:A:4757:ILE:HD11	1:J:4767:GLN:HB3	1.79	0.64
1:D:4097:PHE:CE2	1:D:4152:GLU:CB	2.70	0.64
1:G:739:ARG:HH21	1:G:1535:PRO:HG3	1.62	0.64
1:J:4084:PHE:O	1:J:4088:PHE:HB2	1.98	0.64
1:A:4097:PHE:CD2	1:A:4152:GLU:HG3	2.32	0.64
1:D:4767:GLN:HB3	1:G:4757:ILE:HD11	1.79	0.64
1:G:649:VAL:HG11	1:G:713:TRP:HB3	1.79	0.64
1:G:4097:PHE:CD2	1:G:4152:GLU:HG3	2.32	0.64
1:J:4573:LEU:CD2	1:J:4737:ASN:ND2	2.52	0.64
1:A:4903:PRO:CA	1:J:4955:ALA:HB1	2.28	0.64
1:J:4097:PHE:CD2	1:J:4152:GLU:HG3	2.33	0.64
1:D:1304:LEU:HB3	1:D:1541:PRO:HG2	1.80	0.64
1:J:1589:GLN:NE2	1:J:1634:GLU:OE1	2.31	0.64
1:A:649:VAL:HG11	1:A:713:TRP:HB3	1.79	0.63
1:A:4904:HIS:NE2	1:J:4184:LYS:HA	2.13	0.63
1:D:4020:MET:CE	1:D:4066:PHE:HE2	2.11	0.63
1:J:4070:CYS:SG	1:J:4088:PHE:CZ	2.91	0.63
1:A:1304:LEU:HB3	1:A:1541:PRO:HG2	1.80	0.63
1:D:4020:MET:CE	1:D:4066:PHE:HD2	2.06	0.63
1:A:4515:ASN:ND2	1:A:4744:LEU:CD2	2.41	0.63
1:A:4767:GLN:HB3	1:D:4757:ILE:HD11	1.79	0.63
1:J:419:ILE:HD13	1:J:492:GLU:HG3	1.81	0.63
1:D:649:VAL:HG11	1:D:713:TRP:HB3	1.79	0.63
1:D:1589:GLN:NE2	1:D:1634:GLU:OE1	2.31	0.63
1:A:1267:HIS:H	1:A:1294:ASN:HD21	1.46	0.63
1:D:279:THR:O	1:D:296:ARG:NH2	2.32	0.63
1:G:1589:GLN:NE2	1:G:1634:GLU:OE1	2.31	0.63
1:J:1092:LYS:H	1:J:1250:TRP:HZ3	1.47	0.63
1:A:1092:LYS:H	1:A:1250:TRP:HZ3	1.47	0.63
1:D:1092:LYS:H	1:D:1250:TRP:HZ3	1.47	0.63
1:J:1267:HIS:H	1:J:1294:ASN:HD21	1.46	0.63
1:G:1092:LYS:H	1:G:1250:TRP:HZ3	1.47	0.62
1:D:2416:GLU:O	1:D:2420:ILE:HD12	1.98	0.62
1:G:4767:GLN:HB3	1:J:4757:ILE:HD11	1.80	0.62
1:A:1589:GLN:NE2	1:A:1634:GLU:OE1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3160:LEU:O	1:D:3164:ALA:HB2	1.99	0.62
1:G:1510:VAL:HG12	1:G:1511:VAL:HG23	1.82	0.62
1:J:279:THR:O	1:J:296:ARG:NH2	2.32	0.62
1:A:279:THR:O	1:A:296:ARG:NH2	2.32	0.62
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.82	0.62
1:J:1304:LEU:HB3	1:J:1541:PRO:HG2	1.80	0.62
1:J:4052:ALA:O	1:J:4056:HIS:ND1	2.33	0.62
1:A:246:THR:OG1	1:A:272:ARG:NH1	2.33	0.62
1:A:1267:HIS:HD2	1:A:1293:GLN:HB2	1.65	0.62
1:A:3160:LEU:O	1:A:3164:ALA:HB2	1.99	0.62
1:G:247:VAL:O	1:G:272:ARG:NH1	2.31	0.62
1:J:1267:HIS:HD2	1:J:1293:GLN:HB2	1.65	0.62
1:J:1510:VAL:HG12	1:J:1511:VAL:HG23	1.82	0.62
1:D:246:THR:OG1	1:D:272:ARG:NH1	2.33	0.62
1:G:1267:HIS:HD2	1:G:1293:GLN:HB2	1.65	0.62
1:G:4052:ALA:O	1:G:4056:HIS:ND1	2.33	0.62
1:J:3160:LEU:O	1:J:3164:ALA:HB2	1.99	0.62
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.33	0.62
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.82	0.62
1:G:279:THR:O	1:G:296:ARG:NH2	2.32	0.62
1:G:4573:LEU:CD2	1:G:4737:ASN:ND2	2.52	0.62
1:A:1706:LEU:HD22	1:A:1824:LEU:HD11	1.82	0.62
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.68	0.62
1:G:246:THR:OG1	1:G:272:ARG:NH1	2.33	0.62
1:G:249:SER:HG	1:G:252:HIS:HE2	1.48	0.62
1:D:419:ILE:HD13	1:D:492:GLU:HG3	1.81	0.62
1:D:2241:LEU:HD12	1:D:2298:ARG:HG3	1.81	0.62
1:G:419:ILE:HD13	1:G:492:GLU:HG3	1.81	0.62
1:A:4020:MET:CE	1:A:4066:PHE:HE2	2.11	0.61
1:J:1680:VAL:HG13	1:J:1685:LEU:HD11	1.82	0.61
1:A:2241:LEU:HD12	1:A:2298:ARG:HG3	1.81	0.61
1:D:4046:LYS:H	1:D:4077:GLU:HB3	1.66	0.61
1:G:4084:PHE:O	1:G:4088:PHE:HB2	2.01	0.61
1:J:258:ARG:NH1	1:J:317:MET:SD	2.73	0.61
1:J:4621:GLN:HE22	1:J:4633:ARG:HH12	1.48	0.61
1:A:4046:LYS:H	1:A:4077:GLU:HB3	1.66	0.61
1:D:1267:HIS:H	1:D:1294:ASN:HD21	1.46	0.61
1:G:258:ARG:NH1	1:G:317:MET:SD	2.73	0.61
1:D:4086:LYS:HB3	1:D:4086:LYS:HZ3	1.61	0.61
1:G:1267:HIS:H	1:G:1294:ASN:HD21	1.46	0.61
1:A:1680:VAL:HG13	1:A:1685:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:NH1	1:D:317:MET:SD	2.73	0.61
1:D:1904:LYS:HG3	1:D:2081:LEU:HD11	1.83	0.61
1:G:1304:LEU:HB3	1:G:1541:PRO:HG2	1.81	0.61
1:J:247:VAL:O	1:J:272:ARG:NH1	2.31	0.61
1:J:1904:LYS:HG3	1:J:2081:LEU:HD11	1.83	0.61
1:A:123:HIS:HD2	1:A:126:SER:H	1.49	0.61
1:A:258:ARG:NH1	1:A:317:MET:SD	2.73	0.61
1:D:1706:LEU:HD22	1:D:1824:LEU:HD11	1.82	0.61
1:G:1904:LYS:HG3	1:G:2081:LEU:HD11	1.83	0.61
1:G:3805:ASP:OD2	1:G:3809:PHE:N	2.33	0.61
1:J:1106:GLU:OE1	1:J:1214:ARG:NH1	2.34	0.61
1:J:4046:LYS:H	1:J:4077:GLU:HB3	1.66	0.61
1:A:4020:MET:CE	1:A:4066:PHE:HD2	2.06	0.61
1:A:4955:ALA:HB1	1:D:4903:PRO:CA	2.30	0.61
1:D:1267:HIS:HD2	1:D:1293:GLN:HB2	1.65	0.61
1:D:4184:LYS:HA	1:G:4904:HIS:NE2	2.16	0.61
1:G:3160:LEU:O	1:G:3164:ALA:HB2	1.99	0.61
1:G:4046:LYS:H	1:G:4077:GLU:HB3	1.66	0.61
1:G:495:ILE:O	1:G:499:LEU:HB2	2.01	0.61
1:G:1706:LEU:HD22	1:G:1824:LEU:HD11	1.82	0.61
1:G:2241:LEU:HD12	1:G:2298:ARG:HG3	1.81	0.61
3:I:56:VAL:HG11	3:I:64:ILE:HA	1.83	0.61
1:J:246:THR:OG1	1:J:272:ARG:NH1	2.33	0.61
1:J:4087:ARG:HD2	1:J:4087:ARG:O	2.00	0.61
3:L:56:VAL:HG11	3:L:64:ILE:HA	1.83	0.61
1:A:3805:ASP:OD2	1:A:3809:PHE:N	2.33	0.61
1:D:123:HIS:HD2	1:D:126:SER:H	1.49	0.61
1:D:495:ILE:O	1:D:499:LEU:HB2	2.01	0.61
3:F:56:VAL:HG11	3:F:64:ILE:HA	1.83	0.61
1:G:1106:GLU:OE1	1:G:1214:ARG:NH1	2.34	0.61
1:G:1680:VAL:HG13	1:G:1685:LEU:HD11	1.82	0.61
1:J:841:LYS:HB2	1:J:848:ARG:HD3	1.83	0.61
1:A:419:ILE:HD13	1:A:492:GLU:HG3	1.81	0.61
1:A:4903:PRO:HA	1:J:4955:ALA:CB	2.31	0.61
1:D:4621:GLN:HE22	1:D:4633:ARG:HH12	1.48	0.61
1:J:123:HIS:HD2	1:J:126:SER:H	1.49	0.61
1:J:495:ILE:O	1:J:499:LEU:HB2	2.01	0.61
1:A:3615:HIS:NE2	3:C:7:GLU:OE2	2.35	0.60
1:G:4020:MET:CE	1:G:4066:PHE:HE2	2.11	0.60
1:A:4490:GLN:NE2	1:A:4494:ASN:OD1	2.35	0.60
1:A:4621:GLN:HE22	1:A:4633:ARG:HH12	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4184:LYS:HA	1:J:4904:HIS:NE2	2.16	0.60
1:J:4490:GLN:NE2	1:J:4494:ASN:OD1	2.35	0.60
1:A:4184:LYS:HA	1:D:4904:HIS:NE2	2.16	0.60
1:D:1680:VAL:HG13	1:D:1685:LEU:HD11	1.82	0.60
1:G:123:HIS:HD2	1:G:126:SER:H	1.49	0.60
1:G:4490:GLN:NE2	1:G:4494:ASN:OD1	2.35	0.60
1:G:4621:GLN:HE22	1:G:4633:ARG:HH12	1.48	0.60
1:A:495:ILE:O	1:A:499:LEU:HB2	2.01	0.60
1:A:1904:LYS:HG3	1:A:2081:LEU:HD11	1.83	0.60
3:C:56:VAL:HG11	3:C:64:ILE:HA	1.83	0.60
1:J:3615:HIS:NE2	3:L:7:GLU:OE2	2.34	0.60
1:A:4087:ARG:HH11	1:A:4087:ARG:CG	2.14	0.60
1:D:841:LYS:HB2	1:D:848:ARG:HD3	1.83	0.60
1:D:1106:GLU:OE1	1:D:1214:ARG:NH1	2.34	0.60
1:D:4490:GLN:NE2	1:D:4494:ASN:OD1	2.34	0.60
1:A:247:VAL:O	1:A:272:ARG:NH1	2.31	0.60
1:A:365:HIS:HD2	1:A:368:THR:H	1.49	0.60
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.33	0.60
1:G:365:HIS:HD2	1:G:368:THR:H	1.49	0.60
1:J:2241:LEU:HD12	1:J:2298:ARG:HG3	1.81	0.60
1:A:1106:GLU:OE1	1:A:1214:ARG:NH1	2.34	0.60
1:D:4087:ARG:HH11	1:D:4087:ARG:CG	2.14	0.60
1:D:4955:ALA:HB1	1:G:4903:PRO:CA	2.30	0.60
1:G:841:LYS:HB2	1:G:848:ARG:HD3	1.83	0.60
1:D:3613:PRO:HD2	1:D:3616:ARG:HD3	1.83	0.60
1:D:247:VAL:O	1:D:272:ARG:NH1	2.31	0.59
1:J:983:LEU:HB3	1:J:1055:ARG:HB3	1.84	0.59
1:J:1706:LEU:HD22	1:J:1824:LEU:HD11	1.82	0.59
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.85	0.59
1:G:4588:ILE:HG22	1:G:4723:LEU:HB3	1.85	0.59
1:J:1645:THR:HG22	1:J:1695:PRO:HG3	1.85	0.59
1:D:3593:SER:O	1:D:3597:LYS:NZ	2.35	0.59
1:G:3613:PRO:HD2	1:G:3616:ARG:HD3	1.83	0.59
1:D:1445:TRP:HB2	1:D:1487:MET:HG3	1.84	0.59
1:D:4826:GLY:O	1:G:4823:ARG:NH1	2.35	0.59
1:G:1445:TRP:HB2	1:G:1487:MET:HG3	1.84	0.59
1:G:4955:ALA:HB1	1:J:4903:PRO:CA	2.31	0.59
1:J:3613:PRO:HD2	1:J:3616:ARG:HD3	1.83	0.59
1:A:4573:LEU:CD2	1:A:4737:ASN:ND2	2.52	0.59
1:A:4588:ILE:HG22	1:A:4723:LEU:HB3	1.85	0.59
1:D:660:PHE:HB3	1:D:787:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3615:HIS:NE2	3:F:7:GLU:OE2	2.34	0.59
1:J:365:HIS:HD2	1:J:368:THR:H	1.49	0.59
1:J:660:PHE:HB3	1:J:787:LEU:HD22	1.84	0.59
1:A:983:LEU:HB3	1:A:1055:ARG:HB3	1.84	0.59
1:A:4955:ALA:CB	1:D:4903:PRO:HA	2.31	0.59
1:J:676:GLU:HB2	1:J:803:LEU:HB2	1.85	0.59
1:A:3593:SER:O	1:A:3597:LYS:NZ	2.35	0.59
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.85	0.59
1:D:3775:GLN:NE2	1:D:3846:LEU:O	2.34	0.59
1:J:4588:ILE:HG22	1:J:4723:LEU:HB3	1.85	0.59
1:A:4826:GLY:O	1:D:4823:ARG:NH1	2.36	0.59
1:G:1645:THR:HG22	1:G:1695:PRO:HG3	1.84	0.59
1:G:4021:PHE:CE2	1:G:4088:PHE:CD1	2.91	0.59
1:A:3613:PRO:HD2	1:A:3616:ARG:HD3	1.83	0.59
1:D:365:HIS:HD2	1:D:368:THR:H	1.49	0.59
1:D:4588:ILE:HG22	1:D:4723:LEU:HB3	1.85	0.59
1:G:3615:HIS:NE2	3:I:7:GLU:OE2	2.34	0.59
1:A:143:LEU:HD21	1:D:2427:LEU:CD1	2.32	0.58
1:A:3956:GLN:NE2	1:A:3973:MET:SD	2.76	0.58
1:J:4835:PRO:HB2	1:J:4841:GLU:HG3	1.84	0.58
1:A:2083:ARG:NH2	1:A:3686:ASP:OD1	2.36	0.58
1:J:802:PHE:HB2	1:J:1617:TRP:HB2	1.84	0.58
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.85	0.58
1:A:875:PRO:HD2	1:A:878:LEU:HD12	1.85	0.58
1:D:3956:GLN:NE2	1:D:3973:MET:SD	2.76	0.58
1:G:4087:ARG:HH11	1:G:4087:ARG:CG	2.14	0.58
1:J:1104:GLU:HG2	1:J:1216:ASN:HD22	1.68	0.58
1:J:1445:TRP:HB2	1:J:1487:MET:HG3	1.84	0.58
1:A:4903:PRO:CA	1:J:4955:ALA:CB	2.81	0.58
1:G:4955:ALA:CB	1:J:4903:PRO:HA	2.34	0.58
1:J:3956:GLN:NE2	1:J:3973:MET:SD	2.76	0.58
1:G:3956:GLN:NE2	1:G:3973:MET:SD	2.76	0.58
1:J:3805:ASP:OD2	1:J:3809:PHE:N	2.33	0.58
1:A:1104:GLU:HG2	1:A:1216:ASN:HD22	1.68	0.58
1:A:4835:PRO:HB2	1:A:4841:GLU:HG3	1.84	0.58
1:D:983:LEU:HB3	1:D:1055:ARG:HB3	1.84	0.58
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.84	0.58
1:A:841:LYS:HB2	1:A:848:ARG:HD3	1.83	0.58
1:G:660:PHE:HB3	1:G:787:LEU:HD22	1.84	0.58
1:G:4835:PRO:HB2	1:G:4841:GLU:HG3	1.84	0.58
1:A:1445:TRP:HB2	1:A:1487:MET:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4835:PRO:HB2	1:D:4841:GLU:HG3	1.84	0.58
1:D:4955:ALA:HB3	1:G:4903:PRO:CB	2.29	0.58
1:A:1993:ILE:HG12	3:C:112:ASN:HA	1.86	0.58
1:A:3903:GLY:O	1:A:3907:PHE:HB2	2.04	0.58
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.84	0.58
1:D:1993:ILE:HG12	3:F:112:ASN:HA	1.86	0.58
1:D:3903:GLY:O	1:D:3907:PHE:HB2	2.04	0.58
1:G:802:PHE:HB2	1:G:1617:TRP:HB2	1.84	0.58
1:G:1993:ILE:HG12	3:I:112:ASN:HA	1.86	0.58
1:J:4733:GLY:HA3	1:J:4740:PHE:HD1	1.61	0.58
1:D:4955:ALA:CB	1:G:4903:PRO:HA	2.32	0.58
1:G:983:LEU:HB3	1:G:1055:ARG:HB3	1.84	0.58
1:A:660:PHE:HB3	1:A:787:LEU:HD22	1.84	0.57
1:D:1104:GLU:HG2	1:D:1216:ASN:HD22	1.68	0.57
1:D:3960:SER:HB2	1:D:4088:PHE:CE1	2.38	0.57
1:G:875:PRO:HD2	1:G:878:LEU:HD12	1.85	0.57
1:G:2304:ARG:HH21	1:G:2402:ARG:HH12	1.52	0.57
1:G:2083:ARG:NH2	1:G:3686:ASP:OD1	2.36	0.57
1:A:2427:LEU:CD1	1:J:143:LEU:HD21	2.35	0.57
1:A:4955:ALA:CB	1:D:4903:PRO:CA	2.82	0.57
1:G:4011:VAL:HA	1:G:4014:ILE:HG12	1.86	0.57
1:J:875:PRO:HD2	1:J:878:LEU:HD12	1.85	0.57
1:J:1993:ILE:HG12	3:L:112:ASN:HA	1.86	0.57
1:A:4823:ARG:NH1	1:J:4826:GLY:O	2.37	0.57
1:D:875:PRO:HD2	1:D:878:LEU:HD12	1.85	0.57
1:G:3593:SER:O	1:G:3597:LYS:NZ	2.35	0.57
1:J:3775:GLN:NE2	1:J:3846:LEU:O	2.34	0.57
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.87	0.57
1:D:3805:ASP:OD2	1:D:3809:PHE:N	2.33	0.57
1:D:4011:VAL:HA	1:D:4014:ILE:HG12	1.86	0.57
1:G:4826:GLY:O	1:J:4823:ARG:NH1	2.37	0.57
1:J:290:ARG:H	1:J:293:GLN:HE21	1.53	0.57
1:J:433:LEU:HD12	1:J:447:LEU:HD11	1.87	0.57
1:J:2083:ARG:NH2	1:J:3686:ASP:OD1	2.36	0.57
1:J:2304:ARG:HH21	1:J:2402:ARG:HH12	1.52	0.57
1:D:4056:HIS:O	1:D:4058:HIS:ND1	2.38	0.57
1:D:4792:LYS:NZ	1:D:4838:ASP:OD2	2.34	0.57
1:J:3593:SER:O	1:J:3597:LYS:NZ	2.35	0.57
1:D:4955:ALA:CB	1:G:4903:PRO:CA	2.83	0.57
1:G:143:LEU:HD21	1:J:2427:LEU:CD1	2.35	0.57
3:I:27:THR:HG22	3:I:65:ASP:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:756:SER:HB3	1:J:769:ARG:HB2	1.87	0.57
1:A:4070:CYS:SG	1:A:4088:PHE:CZ	2.98	0.57
1:D:2304:ARG:HH21	1:D:2402:ARG:HH12	1.52	0.57
1:G:433:LEU:HD12	1:G:447:LEU:HD11	1.87	0.57
1:G:1466:THR:HG22	1:G:1482:ARG:HG2	1.87	0.57
1:G:1487:MET:HE1	1:G:1531:TYR:HB2	1.87	0.57
1:A:290:ARG:H	1:A:293:GLN:HE21	1.53	0.56
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.85	0.56
1:G:290:ARG:H	1:G:293:GLN:HE21	1.53	0.56
1:G:3775:GLN:NE2	1:G:3846:LEU:O	2.34	0.56
1:G:4087:ARG:HD2	1:G:4087:ARG:O	2.04	0.56
1:G:676:GLU:HB2	1:G:803:LEU:HB2	1.85	0.56
1:G:4056:HIS:O	1:G:4058:HIS:ND1	2.38	0.56
1:J:1106:GLU:HA	1:J:1161:VAL:HA	1.87	0.56
1:A:411:GLU:OE2	1:A:484:ASN:ND2	2.38	0.56
1:A:4011:VAL:HA	1:A:4014:ILE:HG12	1.86	0.56
1:A:4819:TYR:O	1:A:4823:ARG:HD3	2.06	0.56
1:D:15:ARG:HD3	1:D:110:HIS:HB3	1.88	0.56
1:D:411:GLU:OE2	1:D:484:ASN:ND2	2.38	0.56
1:D:756:SER:HB3	1:D:769:ARG:HB2	1.87	0.56
1:D:1128:LEU:HD21	1:D:1136:ALA:HB3	1.88	0.56
1:D:1466:THR:HG22	1:D:1482:ARG:HG2	1.87	0.56
1:D:2083:ARG:NH2	1:D:3686:ASP:OD1	2.36	0.56
1:G:1104:GLU:HG2	1:G:1216:ASN:HD22	1.69	0.56
1:G:1128:LEU:HD21	1:G:1136:ALA:HB3	1.88	0.56
1:G:3903:GLY:O	1:G:3907:PHE:HB2	2.04	0.56
1:G:4955:ALA:HB3	1:J:4903:PRO:CB	2.29	0.56
3:I:119:ASP:O	3:I:123:ASP:HB2	2.05	0.56
1:J:1106:GLU:HB3	1:J:1214:ARG:HB3	1.87	0.56
1:J:1466:THR:HG22	1:J:1482:ARG:HG2	1.87	0.56
1:J:4011:VAL:HA	1:J:4014:ILE:HG12	1.86	0.56
1:D:4819:TYR:O	1:D:4823:ARG:HD3	2.06	0.56
3:F:27:THR:HG22	3:F:65:ASP:HB3	1.87	0.56
1:J:15:ARG:HD3	1:J:110:HIS:HB3	1.88	0.56
1:A:15:ARG:HD3	1:A:110:HIS:HB3	1.88	0.56
1:A:1106:GLU:HB3	1:A:1214:ARG:HB3	1.87	0.56
3:C:27:THR:HG22	3:C:65:ASP:HB3	1.87	0.56
3:L:119:ASP:O	3:L:123:ASP:HB2	2.05	0.56
1:A:2304:ARG:HH21	1:A:2402:ARG:HH12	1.52	0.56
1:A:4759:SER:HA	1:A:4762:THR:HG22	1.88	0.56
1:D:2316:GLU:O	1:D:3811:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4873:GLU:CB	1:G:4875:ARG:NH1	2.64	0.56
1:G:1106:GLU:HA	1:G:1161:VAL:HA	1.87	0.56
1:G:2316:GLU:O	1:G:3811:ARG:NH2	2.39	0.56
1:G:4090:GLU:CB	1:G:4091:PRO:HD3	2.17	0.56
1:A:1487:MET:HE1	1:A:1531:TYR:HB2	1.87	0.56
1:A:2316:GLU:O	1:A:3811:ARG:NH2	2.39	0.56
1:A:4875:ARG:NH1	1:J:4873:GLU:CB	2.64	0.56
1:D:4070:CYS:SG	1:D:4088:PHE:CZ	2.99	0.56
1:G:15:ARG:HD3	1:G:110:HIS:HB3	1.88	0.56
1:G:411:GLU:OE2	1:G:484:ASN:ND2	2.38	0.56
1:J:411:GLU:OE2	1:J:484:ASN:ND2	2.38	0.56
1:J:4020:MET:CE	1:J:4066:PHE:HE2	2.11	0.56
1:J:4056:HIS:O	1:J:4058:HIS:ND1	2.38	0.56
1:A:433:LEU:HD12	1:A:447:LEU:HD11	1.87	0.56
1:A:1431:ARG:HE	1:A:1505:LEU:HD21	1.71	0.56
1:D:433:LEU:HD12	1:D:447:LEU:HD11	1.87	0.56
1:J:1431:ARG:HE	1:J:1505:LEU:HD21	1.71	0.56
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.88	0.56
1:A:3960:SER:HB2	1:A:4088:PHE:CE1	2.38	0.56
3:C:119:ASP:O	3:C:123:ASP:HB2	2.05	0.56
3:F:119:ASP:O	3:F:123:ASP:HB2	2.05	0.56
1:G:1106:GLU:HB3	1:G:1214:ARG:HB3	1.87	0.56
1:G:4819:TYR:O	1:G:4823:ARG:HD3	2.06	0.56
1:A:436:LEU:HD21	1:A:445:VAL:HB	1.88	0.56
1:D:679:VAL:HA	1:D:800:VAL:HG12	1.88	0.56
1:D:1431:ARG:HE	1:D:1505:LEU:HD21	1.71	0.56
1:J:3903:GLY:O	1:J:3907:PHE:HB2	2.04	0.56
1:A:1106:GLU:HA	1:A:1161:VAL:HA	1.87	0.55
1:A:1466:THR:HG22	1:A:1482:ARG:HG2	1.87	0.55
1:D:290:ARG:H	1:D:293:GLN:HE21	1.53	0.55
1:J:2316:GLU:O	1:J:3811:ARG:NH2	2.39	0.55
1:J:4759:SER:HA	1:J:4762:THR:HG22	1.88	0.55
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.72	0.55
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.39	0.55
1:A:4056:HIS:O	1:A:4058:HIS:ND1	2.38	0.55
1:A:4733:GLY:CA	1:A:4740:PHE:HD1	2.18	0.55
1:J:4819:TYR:O	1:J:4823:ARG:HD3	2.06	0.55
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.72	0.55
1:D:1487:MET:HE1	1:D:1531:TYR:HB2	1.87	0.55
1:G:756:SER:HB3	1:G:769:ARG:HB2	1.87	0.55
3:L:100:TYR:HB3	3:L:136:GLN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4903:PRO:CB	1:J:4955:ALA:HB3	2.26	0.55
1:A:4955:ALA:HB3	1:D:4903:PRO:CB	2.28	0.55
3:F:100:TYR:HB3	3:F:136:GLN:HB3	1.89	0.55
1:G:1091:GLU:HB3	1:G:1094:TYR:HD2	1.72	0.55
1:G:1714:TYR:OH	1:G:1718:ARG:NH2	2.40	0.55
1:G:4759:SER:HA	1:G:4762:THR:HG22	1.88	0.55
1:J:695:VAL:HA	1:J:792:VAL:HG22	1.89	0.55
3:C:100:TYR:HB3	3:C:136:GLN:HB3	1.89	0.55
1:D:25:THR:HG22	1:D:34:LYS:HG2	1.89	0.55
1:D:1106:GLU:HB3	1:D:1214:ARG:HB3	1.87	0.55
1:G:4955:ALA:CB	1:J:4903:PRO:CA	2.84	0.55
1:D:436:LEU:HD21	1:D:445:VAL:HB	1.88	0.55
1:D:4733:GLY:HA3	1:D:4740:PHE:HD1	1.61	0.55
1:J:1487:MET:HE1	1:J:1531:TYR:HB2	1.87	0.55
1:D:1106:GLU:HA	1:D:1161:VAL:HA	1.87	0.55
1:D:1714:TYR:OH	1:D:1718:ARG:NH2	2.40	0.55
1:G:2832:VAL:O	1:G:2895:LYS:NZ	2.40	0.55
1:J:1091:GLU:HB3	1:J:1094:TYR:HD2	1.72	0.55
1:A:1714:TYR:OH	1:A:1718:ARG:NH2	2.40	0.55
1:A:4823:ARG:CZ	1:A:4823:ARG:CB	2.85	0.55
1:D:695:VAL:HA	1:D:792:VAL:HG22	1.89	0.55
1:G:679:VAL:HA	1:G:800:VAL:HG12	1.88	0.55
1:A:476:GLN:NE2	1:A:3679:GLU:OE1	2.40	0.55
1:D:4759:SER:HA	1:D:4762:THR:HG22	1.88	0.55
1:J:476:GLN:NE2	1:J:3679:GLU:OE1	2.40	0.55
3:L:27:THR:HG22	3:L:65:ASP:HB3	1.87	0.55
1:A:4767:GLN:CB	1:D:4757:ILE:HD11	2.37	0.54
1:D:1990:PRO:HA	1:D:1993:ILE:HB	1.89	0.54
1:G:4021:PHE:CE2	1:G:4088:PHE:HD1	2.25	0.54
1:A:1128:LEU:HD21	1:A:1136:ALA:HB3	1.88	0.54
1:A:1990:PRO:HA	1:A:1993:ILE:HB	1.89	0.54
1:D:4823:ARG:CZ	1:D:4823:ARG:CB	2.85	0.54
1:G:25:THR:HG22	1:G:34:LYS:HG2	1.89	0.54
1:G:1119:ARG:NH2	1:G:1196:ASP:O	2.40	0.54
1:G:476:GLN:NE2	1:G:3679:GLU:OE1	2.40	0.54
1:J:1128:LEU:HD21	1:J:1136:ALA:HB3	1.88	0.54
1:D:476:GLN:NE2	1:D:3679:GLU:OE1	2.40	0.54
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.40	0.54
1:G:1734:LYS:HE2	1:G:1931:ASP:HB3	1.89	0.54
1:J:169:ARG:NH1	1:J:179:ASP:OD1	2.41	0.54
1:J:436:LEU:HD21	1:J:445:VAL:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:679:VAL:HA	1:J:800:VAL:HG12	1.88	0.54
1:J:4823:ARG:CZ	1:J:4823:ARG:CB	2.85	0.54
1:A:25:THR:HG22	1:A:34:LYS:HG2	1.89	0.54
1:D:2832:VAL:O	1:D:2895:LYS:NZ	2.40	0.54
1:D:4188:GLU:OE2	1:D:4948:ARG:NH2	2.41	0.54
3:I:100:TYR:HB3	3:I:136:GLN:HB3	1.89	0.54
1:J:70:GLU:OE2	1:J:122:ARG:NH1	2.41	0.54
1:J:1119:ARG:NH2	1:J:1196:ASP:O	2.40	0.54
1:A:3775:GLN:NE2	1:A:3846:LEU:O	2.34	0.54
1:D:3729:GLN:O	1:D:3733:HIS:ND1	2.39	0.54
1:G:1431:ARG:HE	1:G:1505:LEU:HD21	1.71	0.54
1:G:4823:ARG:CZ	1:G:4823:ARG:CB	2.85	0.54
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.34	0.54
1:J:25:THR:HG22	1:J:34:LYS:HG2	1.89	0.54
1:D:70:GLU:OE2	1:D:122:ARG:NH1	2.41	0.54
1:D:3686:ASP:HB2	1:D:3755:MET:HE1	1.90	0.54
1:G:70:GLU:OE2	1:G:122:ARG:NH1	2.41	0.54
1:G:695:VAL:HA	1:G:792:VAL:HG22	1.89	0.54
1:G:1990:PRO:HA	1:G:1993:ILE:HB	1.89	0.54
1:G:4085:VAL:O	1:G:4089:HIS:N	2.40	0.54
1:D:1443:VAL:HG22	1:D:1543:VAL:HG22	1.89	0.54
1:G:228:LEU:HB3	1:G:289:ILE:HB	1.90	0.54
1:G:436:LEU:HD21	1:G:445:VAL:HB	1.88	0.54
1:G:3686:ASP:HB2	1:G:3755:MET:HE1	1.90	0.54
1:G:4733:GLY:CA	1:G:4740:PHE:HD1	2.18	0.54
1:A:4757:ILE:HD11	1:J:4767:GLN:CB	2.38	0.54
1:G:4188:GLU:OE2	1:G:4948:ARG:NH2	2.41	0.54
1:G:4873:GLU:CB	1:J:4875:ARG:NH1	2.66	0.54
1:G:4911:LEU:O	1:G:4915:ASN:ND2	2.41	0.54
1:J:1990:PRO:HA	1:J:1993:ILE:HB	1.90	0.54
1:A:695:VAL:HA	1:A:792:VAL:HG22	1.89	0.54
1:A:4188:GLU:OE2	1:A:4948:ARG:NH2	2.41	0.54
1:A:70:GLU:OE2	1:A:122:ARG:NH1	2.41	0.53
1:A:4733:GLY:HA3	1:A:4740:PHE:HD1	1.61	0.53
1:A:4911:LEU:O	1:A:4915:ASN:ND2	2.41	0.53
1:G:169:ARG:NH1	1:G:179:ASP:OD1	2.41	0.53
1:J:1734:LYS:HE2	1:J:1931:ASP:HB3	1.89	0.53
1:J:3686:ASP:HB2	1:J:3755:MET:HE1	1.90	0.53
1:J:4188:GLU:OE2	1:J:4948:ARG:NH2	2.41	0.53
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.40	0.53
1:A:1443:VAL:HG22	1:A:1543:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3800:SER:OG	1:A:3801:CYS:N	2.41	0.53
1:D:1734:LYS:HE2	1:D:1931:ASP:HB3	1.89	0.53
1:D:4911:LEU:O	1:D:4915:ASN:ND2	2.41	0.53
1:G:1443:VAL:HG22	1:G:1543:VAL:HG22	1.89	0.53
1:J:228:LEU:HB3	1:J:289:ILE:HB	1.90	0.53
1:A:169:ARG:NH1	1:A:179:ASP:OD1	2.41	0.53
2:B:40:ARG:NH2	2:B:102:GLU:OE1	2.35	0.53
1:A:1288:LYS:HE3	1:A:1555:PHE:HD2	1.74	0.53
1:A:3984:LEU:HD11	1:A:4101:VAL:HG12	1.91	0.53
1:D:143:LEU:HD21	1:G:2427:LEU:CD1	2.35	0.53
1:J:1166:VAL:HG22	1:J:1173:MET:HG3	1.91	0.53
1:J:1288:LYS:HE3	1:J:1555:PHE:HD2	1.74	0.53
1:A:3686:ASP:HB2	1:A:3755:MET:HE1	1.90	0.53
1:D:4767:GLN:CB	1:G:4757:ILE:HD11	2.37	0.53
1:G:4086:LYS:C	1:G:4088:PHE:H	2.16	0.53
1:J:1443:VAL:HG22	1:J:1543:VAL:HG22	1.89	0.53
1:J:3804:LEU:HD13	1:J:3910:ALA:HB2	1.91	0.53
1:A:228:LEU:HB3	1:A:289:ILE:HB	1.90	0.53
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	1.91	0.53
1:J:3800:SER:OG	1:J:3801:CYS:N	2.41	0.53
1:A:1166:VAL:HG22	1:A:1173:MET:HG3	1.91	0.53
1:A:2834:LEU:HD13	1:A:2838:LEU:HB3	1.91	0.53
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.91	0.53
1:D:2834:LEU:HD13	1:D:2838:LEU:HB3	1.91	0.53
1:J:4911:LEU:O	1:J:4915:ASN:ND2	2.41	0.53
1:G:4767:GLN:CB	1:J:4757:ILE:HD11	2.39	0.53
1:J:1714:TYR:OH	1:J:1718:ARG:NH2	2.40	0.53
1:J:4844:ARG:HH12	1:J:4848:ASP:HB2	1.74	0.53
1:A:238:HIS:HB3	1:A:243:GLU:HB3	1.91	0.53
1:A:4097:PHE:HE2	1:A:4152:GLU:HB2	1.72	0.53
1:D:169:ARG:NH1	1:D:179:ASP:OD1	2.41	0.53
1:D:4844:ARG:HH12	1:D:4848:ASP:HB2	1.74	0.53
1:A:1734:LYS:HE2	1:A:1931:ASP:HB3	1.89	0.52
1:D:1288:LYS:HE3	1:D:1555:PHE:HD2	1.74	0.52
1:A:4808:ASP:HB2	1:D:4523:VAL:HG21	1.91	0.52
2:E:27:THR:HG23	2:E:100:ASP:HB3	1.92	0.52
1:J:3729:GLN:O	1:J:3733:HIS:ND1	2.39	0.52
1:D:228:LEU:HB3	1:D:289:ILE:HB	1.90	0.52
1:D:651:HIS:HE1	1:D:1604:LEU:HD23	1.74	0.52
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.35	0.52
1:G:651:HIS:HE1	1:G:1604:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1166:VAL:HG22	1:G:1173:MET:HG3	1.91	0.52
1:A:651:HIS:HE1	1:A:1604:LEU:HD23	1.74	0.52
2:B:27:THR:HG23	2:B:100:ASP:HB3	1.92	0.52
1:D:238:HIS:HB3	1:D:243:GLU:HB3	1.91	0.52
1:G:849:ASP:OD1	1:G:1214:ARG:NE	2.41	0.52
1:A:2999:ASN:O	1:A:3003:GLU:CB	2.57	0.52
1:G:238:HIS:HB3	1:G:243:GLU:HB3	1.91	0.52
1:G:263:GLU:HB3	1:G:267:VAL:HG11	1.92	0.52
1:D:263:GLU:HB3	1:D:267:VAL:HG11	1.92	0.52
1:D:693:LEU:HD21	1:D:798:ILE:HG21	1.92	0.52
1:D:2999:ASN:O	1:D:3003:GLU:CB	2.57	0.52
1:G:2999:ASN:O	1:G:3003:GLU:CB	2.57	0.52
1:J:1729:MET:HE1	1:J:3614:ARG:HG2	1.91	0.52
1:J:4097:PHE:HE2	1:J:4152:GLU:HB2	1.73	0.52
1:D:1166:VAL:HG22	1:D:1173:MET:HG3	1.91	0.52
1:J:238:HIS:HB3	1:J:243:GLU:HB3	1.91	0.52
1:J:651:HIS:HE1	1:J:1604:LEU:HD23	1.74	0.52
1:J:2999:ASN:O	1:J:3003:GLU:CB	2.57	0.52
1:G:2834:LEU:HD13	1:G:2838:LEU:HB3	1.91	0.52
1:G:3729:GLN:O	1:G:3733:HIS:ND1	2.39	0.52
1:J:54:ASN:HB3	1:J:57:ASN:HB3	1.92	0.52
1:J:365:HIS:CD2	1:J:368:THR:H	2.28	0.52
1:A:4095:ILE:CD1	1:A:4095:ILE:N	2.73	0.52
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.91	0.52
1:G:1288:LYS:HE3	1:G:1555:PHE:HD2	1.74	0.52
1:A:54:ASN:HB3	1:A:57:ASN:HB3	1.92	0.51
1:A:4792:LYS:NZ	1:A:4838:ASP:OD2	2.34	0.51
1:D:1511:VAL:HA	1:D:1517:LEU:H	1.75	0.51
1:D:3921:LEU:HD22	1:D:3936:LEU:HD11	1.93	0.51
1:G:693:LEU:HD21	1:G:798:ILE:HG21	1.92	0.51
1:G:4095:ILE:N	1:G:4095:ILE:CD1	2.73	0.51
1:J:2834:LEU:HD13	1:J:2838:LEU:HB3	1.91	0.51
1:A:1511:VAL:HA	1:A:1517:LEU:H	1.75	0.51
1:A:1729:MET:HE1	1:A:3614:ARG:HG2	1.91	0.51
1:G:3984:LEU:HD11	1:G:4101:VAL:HG12	1.92	0.51
2:H:27:THR:HG23	2:H:100:ASP:HB3	1.92	0.51
1:J:3921:LEU:HD22	1:J:3936:LEU:HD11	1.93	0.51
1:A:263:GLU:HB3	1:A:267:VAL:HG11	1.92	0.51
1:A:3921:LEU:HD22	1:A:3936:LEU:HD11	1.93	0.51
1:D:503:ASP:OD1	1:D:557:TRP:NE1	2.37	0.51
1:G:1729:MET:HE1	1:G:3614:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3921:LEU:HD22	1:G:3936:LEU:HD11	1.93	0.51
1:J:3984:LEU:HD11	1:J:4101:VAL:HG12	1.92	0.51
2:K:27:THR:HG23	2:K:100:ASP:HB3	1.92	0.51
1:A:693:LEU:HD21	1:A:798:ILE:HG21	1.92	0.51
1:A:4844:ARG:HH12	1:A:4848:ASP:HB2	1.74	0.51
1:G:1426:TYR:HD2	1:G:1574:GLU:HB2	1.75	0.51
1:A:365:HIS:CD2	1:A:368:THR:H	2.28	0.51
1:D:1426:TYR:HD2	1:D:1574:GLU:HB2	1.75	0.51
1:D:3984:LEU:HD11	1:D:4101:VAL:HG12	1.91	0.51
1:D:4095:ILE:CD1	1:D:4095:ILE:N	2.73	0.51
1:J:4095:ILE:N	1:J:4095:ILE:CD1	2.73	0.51
1:A:3925:ILE:HD11	1:A:3936:LEU:HD13	1.93	0.51
1:D:3925:ILE:HD11	1:D:3936:LEU:HD13	1.93	0.51
1:G:4844:ARG:HH12	1:G:4848:ASP:HB2	1.74	0.51
1:J:4515:ASN:ND2	1:J:4744:LEU:CD2	2.41	0.51
1:A:849:ASP:OD1	1:A:1214:ARG:NE	2.41	0.51
1:D:4808:ASP:HB2	1:G:4523:VAL:HG21	1.92	0.51
1:G:54:ASN:HB3	1:G:57:ASN:HB3	1.92	0.51
1:J:263:GLU:HB3	1:J:267:VAL:HG11	1.92	0.51
1:J:693:LEU:HD21	1:J:798:ILE:HG21	1.92	0.51
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.40	0.50
1:A:4523:VAL:HG21	1:J:4808:ASP:HB2	1.93	0.50
1:J:1511:VAL:HA	1:J:1517:LEU:H	1.75	0.50
1:A:1787:LEU:HD21	1:A:1824:LEU:HD21	1.93	0.50
1:D:289:ILE:HG22	1:D:354:ILE:HD12	1.93	0.50
1:D:1729:MET:HE1	1:D:3614:ARG:HG2	1.91	0.50
1:J:4021:PHE:CE2	1:J:4088:PHE:HD1	2.30	0.50
1:A:1218:GLY:HA3	1:A:1240:ALA:H	1.77	0.50
1:A:1426:TYR:HD2	1:A:1574:GLU:HB2	1.75	0.50
1:A:4097:PHE:CE2	1:A:4152:GLU:HB2	2.47	0.50
1:D:54:ASN:HB3	1:D:57:ASN:HB3	1.92	0.50
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.30	0.50
1:A:4873:GLU:CB	1:D:4875:ARG:NH1	2.65	0.50
1:D:1218:GLY:HA3	1:D:1240:ALA:H	1.77	0.50
1:G:1511:VAL:HA	1:G:1517:LEU:H	1.75	0.50
1:J:1218:GLY:HA3	1:J:1240:ALA:H	1.77	0.50
1:G:3160:LEU:O	1:G:3164:ALA:CB	2.60	0.50
1:G:4808:ASP:HB2	1:J:4523:VAL:HG21	1.92	0.50
1:J:3986:MET:HG2	1:J:3996:ILE:HD11	1.94	0.50
1:D:1787:LEU:HD21	1:D:1824:LEU:HD21	1.93	0.50
1:J:849:ASP:OD1	1:J:1214:ARG:NE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3160:LEU:O	1:A:3164:ALA:CB	2.60	0.50
1:D:2521:LEU:HD22	1:D:2565:ALA:HB2	1.94	0.50
1:D:3986:MET:HG2	1:D:3996:ILE:HD11	1.94	0.50
1:J:843:GLU:HA	1:J:848:ARG:HG2	1.94	0.50
1:J:1426:TYR:HD2	1:J:1574:GLU:HB2	1.75	0.50
1:J:4733:GLY:CA	1:J:4740:PHE:HD1	2.18	0.50
1:A:289:ILE:HG22	1:A:354:ILE:HD12	1.93	0.50
1:A:503:ASP:OD1	1:A:557:TRP:NE1	2.37	0.50
1:G:70:GLU:HG3	1:G:129:TYR:HE1	1.77	0.50
1:G:1218:GLY:HA3	1:G:1240:ALA:H	1.77	0.50
1:J:70:GLU:HG3	1:J:129:TYR:HE1	1.77	0.50
1:J:3160:LEU:O	1:J:3164:ALA:CB	2.60	0.50
2:K:40:ARG:NH2	2:K:102:GLU:OE1	2.35	0.50
1:A:70:GLU:HG3	1:A:129:TYR:HE1	1.77	0.50
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.94	0.50
1:A:4020:MET:SD	1:A:4066:PHE:CD2	3.05	0.50
1:D:4086:LYS:HB3	1:D:4086:LYS:HZ2	1.76	0.50
1:G:289:ILE:HG22	1:G:354:ILE:HD12	1.93	0.50
1:G:1689:ILE:HA	1:G:1703:TYR:HE1	1.77	0.50
1:G:3925:ILE:HD11	1:G:3936:LEU:HD13	1.93	0.50
1:G:4020:MET:HE1	1:G:4067:LEU:HD12	1.94	0.50
1:J:3925:ILE:HD11	1:J:3936:LEU:HD13	1.93	0.50
1:J:4635:VAL:O	1:J:4638:THR:OG1	2.25	0.50
1:G:1510:VAL:HA	1:G:1518:LEU:HD23	1.94	0.49
1:D:335:LYS:NZ	1:D:398:HIS:O	2.37	0.49
1:D:1689:ILE:HA	1:D:1703:TYR:HE1	1.77	0.49
1:G:503:ASP:OD1	1:G:557:TRP:NE1	2.37	0.49
1:A:4021:PHE:CE1	1:A:4088:PHE:HB3	2.47	0.49
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.31	0.49
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.94	0.49
1:D:849:ASP:OD1	1:D:1214:ARG:NE	2.41	0.49
1:D:1510:VAL:HA	1:D:1518:LEU:HD23	1.94	0.49
1:G:843:GLU:HA	1:G:848:ARG:HG2	1.94	0.49
1:G:4792:LYS:NZ	1:G:4838:ASP:OD2	2.34	0.49
1:J:4020:MET:SD	1:J:4066:PHE:CD2	3.05	0.49
1:D:3951:VAL:O	1:D:3955:MET:HB2	2.12	0.49
1:G:1184:ASP:OD2	1:G:1188:SER:OG	2.30	0.49
1:G:1787:LEU:HD21	1:G:1824:LEU:HD21	1.93	0.49
1:G:3986:MET:HG2	1:G:3996:ILE:HD11	1.94	0.49
1:G:4020:MET:SD	1:G:4066:PHE:CD2	3.05	0.49
1:J:1184:ASP:OD2	1:J:1188:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.30	0.49
1:A:1689:ILE:HA	1:A:1703:TYR:HE1	1.77	0.49
1:D:365:HIS:CD2	1:D:368:THR:H	2.28	0.49
1:G:626:ARG:HD2	1:G:2133:VAL:HG21	1.95	0.49
1:G:4889:CYS:SG	1:G:4890:PHE:N	2.86	0.49
1:J:123:HIS:CD2	1:J:126:SER:H	2.29	0.49
1:J:626:ARG:HD2	1:J:2133:VAL:HG21	1.94	0.49
1:J:1689:ILE:HA	1:J:1703:TYR:HE1	1.77	0.49
1:J:2832:VAL:O	1:J:2895:LYS:NZ	2.40	0.49
1:A:58:VAL:HG13	1:A:319:LYS:HB3	1.95	0.49
1:A:626:ARG:HD2	1:A:2133:VAL:HG21	1.94	0.49
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.94	0.49
1:A:3951:VAL:O	1:A:3955:MET:HB2	2.12	0.49
1:D:843:GLU:HA	1:D:848:ARG:HG2	1.94	0.49
1:D:3160:LEU:O	1:D:3164:ALA:CB	2.60	0.49
1:D:4020:MET:SD	1:D:4066:PHE:CD2	3.05	0.49
1:D:4021:PHE:CE1	1:D:4088:PHE:HB3	2.47	0.49
1:G:559:ILE:HD13	1:G:593:HIS:HB3	1.94	0.49
1:G:4085:VAL:O	1:G:4089:HIS:HB3	2.12	0.49
1:J:4021:PHE:CE2	1:J:4088:PHE:CD1	3.01	0.49
1:D:3841:PHE:HB3	1:D:3920:THR:HG21	1.94	0.49
1:J:244:CYS:SG	1:J:245:LEU:N	2.86	0.49
1:J:940:LEU:HD21	1:J:1057:LEU:HD21	1.94	0.49
1:J:2521:LEU:HD22	1:J:2565:ALA:HB2	1.94	0.49
1:A:123:HIS:CD2	1:A:126:SER:H	2.29	0.49
1:A:3638:GLU:HG2	1:A:3698:LYS:HB2	1.95	0.49
1:A:3986:MET:HG2	1:A:3996:ILE:HD11	1.94	0.49
1:G:123:HIS:CD2	1:G:126:SER:H	2.29	0.49
1:G:940:LEU:HD21	1:G:1057:LEU:HD21	1.94	0.49
1:G:1085:PHE:HE2	1:G:1127:GLU:HG2	1.78	0.49
1:G:3951:VAL:O	1:G:3955:MET:HB2	2.12	0.49
1:J:1787:LEU:HD21	1:J:1824:LEU:HD21	1.93	0.49
1:J:2161:ASN:OD1	1:J:2164:ARG:NH2	2.41	0.49
1:J:4617:TYR:OH	1:J:4629:GLY:O	2.31	0.49
1:A:196:TYR:HA	1:A:201:LEU:HD23	1.95	0.49
1:A:244:CYS:SG	1:A:245:LEU:N	2.86	0.49
1:A:2106:THR:HG23	1:A:3622:LEU:HD11	1.95	0.49
1:A:2120:LEU:HD21	1:A:2163:MET:HE1	1.95	0.49
1:A:4086:LYS:HB3	1:A:4086:LYS:HZ2	1.78	0.49
1:D:58:VAL:HG13	1:D:319:LYS:HB3	1.95	0.49
1:D:355:LYS:HD3	1:D:358:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:940:LEU:HD21	1:D:1057:LEU:HD21	1.94	0.49
1:D:2120:LEU:HD21	1:D:2163:MET:HE1	1.95	0.49
1:D:2264:GLU:HA	1:D:2267:VAL:HG22	1.95	0.49
1:D:4889:CYS:SG	1:D:4890:PHE:N	2.86	0.49
1:G:2521:LEU:HD22	1:G:2565:ALA:HB2	1.94	0.49
1:J:3951:VAL:O	1:J:3955:MET:HB2	2.12	0.49
1:D:337:LYS:HA	1:D:364:GLN:HE22	1.78	0.49
1:G:365:HIS:CD2	1:G:368:THR:H	2.28	0.49
1:J:4097:PHE:CE2	1:J:4152:GLU:HB2	2.48	0.49
1:A:337:LYS:HA	1:A:364:GLN:HE22	1.78	0.48
1:A:894:VAL:HG11	1:A:976:TYR:HD2	1.78	0.48
1:A:940:LEU:HD21	1:A:1057:LEU:HD21	1.94	0.48
1:D:3854:ASP:OD1	1:D:3854:ASP:N	2.46	0.48
1:D:4174:ILE:HG23	1:D:4885:MET:HE3	1.95	0.48
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.31	0.48
1:J:289:ILE:HG22	1:J:354:ILE:HD12	1.93	0.48
1:J:337:LYS:HA	1:J:364:GLN:HE22	1.78	0.48
1:J:559:ILE:HD13	1:J:593:HIS:HB3	1.94	0.48
1:J:1085:PHE:HE2	1:J:1127:GLU:HG2	1.78	0.48
1:A:2433:LEU:HD22	1:A:2488:LEU:HD21	1.95	0.48
1:A:2521:LEU:HD22	1:A:2565:ALA:HB2	1.94	0.48
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	1.94	0.48
1:D:52:THR:O	1:D:55:SER:OG	2.32	0.48
1:D:244:CYS:SG	1:D:245:LEU:N	2.86	0.48
1:D:1085:PHE:HE2	1:D:1127:GLU:HG2	1.78	0.48
1:G:196:TYR:HA	1:G:201:LEU:HD23	1.95	0.48
1:G:4174:ILE:HG23	1:G:4885:MET:HE3	1.95	0.48
1:J:894:VAL:HG11	1:J:976:TYR:HD2	1.78	0.48
1:J:3638:GLU:HG2	1:J:3698:LYS:HB2	1.95	0.48
1:J:4090:GLU:CB	1:J:4091:PRO:CD	2.82	0.48
1:A:678:MET:HE2	1:A:801:ARG:HD3	1.95	0.48
1:A:764:PRO:HG2	1:A:781:ASN:HA	1.95	0.48
1:A:3984:LEU:CD1	1:A:4101:VAL:HG12	2.43	0.48
1:D:196:TYR:HA	1:D:201:LEU:HD23	1.95	0.48
1:D:3984:LEU:CD1	1:D:4101:VAL:HG12	2.43	0.48
1:J:196:TYR:HA	1:J:201:LEU:HD23	1.95	0.48
1:J:2106:THR:HG23	1:J:3622:LEU:HD11	1.95	0.48
1:J:2120:LEU:HD21	1:J:2163:MET:HE1	1.95	0.48
1:J:3854:ASP:OD1	1:J:3854:ASP:N	2.46	0.48
1:A:355:LYS:HD3	1:A:358:ASP:HB2	1.95	0.48
1:A:1274:ASP:HB2	1:A:1286:THR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4889:CYS:SG	1:A:4890:PHE:N	2.86	0.48
1:D:4733:GLY:CA	1:D:4740:PHE:HD1	2.18	0.48
1:D:4806:LYS:NZ	1:D:4808:ASP:OD2	2.46	0.48
1:G:2433:LEU:HD22	1:G:2488:LEU:HD21	1.95	0.48
1:J:764:PRO:HG2	1:J:781:ASN:HA	1.94	0.48
1:J:2433:LEU:HD22	1:J:2488:LEU:HD21	1.95	0.48
1:A:4074:ASP:O	1:A:4078:THR:OG1	2.32	0.48
1:D:764:PRO:HG2	1:D:781:ASN:HA	1.95	0.48
1:D:3638:GLU:HG2	1:D:3698:LYS:HB2	1.95	0.48
1:D:3919:ASN:O	1:D:3922:THR:OG1	2.29	0.48
1:G:337:LYS:HA	1:G:364:GLN:HE22	1.78	0.48
1:G:894:VAL:HG11	1:G:976:TYR:HD2	1.78	0.48
1:G:2264:GLU:HA	1:G:2267:VAL:HG22	1.95	0.48
1:G:3841:PHE:HB3	1:G:3920:THR:HG21	1.94	0.48
1:G:4617:TYR:OH	1:G:4629:GLY:O	2.31	0.48
1:J:1104:GLU:HA	1:J:1163:GLY:HA2	1.95	0.48
1:J:1510:VAL:HA	1:J:1518:LEU:HD23	1.94	0.48
1:J:2124:LEU:HA	1:J:2127:ILE:HG22	1.96	0.48
1:A:700:THR:HG1	1:A:787:LEU:H	1.60	0.48
1:A:4174:ILE:HG23	1:A:4885:MET:HE3	1.95	0.48
1:G:244:CYS:SG	1:G:245:LEU:N	2.86	0.48
1:G:678:MET:HE2	1:G:801:ARG:HD3	1.95	0.48
1:G:1689:ILE:HD11	1:G:1706:LEU:HD13	1.96	0.48
1:J:3841:PHE:HB3	1:J:3920:THR:HG21	1.94	0.48
1:J:4174:ILE:HG23	1:J:4885:MET:HE3	1.95	0.48
1:A:4519:LEU:CD2	1:J:4811:LEU:HD23	2.31	0.48
1:D:70:GLU:HG3	1:D:129:TYR:HE1	1.77	0.48
1:D:626:ARG:HD2	1:D:2133:VAL:HG21	1.94	0.48
1:G:764:PRO:HG2	1:G:781:ASN:HA	1.95	0.48
1:G:2120:LEU:HD21	1:G:2163:MET:HE1	1.95	0.48
1:G:2124:LEU:HA	1:G:2127:ILE:HG22	1.96	0.48
1:G:4804:ASP:OD1	1:G:4804:ASP:N	2.47	0.48
1:J:52:THR:O	1:J:55:SER:OG	2.32	0.48
1:J:1274:ASP:HB2	1:J:1286:THR:HA	1.96	0.48
1:A:717:GLY:O	1:A:735:GLY:N	2.47	0.48
1:A:1510:VAL:HA	1:A:1518:LEU:HD23	1.94	0.48
1:A:1689:ILE:HD11	1:A:1706:LEU:HD13	1.96	0.48
1:A:4804:ASP:OD1	1:A:4804:ASP:N	2.47	0.48
2:B:31:GLN:HB2	2:B:96:THR:HB	1.96	0.48
1:D:34:LYS:H	1:D:53:SER:HG	1.57	0.48
1:D:1689:ILE:HD11	1:D:1706:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2106:THR:HG23	1:D:3622:LEU:HD11	1.95	0.48
1:D:4097:PHE:CE2	1:D:4152:GLU:HB2	2.46	0.48
1:D:4573:LEU:HD22	1:D:4737:ASN:HD21	1.71	0.48
1:G:355:LYS:HD3	1:G:358:ASP:HB2	1.95	0.48
1:G:4136:ARG:HH21	1:G:4148:ARG:CZ	2.27	0.48
1:J:678:MET:HE2	1:J:801:ARG:HD3	1.95	0.48
1:A:2264:GLU:HA	1:A:2267:VAL:HG22	1.95	0.48
1:D:4074:ASP:O	1:D:4078:THR:OG1	2.32	0.48
1:G:4573:LEU:HD22	1:G:4737:ASN:HD21	1.71	0.48
1:J:34:LYS:H	1:J:53:SER:HG	1.56	0.48
1:A:1086:ARG:HD2	1:A:1251:LEU:HD12	1.96	0.48
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.95	0.48
1:D:3927:GLY:O	1:D:3929:CYS:N	2.47	0.48
1:G:58:VAL:HG13	1:G:319:LYS:HB3	1.95	0.48
1:G:2106:THR:HG23	1:G:3622:LEU:HD11	1.95	0.48
1:J:35:LEU:HA	1:J:51:SER:HA	1.96	0.48
1:J:2528:LEU:HD11	1:J:2568:ASP:HA	1.96	0.48
1:J:4806:LYS:NZ	1:J:4808:ASP:OD2	2.46	0.48
1:J:4889:CYS:SG	1:J:4890:PHE:N	2.86	0.48
1:A:646:THR:HA	1:A:1630:LEU:HA	1.96	0.47
1:D:894:VAL:HG11	1:D:976:TYR:HD2	1.78	0.47
1:D:1274:ASP:HB2	1:D:1286:THR:HA	1.96	0.47
1:G:143:LEU:HD21	1:J:2427:LEU:HD13	1.91	0.47
1:G:646:THR:HA	1:G:1630:LEU:HA	1.96	0.47
1:G:4806:LYS:NZ	1:G:4808:ASP:OD2	2.46	0.47
1:J:519:GLY:O	1:J:523:GLY:N	2.47	0.47
1:J:1086:ARG:HD2	1:J:1251:LEU:HD12	1.96	0.47
1:J:1689:ILE:HD11	1:J:1706:LEU:HD13	1.96	0.47
1:J:1756:SER:OG	1:J:1757:LEU:N	2.47	0.47
1:A:3927:GLY:O	1:A:3929:CYS:N	2.47	0.47
1:D:717:GLY:O	1:D:735:GLY:N	2.47	0.47
1:D:2124:LEU:HA	1:D:2127:ILE:HG22	1.96	0.47
1:D:4136:ARG:HH21	1:D:4148:ARG:CZ	2.27	0.47
1:G:52:THR:O	1:G:55:SER:OG	2.32	0.47
1:G:1104:GLU:HA	1:G:1163:GLY:HA2	1.95	0.47
2:K:31:GLN:HB2	2:K:96:THR:HB	1.96	0.47
1:A:4649:PHE:HB3	1:A:4652:ARG:HD2	1.97	0.47
1:A:4655:MET:HE2	1:A:4668:SER:HA	1.97	0.47
1:D:519:GLY:O	1:D:523:GLY:N	2.47	0.47
1:G:1756:SER:OG	1:G:1757:LEU:N	2.47	0.47
1:G:3919:ASN:O	1:G:3922:THR:OG1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4635:VAL:O	1:G:4638:THR:OG1	2.25	0.47
1:J:58:VAL:HG13	1:J:319:LYS:HB3	1.95	0.47
1:J:355:LYS:HD3	1:J:358:ASP:HB2	1.95	0.47
1:J:4655:MET:HE2	1:J:4668:SER:HA	1.97	0.47
1:A:2124:LEU:HA	1:A:2127:ILE:HG22	1.96	0.47
1:D:750:ARG:N	1:D:753:ASP:OD2	2.48	0.47
1:G:2528:LEU:HD11	1:G:2568:ASP:HA	1.96	0.47
3:I:79:ASP:O	3:I:82:SER:OG	2.33	0.47
1:J:646:THR:HA	1:J:1630:LEU:HA	1.96	0.47
1:J:3984:LEU:CD1	1:J:4101:VAL:HG12	2.44	0.47
1:A:1209:VAL:N	1:A:1211:GLN:OE1	2.48	0.47
1:A:1756:SER:OG	1:A:1757:LEU:N	2.47	0.47
1:A:2528:LEU:HD11	1:A:2568:ASP:HA	1.96	0.47
1:D:646:THR:HA	1:D:1630:LEU:HA	1.96	0.47
1:D:2161:ASN:OD1	1:D:2164:ARG:NH2	2.41	0.47
1:G:717:GLY:O	1:G:735:GLY:N	2.47	0.47
1:G:1611:ILE:O	1:G:1620:GLN:N	2.48	0.47
1:G:3638:GLU:HG2	1:G:3698:LYS:HB2	1.95	0.47
1:J:717:GLY:O	1:J:735:GLY:N	2.47	0.47
1:J:3927:GLY:O	1:J:3929:CYS:N	2.47	0.47
1:J:4649:PHE:HB3	1:J:4652:ARG:HD2	1.97	0.47
1:A:275:TRP:HB3	1:A:297:LEU:HD22	1.97	0.47
1:A:799:LYS:HB3	1:A:1620:GLN:HG3	1.97	0.47
1:A:1085:PHE:HE2	1:A:1127:GLU:HG2	1.78	0.47
1:A:4085:VAL:O	1:A:4089:HIS:HB3	2.14	0.47
1:A:4136:ARG:HH21	1:A:4148:ARG:CZ	2.27	0.47
1:A:4808:ASP:O	1:D:4523:VAL:HG22	2.15	0.47
1:D:123:HIS:CD2	1:D:126:SER:H	2.29	0.47
1:D:2433:LEU:HD22	1:D:2488:LEU:HD21	1.95	0.47
1:D:4582:VAL:O	1:D:4586:PHE:HB2	2.15	0.47
1:G:4649:PHE:HB3	1:G:4652:ARG:HD2	1.96	0.47
1:A:52:THR:O	1:A:55:SER:OG	2.32	0.47
1:A:1611:ILE:O	1:A:1620:GLN:N	2.48	0.47
1:A:4154:SER:OG	1:A:4155:GLU:N	2.48	0.47
1:D:34:LYS:O	1:D:52:THR:OG1	2.32	0.47
1:D:275:TRP:HB3	1:D:297:LEU:HD22	1.97	0.47
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.95	0.47
1:D:1209:VAL:N	1:D:1211:GLN:OE1	2.48	0.47
1:D:2834:LEU:HD11	1:D:2894:LEU:HB3	1.97	0.47
1:G:35:LEU:HA	1:G:51:SER:HA	1.96	0.47
1:G:519:GLY:O	1:G:523:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:750:ARG:N	1:G:753:ASP:OD2	2.48	0.47
1:G:3984:LEU:CD1	1:G:4101:VAL:HG12	2.44	0.47
2:H:31:GLN:HB2	2:H:96:THR:HB	1.96	0.47
1:J:1611:ILE:O	1:J:1620:GLN:N	2.48	0.47
1:J:1826:TYR:CZ	1:J:1830:ILE:HD11	2.50	0.47
1:J:2264:GLU:HA	1:J:2267:VAL:HG22	1.95	0.47
1:J:4136:ARG:HH21	1:J:4148:ARG:CZ	2.27	0.47
1:J:4804:ASP:N	1:J:4804:ASP:OD1	2.47	0.47
1:A:779:PHE:HB3	1:A:782:PHE:HZ	1.80	0.47
1:A:2834:LEU:HD11	1:A:2894:LEU:HB3	1.97	0.47
1:A:4582:VAL:O	1:A:4586:PHE:HB2	2.15	0.47
1:A:4662:TYR:HB3	1:A:4666:ARG:HH21	1.80	0.47
1:A:4863:ILE:HG21	1:J:4857:VAL:CG1	2.45	0.47
1:D:678:MET:HE2	1:D:801:ARG:HD3	1.95	0.47
1:D:779:PHE:HB3	1:D:782:PHE:HZ	1.80	0.47
1:D:799:LYS:HB3	1:D:1620:GLN:HG3	1.97	0.47
1:D:1726:ILE:HG13	1:D:1757:LEU:HD23	1.96	0.47
1:D:2528:LEU:HD11	1:D:2568:ASP:HA	1.96	0.47
1:G:1826:TYR:CZ	1:G:1830:ILE:HD11	2.50	0.47
1:G:4097:PHE:CE2	1:G:4152:GLU:HB2	2.47	0.47
1:G:4154:SER:OG	1:G:4155:GLU:N	2.48	0.47
1:G:4582:VAL:O	1:G:4586:PHE:HB2	2.15	0.47
1:J:1129:GLY:O	1:J:1147:GLN:N	2.45	0.47
1:J:4662:TYR:HB3	1:J:4666:ARG:HH21	1.80	0.47
3:L:125:MET:O	3:L:129:ALA:HB2	2.15	0.47
1:A:35:LEU:HA	1:A:51:SER:HA	1.96	0.47
1:A:519:GLY:O	1:A:523:GLY:N	2.47	0.47
1:A:1726:ILE:HG13	1:A:1757:LEU:HD23	1.96	0.47
2:B:23:VAL:HG22	2:B:47:LYS:HG2	1.96	0.47
1:D:4808:ASP:O	1:G:4523:VAL:HG22	2.15	0.47
1:G:1274:ASP:HB2	1:G:1286:THR:HA	1.96	0.47
3:L:78:LYS:HA	3:L:81:ASP:HB2	1.97	0.47
1:A:76:ARG:HB3	1:D:3891:TRP:HB3	1.96	0.47
1:A:750:ARG:N	1:A:753:ASP:OD2	2.48	0.47
1:A:1826:TYR:CZ	1:A:1830:ILE:HD11	2.50	0.47
1:A:2117:THR:HG22	1:A:2155:VAL:HG11	1.97	0.47
1:A:3980:VAL:HA	1:A:3983:LEU:HD23	1.97	0.47
1:D:3980:VAL:HA	1:D:3983:LEU:HD23	1.97	0.47
1:G:1209:VAL:N	1:G:1211:GLN:OE1	2.48	0.47
1:G:4655:MET:HE2	1:G:4668:SER:HA	1.97	0.47
1:A:425:LEU:HD21	1:A:452:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1431:ARG:NH1	1:A:1554:GLN:OE1	2.49	0.46
1:D:4655:MET:HE2	1:D:4668:SER:HA	1.97	0.46
1:G:227:TYR:HE1	1:G:355:LYS:HG2	1.80	0.46
1:G:4074:ASP:O	1:G:4078:THR:OG1	2.32	0.46
1:J:275:TRP:HB3	1:J:297:LEU:HD22	1.97	0.46
1:J:4074:ASP:O	1:J:4078:THR:OG1	2.32	0.46
1:A:2071:ALA:HA	1:A:2076:ILE:HD11	1.98	0.46
1:G:779:PHE:HB3	1:G:782:PHE:HZ	1.80	0.46
1:J:799:LYS:HB3	1:J:1620:GLN:HG3	1.97	0.46
1:J:4582:VAL:O	1:J:4586:PHE:HB2	2.15	0.46
1:A:4573:LEU:HD22	1:A:4737:ASN:HD21	1.71	0.46
3:C:27:THR:HB	3:C:63:THR:HB	1.97	0.46
3:C:78:LYS:HA	3:C:81:ASP:HB2	1.97	0.46
1:D:227:TYR:HE1	1:D:355:LYS:HG2	1.80	0.46
1:D:1086:ARG:HD2	1:D:1251:LEU:HD12	1.96	0.46
1:G:1086:ARG:HD2	1:G:1251:LEU:HD12	1.96	0.46
1:J:227:TYR:HE1	1:J:355:LYS:HG2	1.80	0.46
1:J:779:PHE:HB3	1:J:782:PHE:HZ	1.80	0.46
1:J:2117:THR:HG22	1:J:2155:VAL:HG11	1.98	0.46
1:J:4020:MET:HE1	1:J:4067:LEU:HD12	1.94	0.46
1:J:4573:LEU:HD22	1:J:4737:ASN:HD21	1.71	0.46
1:A:1272:ARG:HH12	1:A:1588:VAL:HA	1.80	0.46
1:A:4806:LYS:NZ	1:A:4808:ASP:OD2	2.46	0.46
1:D:4154:SER:OG	1:D:4155:GLU:N	2.48	0.46
2:E:31:GLN:HB2	2:E:96:THR:HB	1.96	0.46
1:G:2161:ASN:OD1	1:G:2164:ARG:NH2	2.41	0.46
1:G:4808:ASP:O	1:J:4523:VAL:HG22	2.16	0.46
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.96	0.46
3:I:6:THR:H	3:I:9:GLN:HB2	1.81	0.46
1:J:1209:VAL:N	1:J:1211:GLN:OE1	2.48	0.46
1:A:3854:ASP:N	1:A:3854:ASP:OD1	2.46	0.46
1:D:76:ARG:HB3	1:G:3891:TRP:HB3	1.98	0.46
1:D:637:LEU:HB3	1:D:1679:HIS:CE1	2.51	0.46
1:D:1826:TYR:CZ	1:D:1830:ILE:HD11	2.50	0.46
1:G:34:LYS:H	1:G:53:SER:HG	1.58	0.46
1:G:799:LYS:HB3	1:G:1620:GLN:HG3	1.97	0.46
3:I:78:LYS:HA	3:I:81:ASP:HB2	1.97	0.46
3:I:125:MET:O	3:I:129:ALA:HB2	2.15	0.46
1:J:637:LEU:HB3	1:J:1679:HIS:CE1	2.51	0.46
2:K:23:VAL:HG22	2:K:47:LYS:HG2	1.96	0.46
1:A:4861:ALA:HB2	1:D:4864:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HA	1:D:51:SER:HA	1.96	0.46
1:D:754:VAL:HG11	1:D:813:PHE:HD2	1.81	0.46
1:D:1431:ARG:NH1	1:D:1554:GLN:OE1	2.49	0.46
1:G:275:TRP:HB3	1:G:297:LEU:HD22	1.97	0.46
1:G:1108:VAL:HG12	1:G:1109:THR:HG23	1.98	0.46
1:J:425:LEU:HD21	1:J:452:VAL:HG22	1.97	0.46
1:J:754:VAL:HG11	1:J:813:PHE:HD2	1.81	0.46
2:K:49:ARG:HB3	2:K:52:LYS:HE2	1.97	0.46
1:A:677:LEU:HD11	1:A:792:VAL:HG21	1.98	0.46
1:D:677:LEU:HD11	1:D:792:VAL:HG21	1.98	0.46
1:D:4085:VAL:O	1:D:4089:HIS:HB3	2.16	0.46
1:D:4649:PHE:HB3	1:D:4652:ARG:HD2	1.97	0.46
2:E:23:VAL:HG22	2:E:47:LYS:HG2	1.96	0.46
1:G:841:LYS:HD2	1:G:842:GLN:HA	1.98	0.46
1:J:1272:ARG:HH12	1:J:1588:VAL:HA	1.80	0.46
1:A:637:LEU:HB3	1:A:1679:HIS:CE1	2.51	0.46
1:A:1057:LEU:O	1:A:1062:TYR:N	2.49	0.46
2:B:49:ARG:HB3	2:B:52:LYS:HE2	1.97	0.46
1:D:425:LEU:HD21	1:D:452:VAL:HG22	1.97	0.46
1:D:2267:VAL:HG21	1:D:2324:LEU:HB3	1.97	0.46
1:D:4804:ASP:OD1	1:D:4804:ASP:N	2.47	0.46
1:G:1445:TRP:H	1:G:1487:MET:HB2	1.81	0.46
1:G:2235:MET:O	1:G:2298:ARG:NH1	2.35	0.46
1:G:2834:LEU:HD11	1:G:2894:LEU:HB3	1.97	0.46
1:J:750:ARG:N	1:J:753:ASP:OD2	2.48	0.46
1:J:1431:ARG:NH1	1:J:1554:GLN:OE1	2.49	0.46
1:J:2071:ALA:HA	1:J:2076:ILE:HD11	1.98	0.46
1:A:34:LYS:O	1:A:52:THR:OG1	2.32	0.46
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.81	0.46
1:A:4020:MET:HE1	1:A:4067:LEU:HD12	1.94	0.46
1:D:235:ARG:NE	1:D:268:SER:O	2.49	0.46
1:D:1611:ILE:O	1:D:1620:GLN:N	2.48	0.46
1:D:4086:LYS:NZ	1:D:4086:LYS:CB	2.75	0.46
1:G:1726:ILE:HG13	1:G:1757:LEU:HD23	1.96	0.46
1:A:227:TYR:HE1	1:A:355:LYS:HG2	1.80	0.46
1:D:657:PRO:HA	1:D:834:VAL:HA	1.98	0.46
1:D:4662:TYR:HB3	1:D:4666:ARG:HH21	1.80	0.46
1:G:2267:VAL:HG21	1:G:2324:LEU:HB3	1.97	0.46
1:J:2834:LEU:HD11	1:J:2894:LEU:HB3	1.97	0.46
1:A:323:ASP:O	1:A:326:SER:OG	2.35	0.45
1:A:4018:PHE:CE2	1:A:4095:ILE:HG22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:MET:O	3:C:129:ALA:HB2	2.15	0.45
1:D:841:LYS:HD2	1:D:842:GLN:HA	1.98	0.45
1:D:1445:TRP:H	1:D:1487:MET:HB2	1.81	0.45
1:D:4020:MET:HE1	1:D:4067:LEU:HD12	1.94	0.45
1:D:4861:ALA:HB2	1:G:4864:GLN:HG2	1.98	0.45
2:E:49:ARG:HB3	2:E:52:LYS:HE2	1.97	0.45
3:F:6:THR:H	3:F:9:GLN:HB2	1.81	0.45
1:G:1272:ARG:HH12	1:G:1588:VAL:HA	1.80	0.45
1:G:3980:VAL:HA	1:G:3983:LEU:HD23	1.97	0.45
1:J:473:GLU:OE2	1:J:477:ASN:ND2	2.50	0.45
1:D:1108:VAL:HG12	1:D:1109:THR:HG23	1.98	0.45
3:F:78:LYS:HA	3:F:81:ASP:HB2	1.97	0.45
1:G:76:ARG:HB3	1:J:3891:TRP:HB3	1.97	0.45
1:G:425:LEU:HD21	1:G:452:VAL:HG22	1.97	0.45
1:G:637:LEU:HB3	1:G:1679:HIS:CE1	2.51	0.45
1:G:1057:LEU:O	1:G:1062:TYR:N	2.49	0.45
1:G:4021:PHE:CZ	1:G:4088:PHE:CE1	3.04	0.45
1:G:4662:TYR:HB3	1:G:4666:ARG:HH21	1.80	0.45
1:J:1108:VAL:HG12	1:J:1109:THR:HG23	1.98	0.45
1:J:1726:ILE:HG13	1:J:1757:LEU:HD23	1.96	0.45
1:J:4000:MET:HA	1:J:4003:MET:HG2	1.98	0.45
3:L:27:THR:HB	3:L:63:THR:HB	1.97	0.45
1:A:754:VAL:HG11	1:A:813:PHE:HD2	1.81	0.45
2:B:7:ILE:HD11	2:B:73:LYS:HB2	1.99	0.45
1:D:1272:ARG:HH12	1:D:1588:VAL:HA	1.80	0.45
1:D:1756:SER:OG	1:D:1757:LEU:N	2.47	0.45
1:D:2071:ALA:HA	1:D:2076:ILE:HD11	1.98	0.45
1:D:2117:THR:HG22	1:D:2155:VAL:HG11	1.97	0.45
1:G:143:LEU:HD11	1:J:2427:LEU:CD1	2.46	0.45
1:G:527:LYS:NZ	1:G:566:GLU:OE2	2.45	0.45
1:G:1431:ARG:NH1	1:G:1554:GLN:OE1	2.49	0.45
1:G:4000:MET:HA	1:G:4003:MET:HG2	1.98	0.45
1:J:503:ASP:OD1	1:J:557:TRP:NE1	2.37	0.45
1:J:4915:ASN:OD1	1:J:4918:ASN:ND2	2.50	0.45
1:A:64:ILE:H	1:A:64:ILE:HG13	1.69	0.45
1:A:2267:VAL:HG21	1:A:2324:LEU:HB3	1.97	0.45
1:A:4010:ASN:OD1	1:A:4010:ASN:N	2.50	0.45
2:B:92:PRO:HG2	2:B:95:ALA:HB2	1.99	0.45
1:D:4097:PHE:CD2	1:D:4152:GLU:CG	2.92	0.45
2:E:92:PRO:HG2	2:E:95:ALA:HB2	1.99	0.45
3:F:27:THR:HB	3:F:63:THR:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:125:MET:O	3:F:129:ALA:HB2	2.15	0.45
1:G:34:LYS:O	1:G:52:THR:OG1	2.32	0.45
1:G:754:VAL:HG11	1:G:813:PHE:HD2	1.81	0.45
1:G:2117:THR:HG22	1:G:2155:VAL:HG11	1.98	0.45
1:G:2796:GLY:HA3	1:G:2900:ASN:HA	1.99	0.45
1:J:503:ASP:OD1	1:J:561:ARG:NH2	2.50	0.45
1:J:1057:LEU:O	1:J:1062:TYR:N	2.49	0.45
1:J:1445:TRP:H	1:J:1487:MET:HB2	1.81	0.45
1:J:1630:LEU:HD22	1:J:1641:ILE:HD13	1.98	0.45
1:A:441:LYS:HD3	1:A:444:THR:HG21	1.98	0.45
1:A:1630:LEU:HD22	1:A:1641:ILE:HD13	1.98	0.45
1:A:2796:GLY:HA3	1:A:2900:ASN:HA	1.99	0.45
1:A:3977:LYS:HB2	1:A:4095:ILE:HD11	1.99	0.45
1:A:4018:PHE:CE2	1:A:4095:ILE:CG2	2.99	0.45
1:A:4915:ASN:OD1	1:A:4918:ASN:ND2	2.50	0.45
3:C:6:THR:H	3:C:9:GLN:HB2	1.81	0.45
1:D:4635:VAL:O	1:D:4638:THR:OG1	2.25	0.45
1:G:1057:LEU:HB3	1:G:1062:TYR:HB2	1.98	0.45
1:G:4915:ASN:OD1	1:G:4918:ASN:ND2	2.50	0.45
1:J:1057:LEU:HB3	1:J:1062:TYR:HB2	1.98	0.45
1:J:2267:VAL:HG21	1:J:2324:LEU:HB3	1.97	0.45
1:J:2796:GLY:HA3	1:J:2900:ASN:HA	1.99	0.45
1:J:4010:ASN:OD1	1:J:4010:ASN:N	2.50	0.45
3:L:6:THR:H	3:L:9:GLN:HB2	1.81	0.45
1:A:2427:LEU:HD13	1:J:143:LEU:HD21	1.92	0.45
1:A:4864:GLN:HG2	1:J:4861:ALA:HB2	1.99	0.45
1:D:4147:GLU:OE1	1:D:4937:GLN:NE2	2.50	0.45
1:G:836:HIS:CE1	1:G:1610:ARG:HE	2.35	0.45
1:J:657:PRO:HA	1:J:834:VAL:HA	1.98	0.45
1:J:3980:VAL:HA	1:J:3983:LEU:HD23	1.97	0.45
1:A:836:HIS:CE1	1:A:1610:ARG:HE	2.35	0.45
1:A:4061:GLN:O	1:A:4064:THR:OG1	2.25	0.45
1:A:4808:ASP:HB2	1:D:4523:VAL:CG2	2.46	0.45
1:D:441:LYS:HD3	1:D:444:THR:HG21	1.98	0.45
1:D:1057:LEU:O	1:D:1062:TYR:N	2.49	0.45
1:D:2796:GLY:HA3	1:D:2900:ASN:HA	1.99	0.45
1:G:657:PRO:HA	1:G:834:VAL:HA	1.98	0.45
1:G:1951:ALA:HB3	3:I:95:LYS:HE2	1.99	0.45
1:G:2071:ALA:HA	1:G:2076:ILE:HD11	1.98	0.45
3:I:130:ASP:O	3:I:137:VAL:HG22	2.17	0.45
1:J:3919:ASN:O	1:J:3922:THR:OG1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:VAL:HG12	1:A:1109:THR:HG23	1.98	0.45
1:A:4000:MET:HA	1:A:4003:MET:HG2	1.98	0.45
3:C:5:LEU:HB3	3:C:10:ILE:HD11	1.98	0.45
1:D:170:SER:OG	1:D:171:GLU:N	2.50	0.45
1:D:195:SER:OG	1:D:196:TYR:N	2.50	0.45
1:D:3977:LYS:HB2	1:D:4095:ILE:HD11	1.97	0.45
1:D:4857:VAL:CG1	1:G:4863:ILE:HG21	2.47	0.45
1:D:4915:ASN:OD1	1:D:4918:ASN:ND2	2.50	0.45
1:G:417:ARG:HD3	1:G:420:ARG:HH21	1.82	0.45
1:G:677:LEU:HD11	1:G:792:VAL:HG21	1.98	0.45
1:G:4861:ALA:HB2	1:J:4864:GLN:HG2	1.98	0.45
2:H:49:ARG:HB3	2:H:52:LYS:HE2	1.97	0.45
3:I:27:THR:HB	3:I:63:THR:HB	1.97	0.45
1:J:677:LEU:HD11	1:J:792:VAL:HG21	1.98	0.45
3:L:5:LEU:HB3	3:L:10:ILE:HD11	1.98	0.45
1:A:4523:VAL:CG2	1:J:4808:ASP:HB2	2.47	0.45
3:C:130:ASP:O	3:C:137:VAL:HG22	2.17	0.45
1:D:417:ARG:HD3	1:D:420:ARG:HH21	1.82	0.45
1:D:503:ASP:OD1	1:D:561:ARG:NH2	2.50	0.45
1:D:836:HIS:CE1	1:D:1610:ARG:HE	2.35	0.45
1:G:195:SER:OG	1:G:196:TYR:N	2.50	0.45
1:G:249:SER:HG	1:G:252:HIS:CD2	2.35	0.45
1:G:473:GLU:OE2	1:G:477:ASN:ND2	2.50	0.45
1:G:503:ASP:OD1	1:G:561:ARG:NH2	2.50	0.45
1:J:498:VAL:HG13	1:J:533:LEU:HD22	1.99	0.45
1:J:4154:SER:OG	1:J:4155:GLU:N	2.48	0.45
1:A:498:VAL:HG13	1:A:533:LEU:HD22	1.99	0.45
1:A:503:ASP:OD1	1:A:561:ARG:NH2	2.50	0.45
1:A:1951:ALA:HB3	3:C:95:LYS:HE2	1.99	0.45
1:A:4635:VAL:O	1:A:4638:THR:OG1	2.25	0.45
1:A:4753:THR:CG2	1:J:4770:LEU:HD12	2.34	0.45
1:G:811:PHE:HB3	1:G:814:LEU:HD22	1.99	0.45
1:J:1951:ALA:HB3	3:L:95:LYS:HE2	1.99	0.45
1:J:4086:LYS:C	1:J:4088:PHE:H	2.24	0.45
3:L:130:ASP:O	3:L:137:VAL:HG22	2.17	0.45
1:A:452:VAL:O	1:A:456:LEU:HB2	2.17	0.44
1:A:1057:LEU:HB3	1:A:1062:TYR:HB2	1.98	0.44
1:A:4523:VAL:HG22	1:J:4808:ASP:O	2.17	0.44
1:D:473:GLU:OE2	1:D:477:ASN:ND2	2.50	0.44
1:D:1272:ARG:NH2	1:D:1590:PHE:O	2.50	0.44
3:F:5:LEU:HB3	3:F:10:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1272:ARG:NH2	1:G:1590:PHE:O	2.50	0.44
1:J:841:LYS:HD2	1:J:842:GLN:HA	1.98	0.44
2:K:7:ILE:HD11	2:K:73:LYS:HB2	1.99	0.44
1:A:841:LYS:HD2	1:A:842:GLN:HA	1.98	0.44
1:D:143:LEU:HD11	1:G:2427:LEU:CD1	2.46	0.44
1:D:452:VAL:O	1:D:456:LEU:HB2	2.17	0.44
1:G:441:LYS:HD3	1:G:444:THR:HG21	1.98	0.44
1:G:498:VAL:HG13	1:G:533:LEU:HD22	1.99	0.44
1:G:3602:ALA:HA	1:G:3605:ARG:HB3	2.00	0.44
1:G:4203:LEU:HD11	1:G:4597:PRO:HB2	1.99	0.44
1:J:441:LYS:HD3	1:J:444:THR:HG21	1.98	0.44
1:J:4203:LEU:HD11	1:J:4597:PRO:HB2	1.99	0.44
1:A:23:GLN:O	1:A:213:SER:OG	2.32	0.44
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.50	0.44
1:D:847:THR:HG21	1:D:1215:MET:H	1.81	0.44
1:D:1105:PHE:CE2	1:D:1115:VAL:HG21	2.53	0.44
1:D:4018:PHE:CE2	1:D:4095:ILE:CG2	3.01	0.44
1:D:4770:LEU:HD12	1:G:4753:THR:CG2	2.37	0.44
1:D:4808:ASP:HB2	1:G:4523:VAL:CG2	2.47	0.44
1:J:452:VAL:O	1:J:456:LEU:HB2	2.17	0.44
1:J:1272:ARG:NH2	1:J:1590:PHE:O	2.50	0.44
1:J:2548:SER:O	1:J:2552:THR:N	2.51	0.44
1:J:3602:ALA:HA	1:J:3605:ARG:HB3	2.00	0.44
1:A:143:LEU:CD2	1:D:2427:LEU:HD11	2.44	0.44
1:A:657:PRO:HA	1:A:834:VAL:HA	1.98	0.44
1:A:4203:LEU:HD11	1:A:4597:PRO:HB2	1.99	0.44
1:D:1183:LEU:HB3	1:D:1187:GLY:HA2	2.00	0.44
1:D:1951:ALA:HB3	3:F:95:LYS:HE2	1.99	0.44
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.99	0.44
1:G:2088:LEU:HD23	1:G:2088:LEU:HA	1.81	0.44
1:G:3854:ASP:OD1	1:G:3854:ASP:N	2.46	0.44
1:G:4090:GLU:CB	1:G:4091:PRO:CD	2.78	0.44
1:G:4808:ASP:HB2	1:J:4523:VAL:CG2	2.47	0.44
1:J:527:LYS:NZ	1:J:566:GLU:OE2	2.45	0.44
1:J:1053:ALA:O	1:J:1056:THR:OG1	2.29	0.44
2:K:92:PRO:HG2	2:K:95:ALA:HB2	1.99	0.44
1:A:1105:PHE:CE2	1:A:1115:VAL:HG21	2.53	0.44
1:A:1655:TYR:OH	1:A:1659:ARG:NH2	2.45	0.44
1:A:4050:HIS:HD2	1:A:4068:LEU:HD11	1.83	0.44
1:D:1630:LEU:HD22	1:D:1641:ILE:HD13	1.98	0.44
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2548:SER:O	1:D:2552:THR:N	2.51	0.44
1:D:4203:LEU:HD11	1:D:4597:PRO:HB2	1.99	0.44
1:G:1630:LEU:HD22	1:G:1641:ILE:HD13	1.98	0.44
1:G:3927:GLY:O	1:G:3929:CYS:N	2.47	0.44
3:I:132:ASP:OD1	3:I:136:GLN:N	2.47	0.44
1:J:836:HIS:CE1	1:J:1610:ARG:HE	2.35	0.44
1:J:847:THR:HG21	1:J:1215:MET:H	1.81	0.44
1:A:246:THR:OG1	1:A:247:VAL:N	2.51	0.44
1:A:1129:GLY:O	1:A:1147:GLN:N	2.45	0.44
1:A:4147:GLU:OE1	1:A:4937:GLN:NE2	2.50	0.44
1:D:246:THR:OG1	1:D:247:VAL:N	2.51	0.44
1:D:498:VAL:HG13	1:D:533:LEU:HD22	1.99	0.44
3:F:130:ASP:O	3:F:137:VAL:HG22	2.18	0.44
2:H:92:PRO:HG2	2:H:95:ALA:HB2	1.99	0.44
1:A:170:SER:OG	1:A:171:GLU:N	2.50	0.44
1:A:335:LYS:NZ	1:A:398:HIS:O	2.37	0.44
1:A:473:GLU:OE2	1:A:477:ASN:ND2	2.50	0.44
1:A:1757:LEU:HD13	1:A:1757:LEU:HA	1.85	0.44
1:D:323:ASP:O	1:D:326:SER:OG	2.35	0.44
1:D:811:PHE:HB3	1:D:814:LEU:HD22	1.99	0.44
1:D:4000:MET:HA	1:D:4003:MET:HG2	1.98	0.44
1:G:1655:TYR:OH	1:G:1659:ARG:NH2	2.45	0.44
3:I:5:LEU:HB3	3:I:10:ILE:HD11	1.98	0.44
1:A:1256:PRO:O	1:A:1451:HIS:ND1	2.45	0.44
1:A:2088:LEU:HA	1:A:2088:LEU:HD23	1.81	0.44
1:A:3891:TRP:HB3	1:J:76:ARG:HB3	1.99	0.44
1:J:1655:TYR:OH	1:J:1659:ARG:NH2	2.45	0.44
1:A:3596:ARG:NH1	1:A:3817:GLY:O	2.51	0.44
1:A:4515:ASN:HD21	1:A:4744:LEU:HD23	1.73	0.44
1:A:4925:TYR:CZ	1:A:4929:LYS:HD2	2.53	0.44
3:C:79:ASP:O	3:C:82:SER:OG	2.33	0.44
1:D:3602:ALA:HA	1:D:3605:ARG:HB3	2.00	0.44
1:G:847:THR:HG21	1:G:1215:MET:H	1.81	0.44
1:G:3977:LYS:HB2	1:G:4095:ILE:HD11	1.99	0.44
1:G:4857:VAL:CG1	1:J:4863:ILE:HG21	2.48	0.44
1:G:4925:TYR:CZ	1:G:4929:LYS:HD2	2.53	0.44
1:J:836:HIS:HB2	1:J:839:GLU:HG2	2.00	0.44
1:J:4018:PHE:CE2	1:J:4095:ILE:HG22	2.53	0.44
1:J:4925:TYR:CZ	1:J:4929:LYS:HD2	2.53	0.44
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	2.00	0.43
1:A:1907:MET:HE3	1:A:1907:MET:HB2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2622:TYR:O	1:D:2627:GLY:N	2.51	0.43
1:G:1029:ASN:HA	1:G:1030:PRO:HD3	1.87	0.43
1:G:2622:TYR:O	1:G:2627:GLY:N	2.51	0.43
1:J:417:ARG:HD3	1:J:420:ARG:HH21	1.82	0.43
1:J:1629:SER:HA	1:J:1640:ASP:HA	2.00	0.43
1:J:3801:CYS:HB3	1:J:3837:THR:HG22	2.00	0.43
1:A:3786:LYS:HE2	1:A:3786:LYS:HB3	1.86	0.43
1:A:3801:CYS:HB3	1:A:3837:THR:HG22	2.00	0.43
1:D:176:ARG:N	1:D:179:ASP:OD2	2.52	0.43
1:D:1945:TYR:O	1:D:1949:MET:HB2	2.19	0.43
1:D:3596:ARG:NH1	1:D:3817:GLY:O	2.51	0.43
1:G:452:VAL:O	1:G:456:LEU:HB2	2.17	0.43
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.99	0.43
1:J:34:LYS:O	1:J:52:THR:OG1	2.32	0.43
1:J:195:SER:OG	1:J:196:TYR:N	2.50	0.43
1:J:3977:LYS:HB2	1:J:4095:ILE:HD11	2.00	0.43
1:J:4050:HIS:HD2	1:J:4068:LEU:HD11	1.83	0.43
1:A:655:MET:SD	1:A:1610:ARG:HD2	2.59	0.43
1:A:811:PHE:HB3	1:A:814:LEU:HD22	1.99	0.43
1:A:1183:LEU:HB3	1:A:1187:GLY:HA2	2.00	0.43
1:A:1629:SER:HA	1:A:1640:ASP:HA	2.00	0.43
1:A:2548:SER:O	1:A:2552:THR:N	2.51	0.43
1:A:3602:ALA:HA	1:A:3605:ARG:HB3	2.00	0.43
1:D:652:VAL:HG13	1:D:692:HIS:CE1	2.53	0.43
1:D:725:TYR:HD1	1:D:732:LEU:HB3	1.83	0.43
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	2.00	0.43
1:D:4873:GLU:CB	1:G:4875:ARG:HH12	2.17	0.43
1:G:170:SER:OG	1:G:171:GLU:N	2.50	0.43
1:G:836:HIS:HB2	1:G:839:GLU:HG2	2.00	0.43
1:G:1629:SER:HA	1:G:1640:ASP:HA	2.00	0.43
1:G:1944:ARG:HH11	1:G:2024:LEU:HD11	1.83	0.43
1:G:1945:TYR:O	1:G:1949:MET:HB2	2.19	0.43
1:G:3596:ARG:NH1	1:G:3817:GLY:O	2.51	0.43
1:J:811:PHE:HB3	1:J:814:LEU:HD22	1.99	0.43
1:A:847:THR:HG21	1:A:1215:MET:H	1.81	0.43
1:A:1053:ALA:O	1:A:1056:THR:OG1	2.29	0.43
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.29	0.43
1:A:4015:LEU:HD23	1:A:4015:LEU:HA	1.79	0.43
1:D:836:HIS:HB2	1:D:839:GLU:HG2	2.00	0.43
1:D:869:THR:HG22	1:D:1002:ASN:HD21	1.83	0.43
1:D:1220:ASP:HB3	1:D:1223:THR:HG1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1944:ARG:HH11	1:D:2024:LEU:HD11	1.83	0.43
1:D:3797:LEU:HD22	1:D:3836:PHE:HZ	1.83	0.43
1:D:4050:HIS:HD2	1:D:4068:LEU:HD11	1.83	0.43
1:G:655:MET:SD	1:G:1610:ARG:HD2	2.59	0.43
1:G:1261:VAL:HG22	1:G:1594:VAL:HG23	2.01	0.43
1:G:1685:LEU:O	1:G:1689:ILE:HG12	2.18	0.43
1:G:3925:ILE:HG23	1:G:3933:GLN:HG2	2.00	0.43
1:J:1129:GLY:HA3	1:J:1145:TRP:HB3	2.00	0.43
1:J:2463:PRO:O	1:J:2520:TYR:OH	2.32	0.43
1:A:836:HIS:HB2	1:A:839:GLU:HG2	2.00	0.43
1:A:1945:TYR:O	1:A:1949:MET:HB2	2.19	0.43
1:A:3925:ILE:HG23	1:A:3933:GLN:HG2	2.00	0.43
2:B:27:THR:HA	2:B:38:SER:HA	2.00	0.43
1:D:308:LEU:HD21	1:D:370:LEU:HD12	2.01	0.43
1:D:527:LYS:NZ	1:D:566:GLU:OE2	2.45	0.43
1:D:655:MET:SD	1:D:1610:ARG:HD2	2.59	0.43
1:D:1057:LEU:HB3	1:D:1062:TYR:HB2	1.98	0.43
1:D:1629:SER:HA	1:D:1640:ASP:HA	2.00	0.43
1:G:308:LEU:HD21	1:G:370:LEU:HD12	2.01	0.43
1:G:1129:GLY:HA3	1:G:1145:TRP:HB3	2.00	0.43
1:G:1183:LEU:HB3	1:G:1187:GLY:HA2	2.00	0.43
1:G:2548:SER:O	1:G:2552:THR:N	2.51	0.43
1:J:176:ARG:N	1:J:179:ASP:OD2	2.52	0.43
1:J:655:MET:SD	1:J:1610:ARG:HD2	2.59	0.43
1:J:1105:PHE:CE2	1:J:1115:VAL:HG21	2.53	0.43
1:J:1183:LEU:HB3	1:J:1187:GLY:HA2	2.00	0.43
1:J:3797:LEU:HD22	1:J:3836:PHE:HZ	1.83	0.43
1:J:4600:ILE:HD12	1:J:4600:ILE:HA	1.89	0.43
1:A:1714:TYR:CZ	1:A:1761:MET:HB3	2.54	0.43
1:A:2161:ASN:OD1	1:A:2164:ARG:NH2	2.41	0.43
2:B:8:SER:O	2:B:71:ARG:N	2.48	0.43
1:D:281:ARG:NH1	1:D:346:VAL:O	2.52	0.43
1:D:1261:VAL:HG22	1:D:1594:VAL:HG23	2.01	0.43
1:G:176:ARG:N	1:G:179:ASP:OD2	2.52	0.43
1:G:1105:PHE:CE2	1:G:1115:VAL:HG21	2.53	0.43
1:G:2215:MET:HE3	1:G:2215:MET:HB3	1.79	0.43
1:G:4010:ASN:OD1	1:G:4010:ASN:N	2.49	0.43
1:J:796:ALA:HB3	1:J:798:ILE:HG13	2.01	0.43
1:J:869:THR:HG22	1:J:1002:ASN:HD21	1.83	0.43
1:J:1261:VAL:HG22	1:J:1594:VAL:HG23	2.01	0.43
1:J:4618:ILE:HD12	1:J:4667:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:NE	1:A:268:SER:O	2.49	0.43
1:A:700:THR:OG1	1:A:787:LEU:N	2.41	0.43
1:A:842:GLN:NE2	1:A:849:ASP:HB2	2.34	0.43
1:A:4857:VAL:CG1	1:D:4863:ILE:HG21	2.49	0.43
2:B:37:ASP:OD1	2:B:38:SER:N	2.52	0.43
1:D:796:ALA:HB3	1:D:798:ILE:HG13	2.01	0.43
1:D:4925:TYR:CZ	1:D:4929:LYS:HD2	2.53	0.43
1:G:725:TYR:HD1	1:G:732:LEU:HB3	1.83	0.43
1:G:4097:PHE:CD2	1:G:4152:GLU:CG	2.93	0.43
1:G:4147:GLU:OE1	1:G:4937:GLN:NE2	2.50	0.43
1:J:1685:LEU:O	1:J:1689:ILE:HG12	2.18	0.43
1:J:2215:MET:HE3	1:J:2215:MET:HB3	1.79	0.43
1:A:417:ARG:HD3	1:A:420:ARG:HH21	1.82	0.43
1:A:652:VAL:HG13	1:A:692:HIS:CE1	2.53	0.43
1:A:2622:TYR:O	1:A:2627:GLY:N	2.51	0.43
1:D:3801:CYS:HB3	1:D:3837:THR:HG22	2.00	0.43
1:G:3620:LEU:HD13	1:G:3620:LEU:HA	1.92	0.43
1:G:3777:LYS:HE3	1:G:3777:LYS:HB2	1.90	0.43
1:G:3797:LEU:HD22	1:G:3836:PHE:HZ	1.83	0.43
1:G:4018:PHE:CE2	1:G:4095:ILE:HG22	2.54	0.43
1:G:4922:PHE:HE2	1:G:4941:VAL:HG11	1.84	0.43
1:D:1714:TYR:CZ	1:D:1761:MET:HB3	2.54	0.43
1:D:2488:LEU:HA	1:D:2488:LEU:HD23	1.84	0.43
1:D:4018:PHE:CE2	1:D:4095:ILE:HG22	2.53	0.43
1:G:796:ALA:HB3	1:G:798:ILE:HG13	2.01	0.43
1:G:1811:GLY:HA3	1:G:1816:PHE:HB2	2.01	0.43
1:G:2173:MET:HE3	1:G:2173:MET:HB2	1.86	0.43
1:G:3801:CYS:HB3	1:G:3837:THR:HG22	2.00	0.43
1:J:246:THR:OG1	1:J:247:VAL:N	2.51	0.43
1:J:811:PHE:HZ	1:J:823:TYR:HB2	1.83	0.43
1:J:2719:GLU:HG2	1:J:2722:ILE:HD12	2.01	0.43
1:J:3925:ILE:HG23	1:J:3933:GLN:HG2	2.00	0.43
1:A:176:ARG:N	1:A:179:ASP:OD2	2.52	0.43
1:D:1628:MET:HE1	1:D:1684:GLN:HE21	1.84	0.43
1:D:1811:GLY:HA3	1:D:1816:PHE:HB2	2.01	0.43
1:D:2719:GLU:HG2	1:D:2722:ILE:HD12	2.01	0.43
1:D:4766:LYS:O	1:D:4770:LEU:HG	2.19	0.43
2:E:27:THR:HA	2:E:38:SER:HA	2.00	0.43
1:G:4811:LEU:HD23	1:J:4519:LEU:CD2	2.34	0.43
1:J:652:VAL:HG13	1:J:692:HIS:CE1	2.53	0.43
1:J:1220:ASP:HB3	1:J:1223:THR:HG1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3596:ARG:NH1	1:J:3817:GLY:O	2.51	0.43
1:A:869:THR:HG22	1:A:1002:ASN:HD21	1.83	0.42
1:A:4618:ILE:HD12	1:A:4667:ILE:HD12	2.01	0.42
1:A:4811:LEU:HD23	1:D:4519:LEU:CD2	2.34	0.42
1:D:43:GLY:HA2	1:D:454:LEU:HG	2.02	0.42
1:D:765:SER:OG	1:D:780:GLU:OE1	2.34	0.42
1:G:281:ARG:NH1	1:G:346:VAL:O	2.52	0.42
1:G:842:GLN:NE2	1:G:849:ASP:HB2	2.34	0.42
1:G:2719:GLU:HG2	1:G:2722:ILE:HD12	2.01	0.42
1:J:281:ARG:NH1	1:J:346:VAL:O	2.52	0.42
1:J:1945:TYR:O	1:J:1949:MET:HB2	2.19	0.42
1:J:4766:LYS:O	1:J:4770:LEU:HG	2.19	0.42
1:A:1628:MET:HE1	1:A:1684:GLN:HE21	1.84	0.42
1:A:1944:ARG:HH11	1:A:2024:LEU:HD11	1.84	0.42
1:A:2719:GLU:HG2	1:A:2722:ILE:HD12	2.01	0.42
1:A:3922:THR:HG22	1:A:3982:MET:HA	2.01	0.42
1:G:246:THR:OG1	1:G:247:VAL:N	2.51	0.42
1:G:1628:MET:HE1	1:G:1684:GLN:HE21	1.84	0.42
1:G:3893:TYR:HD1	1:G:3893:TYR:HA	1.73	0.42
1:J:289:ILE:HG23	1:J:295:PHE:CE2	2.54	0.42
1:J:725:TYR:HD1	1:J:732:LEU:HB3	1.83	0.42
1:J:2622:TYR:O	1:J:2627:GLY:N	2.51	0.42
1:D:1228:THR:HA	1:D:1232:LEU:HD12	2.01	0.42
1:D:3777:LYS:HE3	1:D:3777:LYS:HB2	1.90	0.42
1:G:289:ILE:HG23	1:G:295:PHE:CE2	2.54	0.42
1:G:869:THR:HG22	1:G:1002:ASN:HD21	1.83	0.42
1:G:1228:THR:HA	1:G:1232:LEU:HD12	2.01	0.42
1:G:1714:TYR:CZ	1:G:1761:MET:HB3	2.54	0.42
1:G:4061:GLN:O	1:G:4064:THR:OG1	2.24	0.42
2:H:27:THR:HA	2:H:38:SER:HA	2.00	0.42
1:J:170:SER:OG	1:J:171:GLU:N	2.50	0.42
1:J:1944:ARG:HH11	1:J:2024:LEU:HD11	1.83	0.42
1:J:3922:THR:HG22	1:J:3982:MET:HA	2.01	0.42
1:J:4922:PHE:HE2	1:J:4941:VAL:HG11	1.84	0.42
2:K:37:ASP:OD1	2:K:38:SER:N	2.52	0.42
1:A:143:LEU:HD11	1:D:2427:LEU:CD1	2.47	0.42
1:A:195:SER:OG	1:A:196:TYR:N	2.50	0.42
1:A:281:ARG:NH1	1:A:346:VAL:O	2.52	0.42
1:A:811:PHE:HZ	1:A:823:TYR:HB2	1.83	0.42
1:A:4873:GLU:CB	1:D:4875:ARG:HH12	2.17	0.42
1:D:811:PHE:HZ	1:D:823:TYR:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4618:ILE:HD12	1:D:4667:ILE:HD12	2.01	0.42
1:D:4922:PHE:HE2	1:D:4941:VAL:HG11	1.84	0.42
1:G:43:GLY:HA2	1:G:454:LEU:HG	2.02	0.42
1:G:335:LYS:NZ	1:G:398:HIS:O	2.37	0.42
1:G:652:VAL:HG13	1:G:692:HIS:CE1	2.53	0.42
1:G:4050:HIS:HD2	1:G:4068:LEU:HD11	1.83	0.42
1:J:308:LEU:HD21	1:J:370:LEU:HD12	2.01	0.42
1:J:1907:MET:HE3	1:J:1907:MET:HB2	1.93	0.42
1:A:249:SER:OG	1:A:252:HIS:NE2	2.49	0.42
1:A:725:TYR:HD1	1:A:732:LEU:HB3	1.83	0.42
1:A:848:ARG:HD2	1:A:1603:PHE:CE2	2.55	0.42
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.18	0.42
1:A:1994:ARG:HA	3:C:113:LEU:HD12	2.01	0.42
1:A:4922:PHE:HE2	1:A:4941:VAL:HG11	1.84	0.42
1:D:1994:ARG:HA	3:F:113:LEU:HD12	2.01	0.42
3:F:79:ASP:O	3:F:82:SER:OG	2.33	0.42
1:G:811:PHE:HZ	1:G:823:TYR:HB2	1.83	0.42
1:G:2024:LEU:HB3	1:G:2025:THR:H	1.74	0.42
1:G:4018:PHE:CE2	1:G:4095:ILE:CG2	3.03	0.42
1:J:64:ILE:H	1:J:64:ILE:HG13	1.69	0.42
1:J:1714:TYR:CZ	1:J:1761:MET:HB3	2.54	0.42
1:J:2390:MET:H	1:J:2390:MET:HG3	1.65	0.42
1:A:308:LEU:HD21	1:A:370:LEU:HD12	2.01	0.42
1:A:796:ALA:HB3	1:A:798:ILE:HG13	2.01	0.42
1:A:1261:VAL:HG22	1:A:1594:VAL:HG23	2.01	0.42
1:A:3797:LEU:HD22	1:A:3836:PHE:HZ	1.83	0.42
1:A:4140:MET:HG2	1:A:4146:ILE:HG12	2.02	0.42
1:D:848:ARG:HD2	1:D:1603:PHE:CE2	2.55	0.42
1:G:848:ARG:HD2	1:G:1603:PHE:CE2	2.55	0.42
1:J:43:GLY:HA2	1:J:454:LEU:HG	2.02	0.42
1:J:848:ARG:HD2	1:J:1603:PHE:CE2	2.55	0.42
1:J:4085:VAL:O	1:J:4089:HIS:CB	2.63	0.42
1:J:4140:MET:HG2	1:J:4146:ILE:HG12	2.02	0.42
1:J:4792:LYS:NZ	1:J:4838:ASP:OD2	2.34	0.42
1:A:1242:ASN:HB2	1:A:1807:ARG:HG2	2.02	0.42
1:D:64:ILE:H	1:D:64:ILE:HG13	1.69	0.42
1:D:2235:MET:O	1:D:2298:ARG:NH1	2.35	0.42
2:E:37:ASP:OD1	2:E:38:SER:N	2.52	0.42
1:G:3794:LEU:HD13	1:G:3844:LEU:HD21	2.01	0.42
1:G:4618:ILE:HD12	1:G:4667:ILE:HD12	2.01	0.42
1:J:842:GLN:NE2	1:J:849:ASP:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1628:MET:HE1	1:J:1684:GLN:HE21	1.84	0.42
1:J:4018:PHE:CE2	1:J:4095:ILE:CG2	3.02	0.42
1:J:4738:PHE:HD1	1:J:4738:PHE:HA	1.63	0.42
1:A:370:LEU:HB2	1:A:393:MET:HE3	2.02	0.42
1:A:1690:GLU:OE2	1:A:1790:LYS:NZ	2.49	0.42
1:A:4766:LYS:O	1:A:4770:LEU:HG	2.19	0.42
1:D:289:ILE:HG23	1:D:295:PHE:CE2	2.54	0.42
1:D:3760:LEU:HD23	1:D:3760:LEU:HA	1.89	0.42
1:G:4766:LYS:O	1:G:4770:LEU:HG	2.19	0.42
1:J:1228:THR:HA	1:J:1232:LEU:HD12	2.01	0.42
2:K:8:SER:O	2:K:71:ARG:N	2.48	0.42
1:A:1001:GLU:HG3	1:A:1035:TYR:HB3	2.02	0.42
1:A:1266:GLU:OE1	1:A:1296:SER:OG	2.37	0.42
1:D:1129:GLY:O	1:D:1147:GLN:N	2.45	0.42
1:D:4518:LEU:HD23	1:D:4738:PHE:HE1	1.70	0.42
1:G:1001:GLU:HG3	1:G:1035:TYR:HB3	2.02	0.42
1:G:1220:ASP:HB3	1:G:1223:THR:HG1	1.85	0.42
1:J:1170:GLU:O	1:J:1172:THR:N	2.52	0.42
1:J:1811:GLY:HA3	1:J:1816:PHE:HB2	2.01	0.42
1:J:3956:GLN:HE22	1:J:3976:GLN:HE21	1.68	0.42
1:J:4761:VAL:HG22	1:J:4867:ILE:HD12	2.02	0.42
1:A:1228:THR:HA	1:A:1232:LEU:HD12	2.01	0.42
1:D:35:LEU:HD13	1:D:49:LEU:HD13	2.02	0.42
1:D:1001:GLU:HG3	1:D:1035:TYR:HB3	2.02	0.42
1:D:3794:LEU:HD13	1:D:3844:LEU:HD21	2.01	0.42
1:D:3800:SER:OG	1:D:3801:CYS:N	2.42	0.42
1:G:323:ASP:O	1:G:326:SER:OG	2.35	0.42
1:G:908:ARG:HA	1:G:916:PRO:HD3	2.01	0.42
1:G:3786:LYS:HE2	1:G:3786:LYS:HB3	1.86	0.42
1:G:4770:LEU:HD12	1:J:4753:THR:CG2	2.38	0.42
1:J:3794:LEU:HD13	1:J:3844:LEU:HD21	2.01	0.42
1:J:4147:GLU:OE1	1:J:4937:GLN:NE2	2.50	0.42
1:A:35:LEU:HD13	1:A:49:LEU:HD13	2.02	0.41
1:A:191:TYR:N	1:A:206:ALA:O	2.53	0.41
1:A:530:LEU:HD23	1:A:530:LEU:HA	1.82	0.41
1:A:1091:GLU:OE1	1:A:1248:THR:OG1	2.38	0.41
1:A:1146:HIS:CD2	1:A:1147:GLN:HG3	2.55	0.41
1:A:1170:GLU:O	1:A:1172:THR:N	2.52	0.41
1:A:2215:MET:HE3	1:A:2215:MET:HB3	1.79	0.41
1:A:2398:ASP:O	1:A:2402:ARG:HG2	2.20	0.41
1:D:191:TYR:N	1:D:206:ALA:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1146:HIS:CD2	1:D:1147:GLN:HG3	2.55	0.41
1:D:1242:ASN:HB2	1:D:1807:ARG:HG2	2.02	0.41
1:D:2215:MET:HE3	1:D:2215:MET:HB3	1.79	0.41
1:D:2734:SER:HB2	1:D:2758:MET:HE1	2.02	0.41
1:D:3922:THR:HG22	1:D:3982:MET:HA	2.01	0.41
1:D:4191:VAL:HG11	1:D:4950:TRP:CH2	2.55	0.41
1:D:4738:PHE:HD1	1:D:4738:PHE:HA	1.63	0.41
1:D:4761:VAL:HG22	1:D:4867:ILE:HD12	2.02	0.41
1:G:630:HIS:CE1	1:G:1671:ARG:HD2	2.55	0.41
1:G:2073:GLU:HG3	1:G:2074:SER:HB3	2.02	0.41
1:G:2304:ARG:NH2	1:G:2402:ARG:HH12	2.18	0.41
1:J:235:ARG:NE	1:J:268:SER:O	2.49	0.41
1:J:908:ARG:HA	1:J:916:PRO:HD3	2.01	0.41
1:A:289:ILE:HG23	1:A:295:PHE:CE2	2.54	0.41
1:D:2398:ASP:O	1:D:2402:ARG:HG2	2.20	0.41
1:G:4573:LEU:HD21	1:G:4737:ASN:CG	2.45	0.41
1:G:4761:VAL:HG22	1:G:4867:ILE:HD12	2.02	0.41
1:J:323:ASP:O	1:J:326:SER:OG	2.35	0.41
1:J:370:LEU:HB2	1:J:393:MET:HE3	2.02	0.41
1:J:630:HIS:CE1	1:J:1671:ARG:HD2	2.55	0.41
1:J:1001:GLU:HG3	1:J:1035:TYR:HB3	2.02	0.41
2:K:27:THR:HA	2:K:38:SER:HA	2.00	0.41
1:A:43:GLY:HA2	1:A:454:LEU:HG	2.02	0.41
1:A:630:HIS:CE1	1:A:1671:ARG:HD2	2.55	0.41
1:A:4086:LYS:NZ	1:A:4086:LYS:CB	2.74	0.41
1:D:842:GLN:NE2	1:D:849:ASP:HB2	2.34	0.41
1:D:2126:GLN:HE21	1:D:2142:LEU:HB3	1.86	0.41
1:D:3794:LEU:HD23	1:D:3794:LEU:HA	1.85	0.41
1:G:541:ILE:HG23	1:G:548:CYS:HB3	2.02	0.41
1:G:1091:GLU:OE1	1:G:1248:THR:OG1	2.38	0.41
1:G:2398:ASP:O	1:G:2402:ARG:HG2	2.20	0.41
1:G:3956:GLN:HE22	1:G:3976:GLN:HE21	1.68	0.41
1:J:1242:ASN:HB2	1:J:1807:ARG:HG2	2.02	0.41
1:A:1811:GLY:HA3	1:A:1816:PHE:HB2	2.01	0.41
1:A:1846:ILE:HG12	1:A:1894:LEU:HD23	2.03	0.41
1:A:3794:LEU:HD13	1:A:3844:LEU:HD21	2.01	0.41
1:A:4761:VAL:HG22	1:A:4867:ILE:HD12	2.02	0.41
1:D:3925:ILE:HG23	1:D:3933:GLN:HG2	2.00	0.41
1:D:4573:LEU:HD21	1:D:4737:ASN:CG	2.45	0.41
1:G:778:MET:HB3	1:G:1467:VAL:HG13	2.02	0.41
1:G:1846:ILE:HG12	1:G:1894:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:LEU:HD13	1:J:49:LEU:HD13	2.02	0.41
1:J:2398:ASP:O	1:J:2402:ARG:HG2	2.20	0.41
1:A:1678:SER:HB2	1:A:1768:PHE:CZ	2.56	0.41
1:A:2173:MET:HE3	1:A:2173:MET:HB2	1.86	0.41
1:A:2734:SER:HB2	1:A:2758:MET:HE1	2.02	0.41
1:A:3956:GLN:HE22	1:A:3976:GLN:HE21	1.68	0.41
1:D:630:HIS:CE1	1:D:1671:ARG:HD2	2.55	0.41
1:D:633:CYS:SG	1:D:1664:VAL:HG11	2.61	0.41
1:D:2173:MET:HB2	1:D:2173:MET:HE3	1.86	0.41
1:D:2304:ARG:NH2	1:D:2402:ARG:HH12	2.18	0.41
3:F:132:ASP:OD1	3:F:136:GLN:N	2.47	0.41
1:G:64:ILE:H	1:G:64:ILE:HG13	1.69	0.41
1:G:3922:THR:HG22	1:G:3982:MET:HA	2.01	0.41
1:J:1678:SER:HB2	1:J:1768:PHE:CZ	2.56	0.41
1:J:1994:ARG:HA	3:L:113:LEU:HD12	2.01	0.41
1:A:4753:THR:CG2	1:J:4770:LEU:HD11	2.06	0.41
1:D:1091:GLU:OE1	1:D:1248:THR:OG1	2.38	0.41
1:D:3737:ALA:HA	1:D:3740:MET:HG2	2.02	0.41
1:G:1678:SER:HB2	1:G:1768:PHE:CZ	2.56	0.41
1:J:541:ILE:HG23	1:J:548:CYS:HB3	2.02	0.41
1:J:633:CYS:SG	1:J:1664:VAL:HG11	2.61	0.41
1:J:695:VAL:N	1:J:725:TYR:O	2.43	0.41
1:J:1250:TRP:HD1	1:J:1601:ASN:C	2.29	0.41
1:J:2073:GLU:HG3	1:J:2074:SER:HB3	2.02	0.41
1:J:2126:GLN:HE21	1:J:2142:LEU:HB3	1.86	0.41
1:J:2235:MET:O	1:J:2298:ARG:NH1	2.35	0.41
1:J:2732:LYS:NZ	1:J:2736:ASP:OD1	2.54	0.41
1:J:4521:TYR:HD1	1:J:4521:TYR:HA	1.73	0.41
1:A:4770:LEU:HD12	1:D:4753:THR:CG2	2.37	0.41
1:D:2073:GLU:HG3	1:D:2074:SER:HB3	2.02	0.41
1:G:1907:MET:HE3	1:G:1907:MET:HB2	1.93	0.41
1:G:2421:ARG:O	1:G:2425:ARG:HG2	2.21	0.41
1:J:778:MET:HB3	1:J:1467:VAL:HG13	2.02	0.41
1:J:1146:HIS:CD2	1:J:1147:GLN:HG3	2.55	0.41
1:J:1705:LEU:HA	1:J:1705:LEU:HD23	1.78	0.41
1:J:2421:ARG:O	1:J:2425:ARG:HG2	2.21	0.41
1:J:3794:LEU:HD23	1:J:3794:LEU:HA	1.85	0.41
3:L:132:ASP:OD1	3:L:136:GLN:N	2.47	0.41
1:A:541:ILE:HG23	1:A:548:CYS:HB3	2.02	0.41
1:A:908:ARG:HA	1:A:916:PRO:HD3	2.01	0.41
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2126:GLN:HE21	1:A:2142:LEU:HB3	1.86	0.41
1:A:2421:ARG:O	1:A:2425:ARG:HG2	2.21	0.41
1:D:2732:LYS:NZ	1:D:2736:ASP:OD1	2.54	0.41
1:G:35:LEU:HD13	1:G:49:LEU:HD13	2.02	0.41
1:G:1146:HIS:CD2	1:G:1147:GLN:HG3	2.55	0.41
1:G:1285:VAL:HG12	1:G:1286:THR:HG23	2.03	0.41
1:G:4086:LYS:C	1:G:4088:PHE:N	2.79	0.41
1:J:1285:VAL:HG12	1:J:1286:THR:HG23	2.03	0.41
1:J:2734:SER:HB2	1:J:2758:MET:HE1	2.02	0.41
1:J:3639:ASP:OD1	1:J:3731:ARG:NH1	2.49	0.41
1:A:307:SER:HA	1:A:327:THR:HB	2.03	0.41
1:A:633:CYS:SG	1:A:1664:VAL:HG11	2.61	0.41
1:A:2732:LYS:NZ	1:A:2736:ASP:OD1	2.54	0.41
1:A:3620:LEU:HD13	1:A:3620:LEU:HA	1.92	0.41
1:A:3690:MET:HE3	1:A:3690:MET:HB3	1.91	0.41
1:A:3921:LEU:HD23	1:A:3921:LEU:HA	1.88	0.41
1:A:4115:ARG:HH11	1:A:4115:ARG:HD3	1.74	0.41
1:D:143:LEU:HD21	1:G:2427:LEU:HD13	1.92	0.41
1:D:370:LEU:HB2	1:D:393:MET:HE3	2.02	0.41
1:D:541:ILE:HG23	1:D:548:CYS:HB3	2.02	0.41
1:D:778:MET:O	1:D:1468:THR:N	2.41	0.41
1:D:1250:TRP:HD1	1:D:1601:ASN:C	2.29	0.41
1:D:1442:TRP:HB2	1:D:1544:PHE:HB2	2.02	0.41
1:D:1640:ASP:OD1	1:D:1640:ASP:N	2.53	0.41
1:D:1842:ILE:HD13	1:D:1842:ILE:HA	1.92	0.41
1:D:4493:LEU:HA	1:D:4496:PHE:HD2	1.86	0.41
1:G:695:VAL:N	1:G:725:TYR:O	2.43	0.41
1:G:1994:ARG:HA	3:I:113:LEU:HD12	2.01	0.41
1:G:2126:GLN:HE21	1:G:2142:LEU:HB3	1.86	0.41
1:G:3737:ALA:HA	1:G:3740:MET:HG2	2.02	0.41
1:G:4191:VAL:HG11	1:G:4950:TRP:CH2	2.55	0.41
1:G:4493:LEU:HA	1:G:4496:PHE:HD2	1.86	0.41
1:G:4515:ASN:HD21	1:G:4744:LEU:HD23	1.73	0.41
1:G:4770:LEU:HD11	1:J:4753:THR:CG2	2.09	0.41
1:J:249:SER:OG	1:J:252:HIS:NE2	2.49	0.41
1:J:394:HIS:NE2	1:J:396:GLU:OE1	2.54	0.41
1:J:899:GLU:HG2	1:J:971:GLN:HE22	1.86	0.41
1:J:2173:MET:HB2	1:J:2173:MET:HE3	1.86	0.41
1:A:228:LEU:HB3	1:A:289:ILE:HD12	2.03	0.41
1:A:287:SER:HA	1:A:349:MET:HA	2.03	0.41
1:A:728:ASP:HA	1:A:748:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLU:HG2	1:A:971:GLN:HE22	1.86	0.41
1:A:1250:TRP:HD1	1:A:1601:ASN:C	2.29	0.41
1:A:1842:ILE:HD13	1:A:1842:ILE:HA	1.92	0.41
1:A:4493:LEU:HA	1:A:4496:PHE:HD2	1.86	0.41
1:A:4573:LEU:HD21	1:A:4737:ASN:CG	2.45	0.41
1:D:899:GLU:HG2	1:D:971:GLN:HE22	1.86	0.41
1:D:908:ARG:HA	1:D:916:PRO:HD3	2.01	0.41
1:D:1267:HIS:CD2	1:D:1293:GLN:HB2	2.52	0.41
1:D:1303:ARG:HB2	1:D:1593:HIS:HB2	2.03	0.41
1:D:2421:ARG:O	1:D:2425:ARG:HG2	2.21	0.41
1:D:3956:GLN:HE22	1:D:3976:GLN:HE21	1.68	0.41
1:G:633:CYS:SG	1:G:1664:VAL:HG11	2.61	0.41
1:G:899:GLU:HG2	1:G:971:GLN:HE22	1.86	0.41
1:G:1242:ASN:HB2	1:G:1807:ARG:HG2	2.02	0.41
1:G:1705:LEU:HA	1:G:1705:LEU:HD23	1.78	0.41
1:G:2060:GLN:NE2	1:G:2092:GLN:O	2.53	0.41
1:G:4140:MET:HG2	1:G:4146:ILE:HG12	2.02	0.41
1:J:191:TYR:N	1:J:206:ALA:O	2.53	0.41
1:J:228:LEU:HB3	1:J:289:ILE:HD12	2.03	0.41
1:J:4191:VAL:HG11	1:J:4950:TRP:CH2	2.55	0.41
1:J:4573:LEU:HD21	1:J:4737:ASN:CG	2.45	0.41
1:A:2427:LEU:CD1	1:J:143:LEU:HD11	2.47	0.40
1:D:307:SER:HA	1:D:327:THR:HB	2.03	0.40
1:D:394:HIS:NE2	1:D:396:GLU:OE1	2.54	0.40
1:D:1809:PRO:HB2	1:D:1817:LEU:HD22	2.02	0.40
1:D:4087:ARG:HG3	1:D:4088:PHE:CD2	2.56	0.40
3:F:23:ASP:OD1	3:F:23:ASP:N	2.54	0.40
1:J:307:SER:HA	1:J:327:THR:HB	2.03	0.40
1:J:533:LEU:HA	1:J:533:LEU:HD23	1.91	0.40
1:J:1809:PRO:HB2	1:J:1817:LEU:HD22	2.02	0.40
1:J:3755:MET:O	1:J:3759:THR:HG23	2.21	0.40
1:J:3786:LYS:HB3	1:J:3786:LYS:HE2	1.86	0.40
1:J:4493:LEU:HA	1:J:4496:PHE:HD2	1.86	0.40
1:A:371:TRP:N	1:A:394:HIS:O	2.54	0.40
1:A:778:MET:O	1:A:1468:THR:N	2.41	0.40
1:A:1705:LEU:HD23	1:A:1705:LEU:HA	1.78	0.40
1:A:2124:LEU:HD11	1:A:2168:MET:HB3	2.04	0.40
1:D:4061:GLN:O	1:D:4064:THR:OG1	2.25	0.40
1:D:4140:MET:HG2	1:D:4146:ILE:HG12	2.02	0.40
1:G:191:TYR:N	1:G:206:ALA:O	2.53	0.40
1:G:2732:LYS:NZ	1:G:2736:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:503:ASP:HA	1:J:561:ARG:HH12	1.86	0.40
1:J:1091:GLU:OE1	1:J:1248:THR:OG1	2.38	0.40
1:J:1299:ILE:HG21	1:J:1299:ILE:HD13	1.86	0.40
1:J:1442:TRP:HB2	1:J:1544:PHE:HB2	2.02	0.40
1:J:2488:LEU:HD23	1:J:2488:LEU:HA	1.84	0.40
1:J:2743:ILE:HG23	1:J:2820:HIS:HB3	2.03	0.40
1:J:3847:LEU:HD23	1:J:3855:PHE:CE2	2.57	0.40
1:A:1442:TRP:HB2	1:A:1544:PHE:HB2	2.02	0.40
3:C:132:ASP:OD1	3:C:136:GLN:N	2.47	0.40
1:D:503:ASP:HA	1:D:561:ARG:HH12	1.86	0.40
1:D:533:LEU:HA	1:D:533:LEU:HD23	1.91	0.40
1:D:1285:VAL:HG12	1:D:1286:THR:HG23	2.03	0.40
1:D:2260:GLU:HG2	1:D:2261:PRO:HD3	2.03	0.40
1:D:4811:LEU:HD23	1:G:4519:LEU:CD2	2.34	0.40
1:G:307:SER:HA	1:G:327:THR:HB	2.03	0.40
1:G:1250:TRP:HD1	1:G:1601:ASN:C	2.29	0.40
1:G:3755:MET:O	1:G:3759:THR:HG23	2.21	0.40
1:J:371:TRP:N	1:J:394:HIS:O	2.54	0.40
1:J:1258:PHE:HB3	1:J:1303:ARG:NH1	2.36	0.40
1:J:1266:GLU:OE1	1:J:1296:SER:OG	2.37	0.40
1:J:1303:ARG:HB2	1:J:1593:HIS:HB2	2.03	0.40
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.93	0.40
1:A:394:HIS:NE2	1:A:396:GLU:OE1	2.54	0.40
1:A:778:MET:HB3	1:A:1467:VAL:HG13	2.02	0.40
1:A:1809:PRO:HB2	1:A:1817:LEU:HD22	2.02	0.40
1:A:2260:GLU:HG2	1:A:2261:PRO:HD3	2.03	0.40
1:A:4907:GLU:CD	1:J:4184:LYS:HB2	2.44	0.40
1:D:530:LEU:HA	1:D:530:LEU:HD23	1.81	0.40
1:D:728:ASP:HA	1:D:748:LEU:HA	2.04	0.40
1:D:1678:SER:HB2	1:D:1768:PHE:CZ	2.56	0.40
2:E:8:SER:O	2:E:71:ARG:N	2.48	0.40
1:G:228:LEU:HB3	1:G:289:ILE:HD12	2.03	0.40
1:G:1086:ARG:HH22	1:G:1254:ARG:HB2	1.87	0.40
1:G:1258:PHE:HB3	1:G:1303:ARG:NH1	2.36	0.40
1:G:1442:TRP:HB2	1:G:1544:PHE:HB2	2.02	0.40
1:G:1690:GLU:OE2	1:G:1790:LYS:NZ	2.49	0.40
1:J:35:LEU:H	1:J:35:LEU:HG	1.66	0.40
1:J:277:LEU:HD13	1:J:289:ILE:HD13	2.03	0.40
1:J:2060:GLN:NE2	1:J:2092:GLN:O	2.53	0.40
1:J:3690:MET:HE3	1:J:3690:MET:HB3	1.91	0.40
1:J:3737:ALA:HA	1:J:3740:MET:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3986:MET:HE2	1:J:3996:ILE:HD11	2.04	0.40
1:A:3737:ALA:HA	1:A:3740:MET:HG2	2.02	0.40
1:D:1086:ARG:HH22	1:D:1254:ARG:HB2	1.87	0.40
1:D:2124:LEU:HD11	1:D:2168:MET:HB3	2.04	0.40
1:D:2743:ILE:HG23	1:D:2820:HIS:HB3	2.03	0.40
1:D:3755:MET:O	1:D:3759:THR:HG23	2.21	0.40
1:G:370:LEU:HB2	1:G:393:MET:HE3	2.02	0.40
1:G:1632:ILE:HD11	1:G:1637:ARG:HG2	2.04	0.40
1:G:2734:SER:HB2	1:G:2758:MET:HE1	2.02	0.40
1:G:3665:LEU:HD12	1:G:3665:LEU:HA	1.94	0.40
1:G:3800:SER:OG	1:G:3801:CYS:N	2.41	0.40
1:G:4097:PHE:C	1:G:4097:PHE:CD1	2.98	0.40
1:G:4732:LEU:HD23	1:G:4732:LEU:HA	1.94	0.40
1:J:1748:LEU:O	1:J:1750:GLY:N	2.55	0.40
1:J:2260:GLU:HG2	1:J:2261:PRO:HD3	2.03	0.40
1:J:2857:LYS:HE3	1:J:2861:LEU:HD21	2.04	0.40
1:J:3983:LEU:HG	1:J:4102:LEU:HD11	2.03	0.40
3:L:23:ASP:OD1	3:L:23:ASP:N	2.54	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	3389/4968 (68%)	3012 (89%)	360 (11%)	17 (0%)	24	57
1	D	3389/4968 (68%)	3013 (89%)	359 (11%)	17 (0%)	24	57
1	G	3389/4968 (68%)	3015 (89%)	356 (10%)	18 (0%)	24	57
1	J	3389/4968 (68%)	3012 (89%)	360 (11%)	17 (0%)	24	57
2	B	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	E	105/108 (97%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	K	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
3	C	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	49
3	F	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	49
3	I	132/149 (89%)	118 (89%)	13 (10%)	1 (1%)	16	49
3	L	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	49
All	All	14504/20900 (69%)	12911 (89%)	1520 (10%)	73 (0%)	26	57

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4916	LEU
1	D	4916	LEU
1	G	4916	LEU
1	J	4916	LEU
1	A	1580	PRO
1	A	1770	SER
3	C	130	ASP
1	D	1580	PRO
1	D	1770	SER
3	F	130	ASP
1	G	1580	PRO
1	G	1770	SER
3	I	130	ASP
1	J	1580	PRO
1	J	1770	SER
3	L	130	ASP
1	A	4071	ALA
1	A	4740	PHE
1	A	4915	ASN
1	D	853	PRO
1	D	4071	ALA
1	D	4740	PHE
1	D	4915	ASN
1	G	4071	ALA
1	G	4740	PHE
1	G	4915	ASN
1	J	4071	ALA
1	J	4740	PHE
1	J	4915	ASN

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Mol	Chain	Res	Type
1	A	853	PRO
1	A	1581	GLN
1	A	3801	CYS
1	A	3802	SER
1	A	4164	PRO
1	D	1581	GLN
1	D	3801	CYS
1	D	3802	SER
1	D	4164	PRO
1	G	853	PRO
1	G	1581	GLN
1	G	3801	CYS
1	G	3802	SER
1	G	4164	PRO
1	J	853	PRO
1	J	1581	GLN
1	J	3801	CYS
1	J	3802	SER
1	J	4164	PRO
1	A	1298	ASP
1	D	1298	ASP
1	G	1298	ASP
1	G	4087	ARG
1	J	1298	ASP
1	A	1535	PRO
1	A	4163	LYS
1	D	1535	PRO
1	D	4163	LYS
1	G	1535	PRO
1	G	4163	LYS
1	J	1535	PRO
1	J	4163	LYS
1	A	1848	PRO
1	D	1848	PRO
1	G	1848	PRO
1	J	1848	PRO
1	A	1769	VAL
1	D	1769	VAL
1	G	1769	VAL
1	J	1769	VAL
1	A	828	PRO
1	D	828	PRO

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Mol	Chain	Res	Type
1	G	828	PRO
1	J	828	PRO

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	2704/4355 (62%)	2674 (99%)	30 (1%)	65	74
1	D	2704/4355 (62%)	2674 (99%)	30 (1%)	65	74
1	G	2704/4355 (62%)	2673 (99%)	31 (1%)	65	74
1	J	2704/4355 (62%)	2675 (99%)	29 (1%)	65	74
2	B	88/89 (99%)	86 (98%)	2 (2%)	44	64
2	E	88/89 (99%)	86 (98%)	2 (2%)	44	64
2	H	88/89 (99%)	86 (98%)	2 (2%)	44	64
2	K	88/89 (99%)	86 (98%)	2 (2%)	44	64
3	C	119/127 (94%)	119 (100%)	0	100	100
3	F	119/127 (94%)	119 (100%)	0	100	100
3	I	119/127 (94%)	119 (100%)	0	100	100
3	L	119/127 (94%)	119 (100%)	0	100	100
All	All	11644/18284 (64%)	11516 (99%)	128 (1%)	63	74

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	234	LEU
1	A	541	ILE
1	A	625	VAL
1	A	646	THR
1	A	728	ASP
1	A	832	LEU
1	A	925	PRO

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Mol	Chain	Res	Type
1	A	990	PRO
1	A	1042	THR
1	A	1054	VAL
1	A	1089	ARG
1	A	1619	VAL
1	A	1821	LEU
1	A	2211	ASN
1	A	2409	LEU
1	A	2420	ILE
1	A	4087	ARG
1	A	4090	GLU
1	A	4094	ASP
1	A	4095	ILE
1	A	4136	ARG
1	A	4499	ASN
1	A	4521	TYR
1	A	4586	PHE
1	A	4738	PHE
1	A	4754	LEU
1	A	4823	ARG
1	A	4858	ILE
1	A	4863	ILE
2	B	27	THR
2	B	41	ASP
1	D	35	LEU
1	D	234	LEU
1	D	541	ILE
1	D	625	VAL
1	D	646	THR
1	D	728	ASP
1	D	832	LEU
1	D	925	PRO
1	D	990	PRO
1	D	1042	THR
1	D	1054	VAL
1	D	1089	ARG
1	D	1619	VAL
1	D	1821	LEU
1	D	2211	ASN
1	D	2409	LEU
1	D	2420	ILE
1	D	4087	ARG

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Mol	Chain	Res	Type
1	D	4090	GLU
1	D	4094	ASP
1	D	4095	ILE
1	D	4136	ARG
1	D	4499	ASN
1	D	4521	TYR
1	D	4586	PHE
1	D	4738	PHE
1	D	4754	LEU
1	D	4823	ARG
1	D	4858	ILE
1	D	4863	ILE
2	E	27	THR
2	E	41	ASP
1	G	35	LEU
1	G	234	LEU
1	G	541	ILE
1	G	625	VAL
1	G	646	THR
1	G	728	ASP
1	G	832	LEU
1	G	925	PRO
1	G	950	VAL
1	G	990	PRO
1	G	1042	THR
1	G	1054	VAL
1	G	1089	ARG
1	G	1619	VAL
1	G	1821	LEU
1	G	2211	ASN
1	G	2409	LEU
1	G	2420	ILE
1	G	4087	ARG
1	G	4090	GLU
1	G	4094	ASP
1	G	4095	ILE
1	G	4136	ARG
1	G	4499	ASN
1	G	4521	TYR
1	G	4586	PHE
1	G	4738	PHE
1	G	4754	LEU

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Mol	Chain	Res	Type
1	G	4823	ARG
1	G	4858	ILE
1	G	4863	ILE
2	H	27	THR
2	H	41	ASP
1	J	35	LEU
1	J	234	LEU
1	J	541	ILE
1	J	625	VAL
1	J	646	THR
1	J	728	ASP
1	J	832	LEU
1	J	925	PRO
1	J	950	VAL
1	J	990	PRO
1	J	1042	THR
1	J	1089	ARG
1	J	1619	VAL
1	J	1821	LEU
1	J	2211	ASN
1	J	2409	LEU
1	J	2420	ILE
1	J	4087	ARG
1	J	4094	ASP
1	J	4095	ILE
1	J	4136	ARG
1	J	4499	ASN
1	J	4521	TYR
1	J	4586	PHE
1	J	4738	PHE
1	J	4754	LEU
1	J	4823	ARG
1	J	4858	ILE
1	J	4863	ILE
2	K	27	THR
2	K	41	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	57	ASN

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Mol	Chain	Res	Type
1	A	110	HIS
1	A	117	HIS
1	A	123	HIS
1	A	150	GLN
1	A	163	HIS
1	A	193	HIS
1	A	293	GLN
1	A	364	GLN
1	A	388	GLN
1	A	394	HIS
1	A	395	HIS
1	A	398	HIS
1	A	487	ASN
1	A	531	ASN
1	A	544	ASN
1	A	576	HIS
1	A	593	HIS
1	A	607	ASN
1	A	621	HIS
1	A	630	HIS
1	A	651	HIS
1	A	888	ASN
1	A	914	GLN
1	A	971	GLN
1	A	1002	ASN
1	A	1143	GLN
1	A	1146	HIS
1	A	1151	HIS
1	A	1216	ASN
1	A	1267	HIS
1	A	1602	GLN
1	A	1620	GLN
1	A	1654	HIS
1	A	1656	HIS
1	A	1679	HIS
1	A	1684	GLN
1	A	1746	HIS
1	A	1918	GLN
1	A	2153	ASN
1	A	2159	HIS
1	A	2196	ASN
1	A	2211	ASN

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Mol	Chain	Res	Type
1	A	2218	HIS
1	A	2317	ASN
1	A	2518	ASN
1	A	2820	HIS
1	A	3667	GLN
1	A	3883	GLN
1	A	3904	GLN
1	A	3916	GLN
1	A	3956	GLN
1	A	4050	HIS
1	A	4172	GLN
1	A	4179	ASN
1	A	4490	GLN
1	A	4494	ASN
1	A	4499	ASN
1	A	4515	ASN
1	A	4621	GLN
1	A	4737	ASN
1	A	4817	HIS
1	A	4880	GLN
2	B	87	HIS
3	C	9	GLN
3	C	50	GLN
3	C	54	ASN
1	D	44	ASN
1	D	57	ASN
1	D	110	HIS
1	D	117	HIS
1	D	123	HIS
1	D	150	GLN
1	D	163	HIS
1	D	193	HIS
1	D	293	GLN
1	D	364	GLN
1	D	394	HIS
1	D	395	HIS
1	D	398	HIS
1	D	487	ASN
1	D	531	ASN
1	D	544	ASN
1	D	576	HIS
1	D	607	ASN

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Mol	Chain	Res	Type
1	D	630	HIS
1	D	651	HIS
1	D	888	ASN
1	D	914	GLN
1	D	971	GLN
1	D	1002	ASN
1	D	1143	GLN
1	D	1151	HIS
1	D	1216	ASN
1	D	1267	HIS
1	D	1602	GLN
1	D	1620	GLN
1	D	1654	HIS
1	D	1656	HIS
1	D	1679	HIS
1	D	1684	GLN
1	D	1746	HIS
1	D	1918	GLN
1	D	2196	ASN
1	D	2211	ASN
1	D	2218	HIS
1	D	2317	ASN
1	D	2518	ASN
1	D	2703	ASN
1	D	2820	HIS
1	D	3667	GLN
1	D	3883	GLN
1	D	3904	GLN
1	D	3916	GLN
1	D	3956	GLN
1	D	4050	HIS
1	D	4172	GLN
1	D	4179	ASN
1	D	4490	GLN
1	D	4494	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4621	GLN
1	D	4737	ASN
1	D	4764	ASN
1	D	4817	HIS
1	D	4880	GLN

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Mol	Chain	Res	Type
2	E	87	HIS
3	F	9	GLN
3	F	50	GLN
3	F	54	ASN
1	G	44	ASN
1	G	57	ASN
1	G	110	HIS
1	G	117	HIS
1	G	123	HIS
1	G	150	GLN
1	G	163	HIS
1	G	193	HIS
1	G	293	GLN
1	G	364	GLN
1	G	388	GLN
1	G	394	HIS
1	G	395	HIS
1	G	398	HIS
1	G	487	ASN
1	G	531	ASN
1	G	544	ASN
1	G	576	HIS
1	G	593	HIS
1	G	607	ASN
1	G	630	HIS
1	G	651	HIS
1	G	842	GLN
1	G	888	ASN
1	G	914	GLN
1	G	971	GLN
1	G	1002	ASN
1	G	1143	GLN
1	G	1146	HIS
1	G	1151	HIS
1	G	1216	ASN
1	G	1267	HIS
1	G	1602	GLN
1	G	1620	GLN
1	G	1654	HIS
1	G	1656	HIS
1	G	1679	HIS
1	G	1684	GLN

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Mol	Chain	Res	Type
1	G	1746	HIS
1	G	1918	GLN
1	G	2126	GLN
1	G	2159	HIS
1	G	2196	ASN
1	G	2211	ASN
1	G	2218	HIS
1	G	2317	ASN
1	G	2518	ASN
1	G	2820	HIS
1	G	3611	ASN
1	G	3667	GLN
1	G	3883	GLN
1	G	3904	GLN
1	G	3916	GLN
1	G	3956	GLN
1	G	4050	HIS
1	G	4172	GLN
1	G	4179	ASN
1	G	4490	GLN
1	G	4494	ASN
1	G	4499	ASN
1	G	4515	ASN
1	G	4621	GLN
1	G	4737	ASN
1	G	4764	ASN
1	G	4817	HIS
1	G	4880	GLN
2	H	87	HIS
3	I	9	GLN
3	I	50	GLN
3	I	54	ASN
1	J	44	ASN
1	J	57	ASN
1	J	110	HIS
1	J	117	HIS
1	J	123	HIS
1	J	163	HIS
1	J	193	HIS
1	J	261	HIS
1	J	293	GLN
1	J	364	GLN

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Mol	Chain	Res	Type
1	J	388	GLN
1	J	394	HIS
1	J	398	HIS
1	J	487	ASN
1	J	531	ASN
1	J	544	ASN
1	J	576	HIS
1	J	593	HIS
1	J	607	ASN
1	J	630	HIS
1	J	651	HIS
1	J	888	ASN
1	J	914	GLN
1	J	971	GLN
1	J	1002	ASN
1	J	1143	GLN
1	J	1146	HIS
1	J	1151	HIS
1	J	1216	ASN
1	J	1267	HIS
1	J	1602	GLN
1	J	1620	GLN
1	J	1654	HIS
1	J	1656	HIS
1	J	1679	HIS
1	J	1684	GLN
1	J	1746	HIS
1	J	1918	GLN
1	J	2153	ASN
1	J	2196	ASN
1	J	2211	ASN
1	J	2218	HIS
1	J	2317	ASN
1	J	2518	ASN
1	J	2820	HIS
1	J	3667	GLN
1	J	3883	GLN
1	J	3904	GLN
1	J	3916	GLN
1	J	3956	GLN
1	J	4050	HIS
1	J	4172	GLN

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Mol	Chain	Res	Type
1	J	4179	ASN
1	J	4490	GLN
1	J	4494	ASN
1	J	4499	ASN
1	J	4515	ASN
1	J	4621	GLN
1	J	4737	ASN
1	J	4817	HIS
1	J	4880	GLN
2	K	87	HIS
3	L	9	GLN
3	L	50	GLN
3	L	54	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

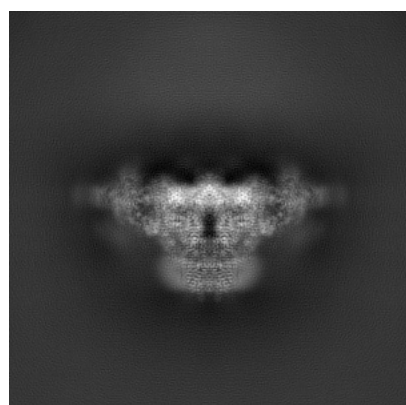
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9833. These allow visual inspection of the internal detail of the map and identification of artifacts.

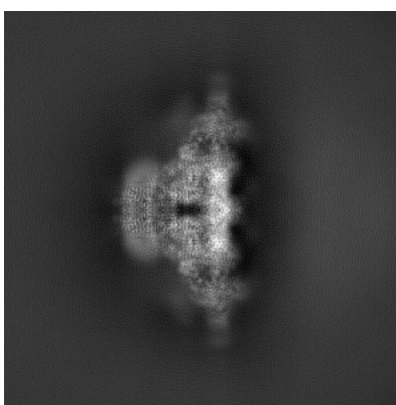
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

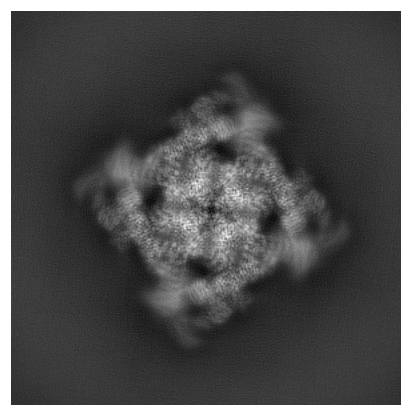
6.1.1 Primary map



X



Y

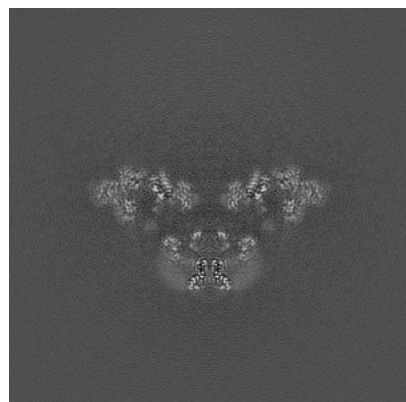


Z

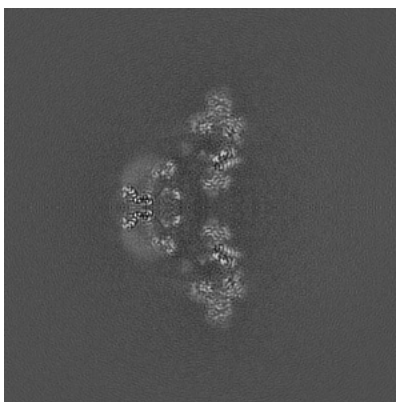
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

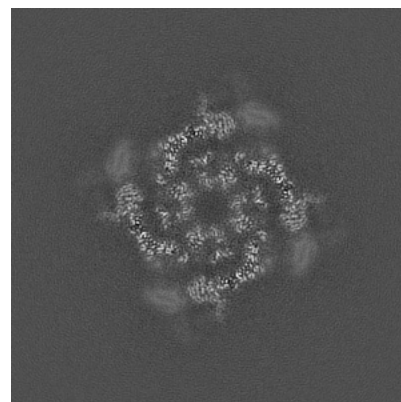
6.2.1 Primary map



X Index: 200



Y Index: 200

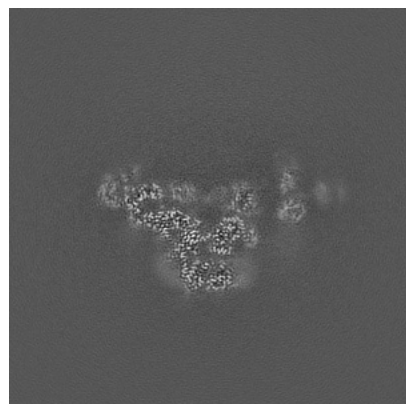


Z Index: 200

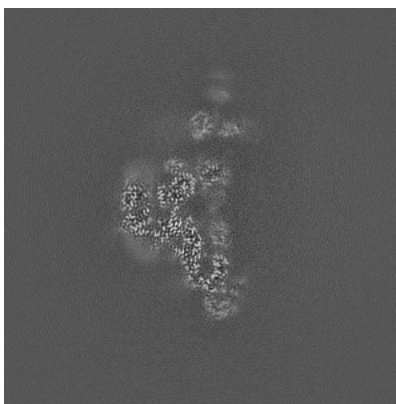
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

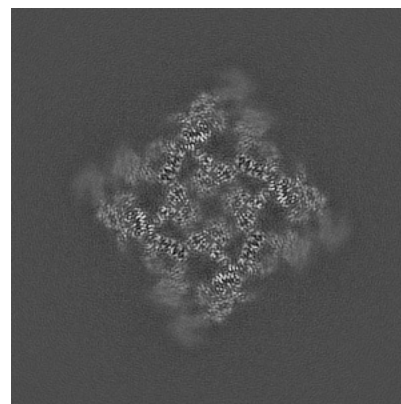
6.3.1 Primary map



X Index: 214



Y Index: 186



Z Index: 209

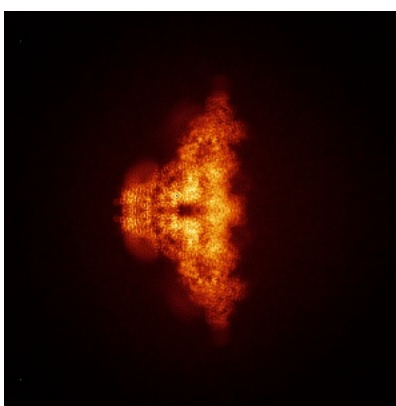
The images above show the largest variance slices of the map in three orthogonal directions.

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

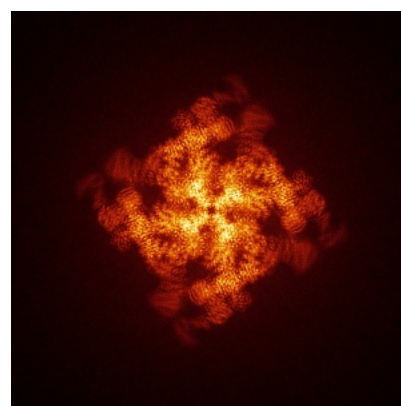
6.4.1 Primary map



X



Y

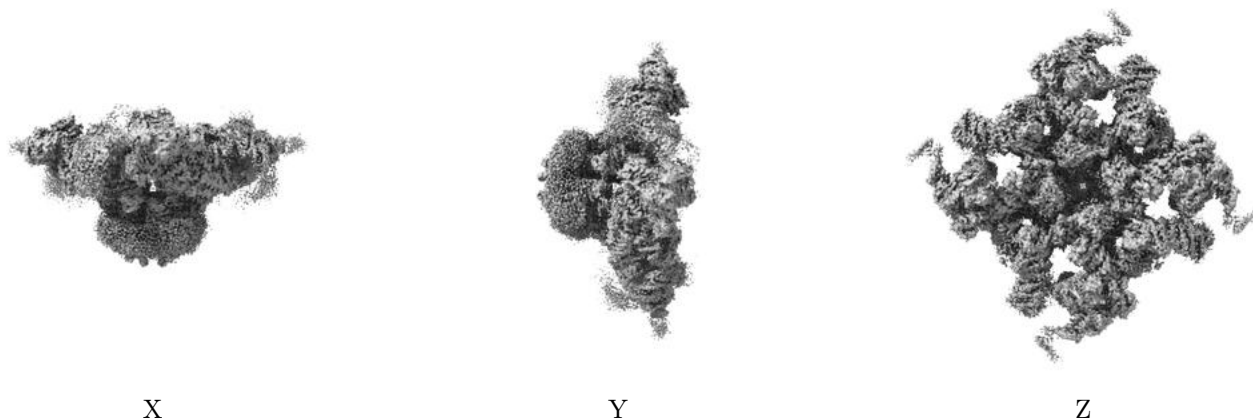


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

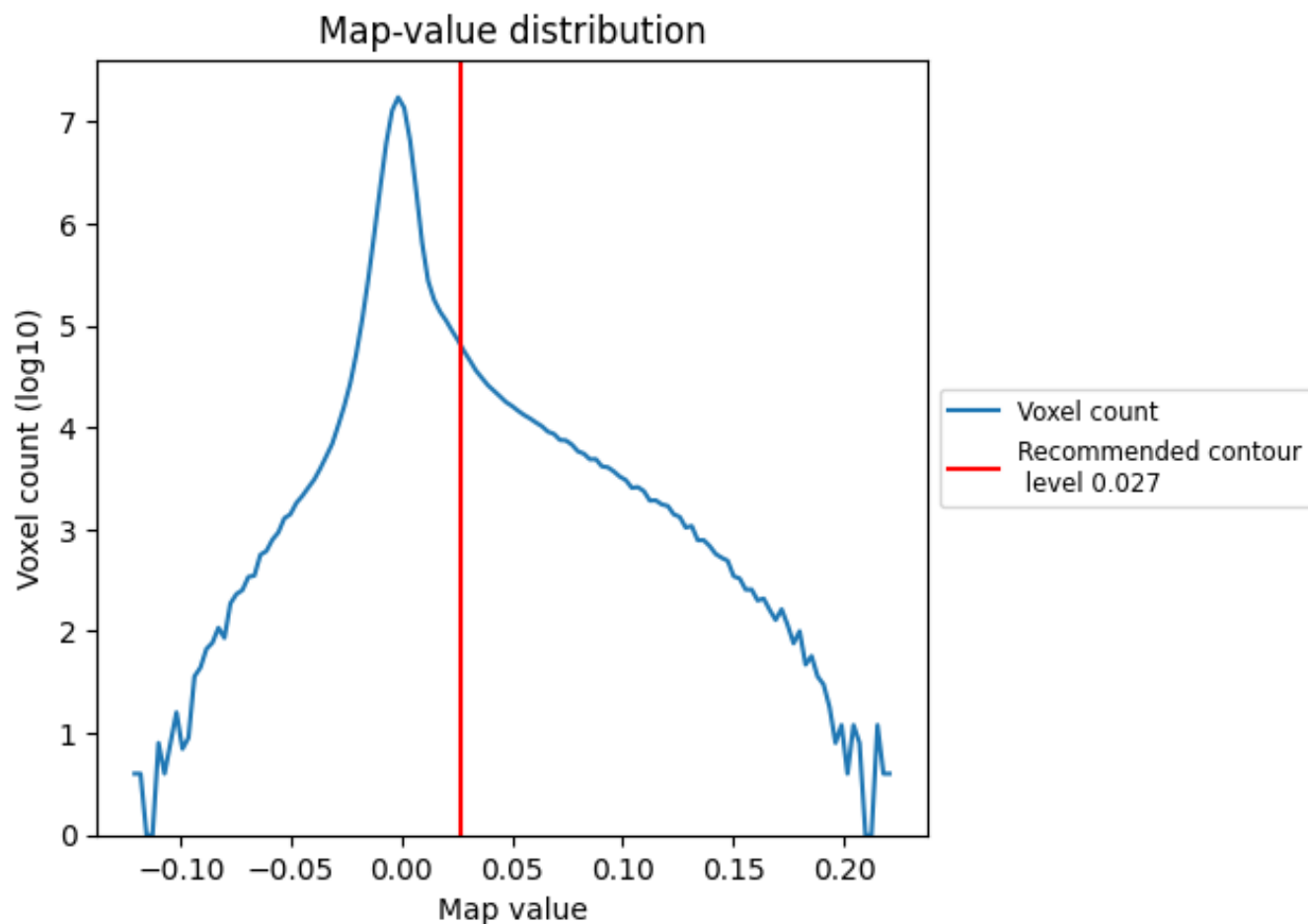
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

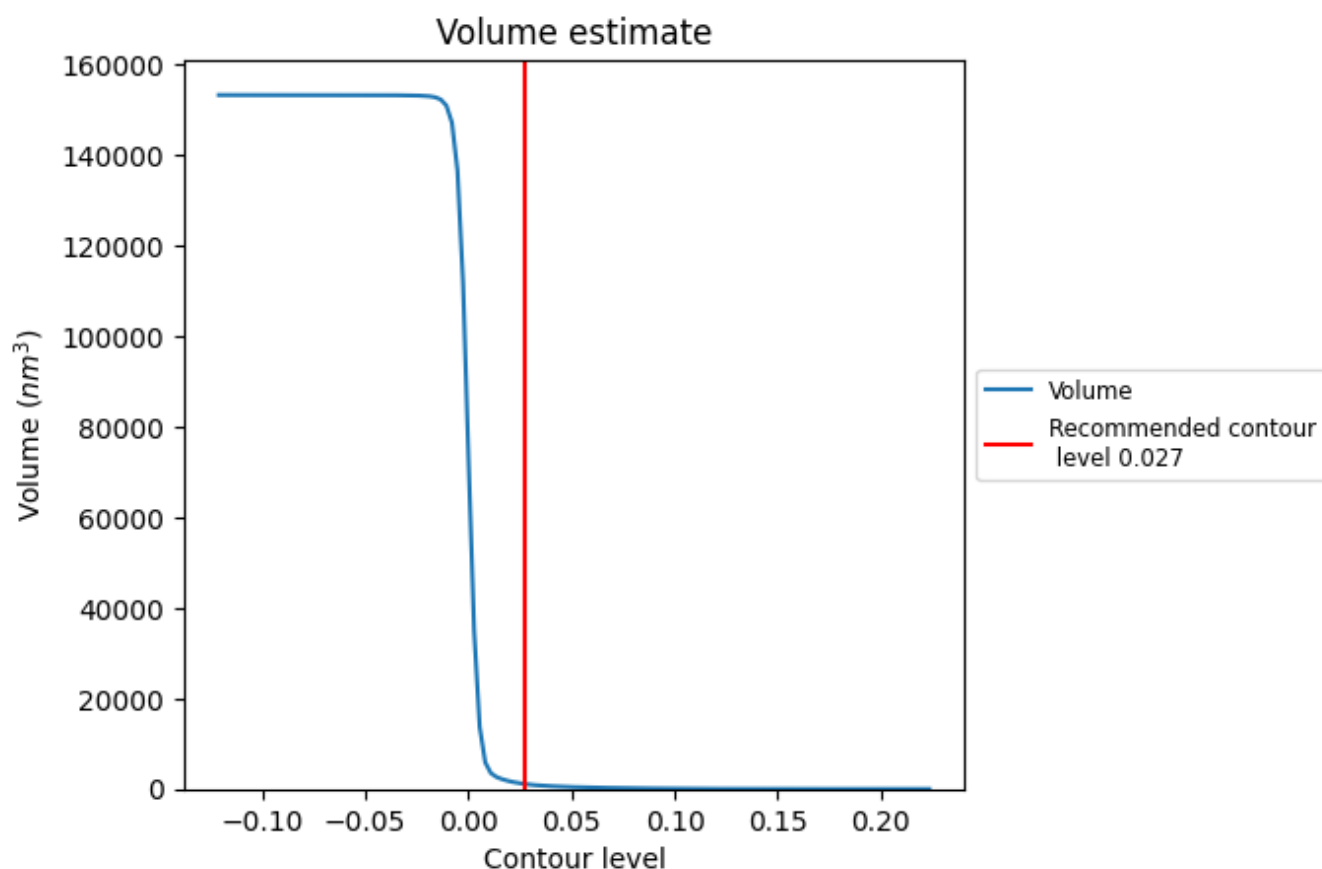
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

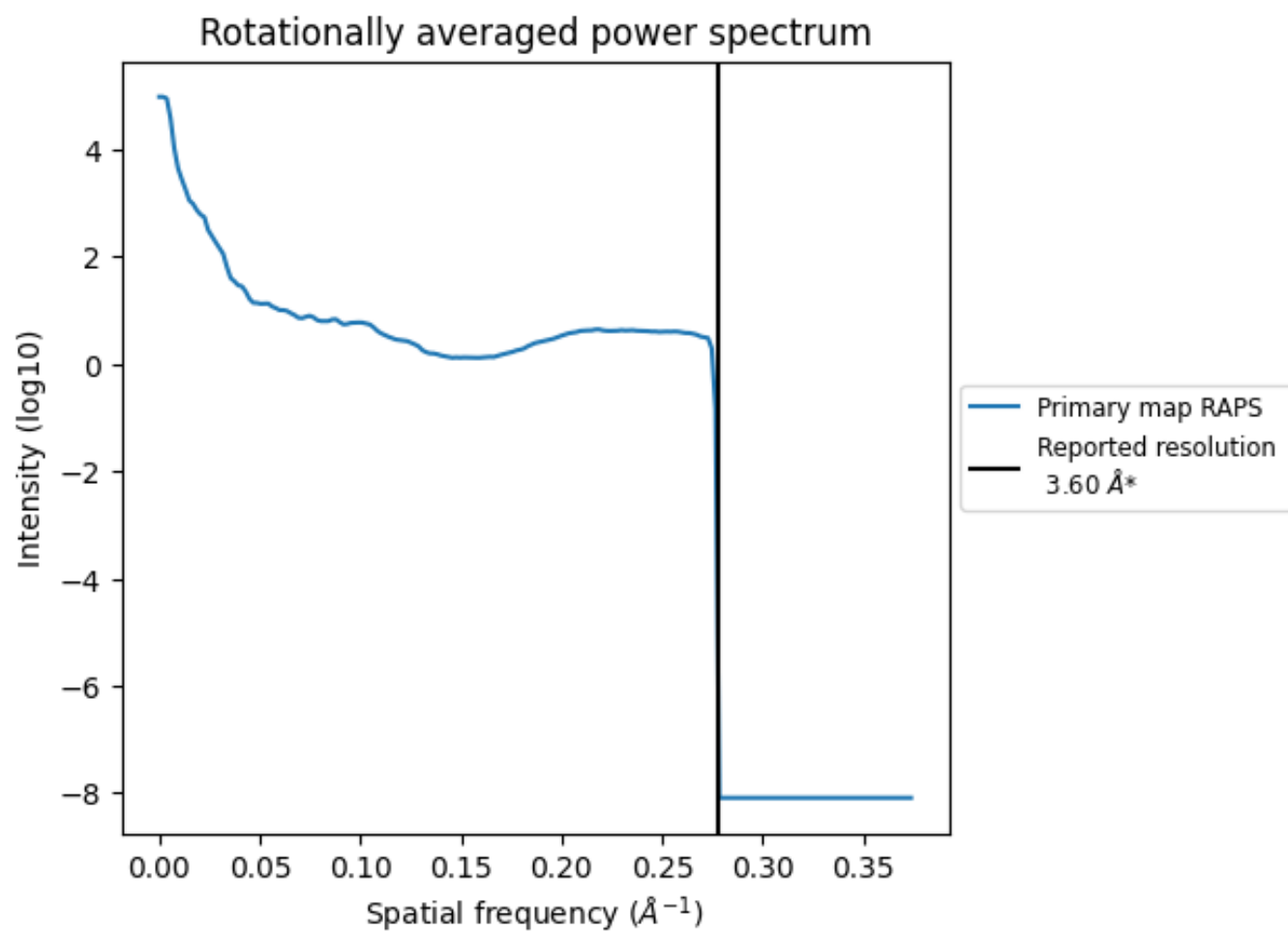
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1114 nm³; this corresponds to an approximate mass of 1007 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

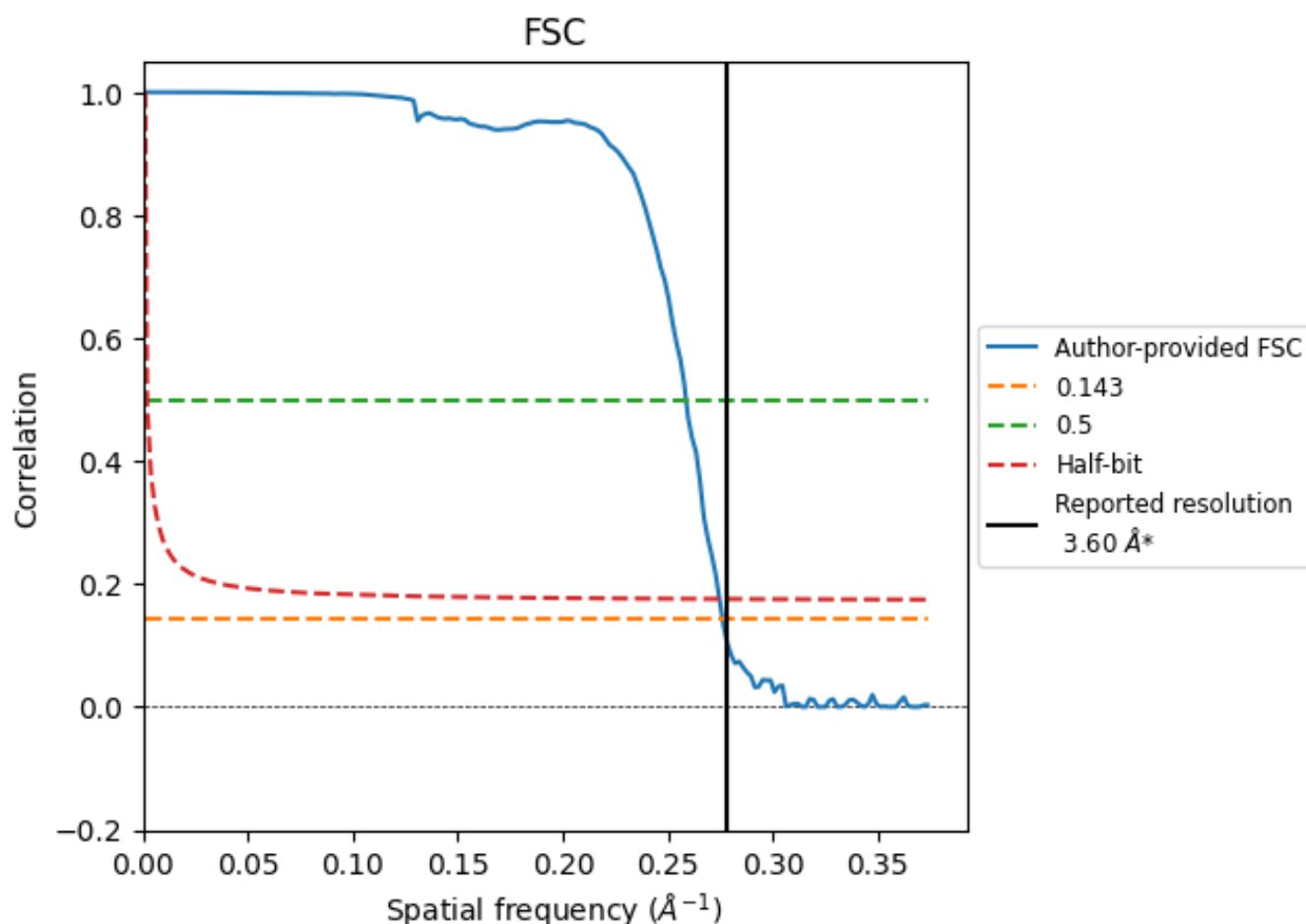


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

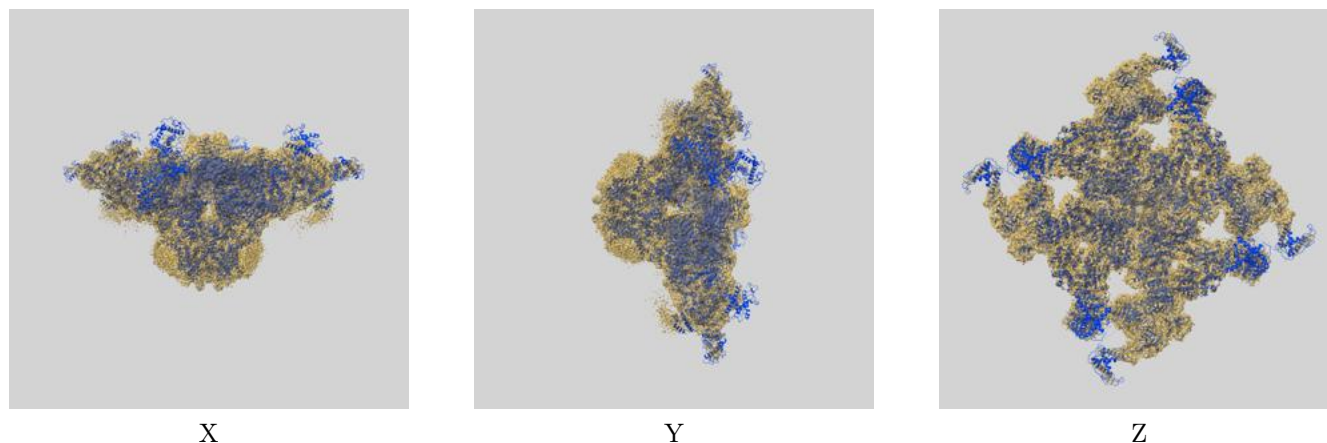
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	3.87	3.64
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

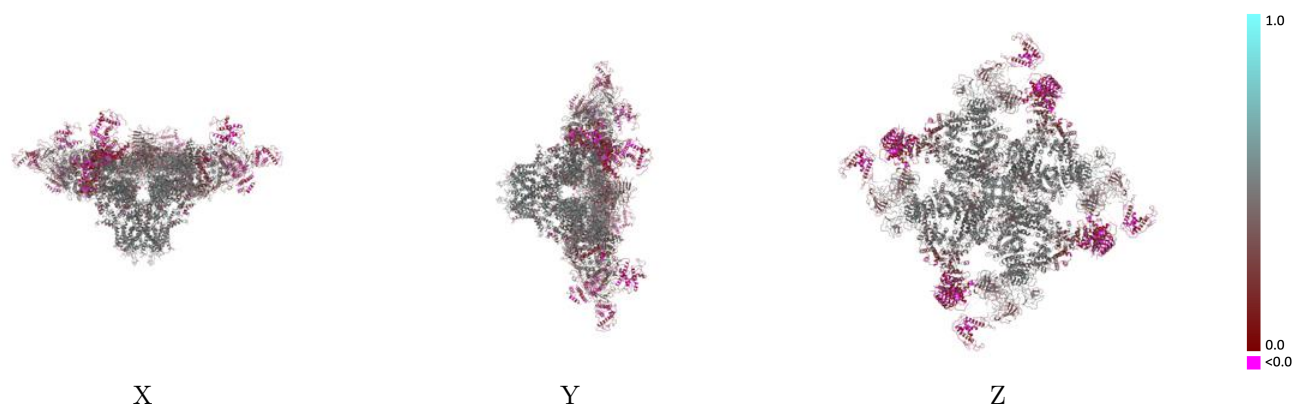
This section contains information regarding the fit between EMDB map EMD-9833 and PDB model 6JI8. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



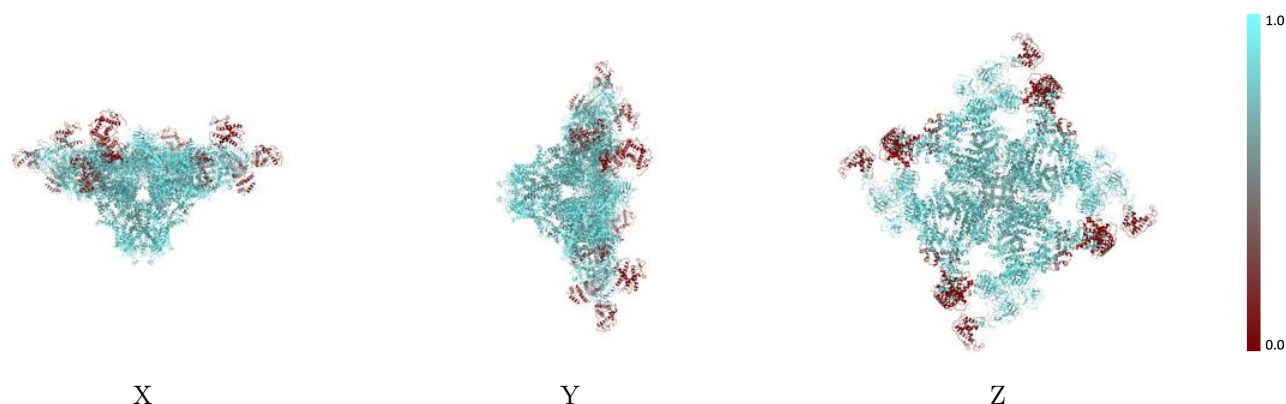
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



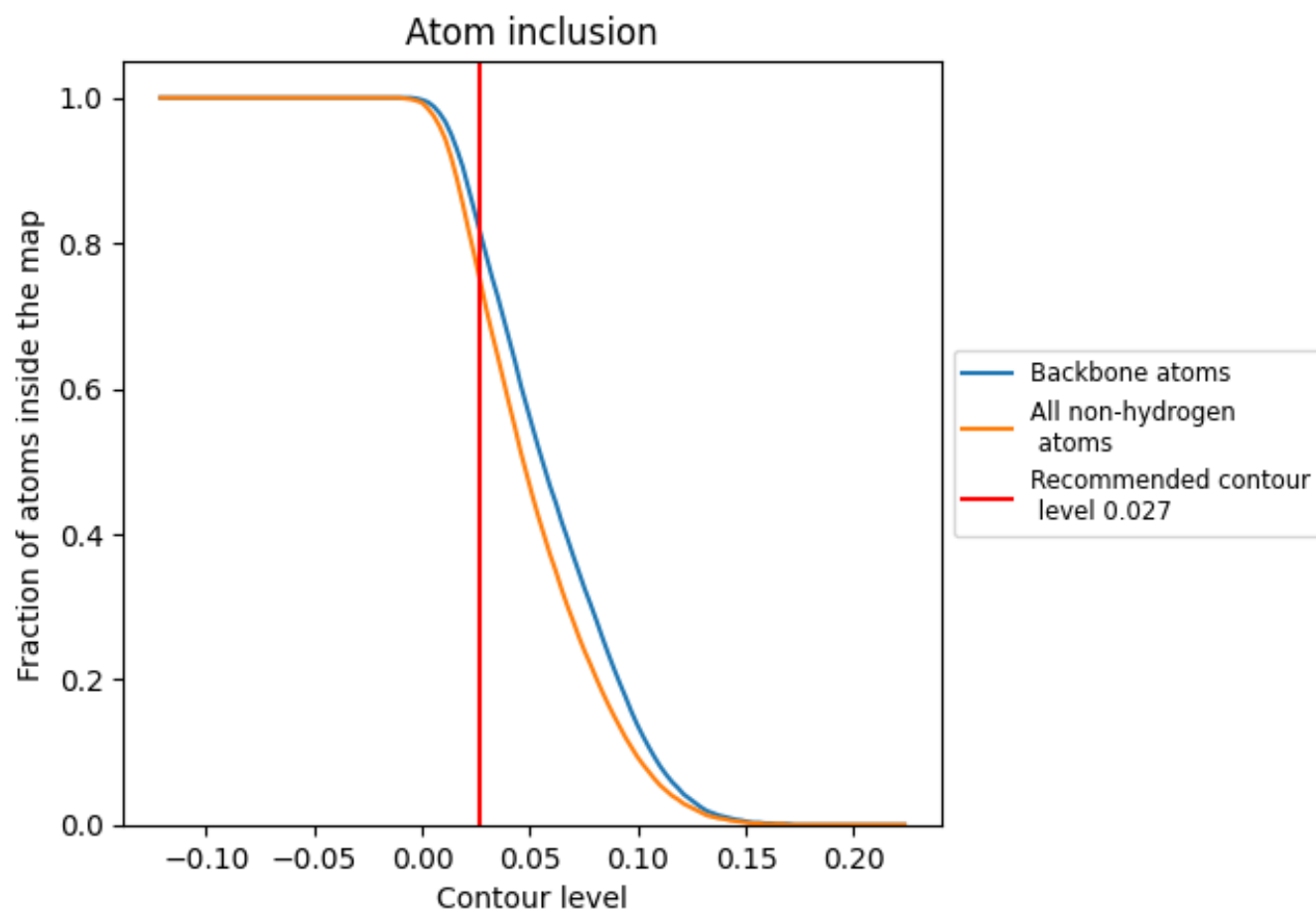
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.3840
A	0.7590	0.3880
B	0.8330	0.4310
C	0.4250	0.2340
D	0.7580	0.3880
E	0.8330	0.4310
F	0.4250	0.2340
G	0.7590	0.3880
H	0.8340	0.4320
I	0.4230	0.2350
J	0.7590	0.3880
K	0.8340	0.4310
L	0.4240	0.2360

1.0

0.0

<0.0