



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 12:57 AM JST

PDB ID : 8IMZ / pdb_00008imz
EMDB ID : EMD-35577
Title : Cryo-EM structure of mouse Piezo1-MDFIC complex (composite map)
Authors : Zhou, Z.; Ma, X.; Lin, Y.; Cheng, D.; Bavi, N.; Li, J.V.; Sutton, D.; Yao, M.;
Harvey, N.; Corry, B.; Zhang, Y.; Cox, C.D.
Deposited on : 2023-03-07
Resolution : 3.66 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 : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

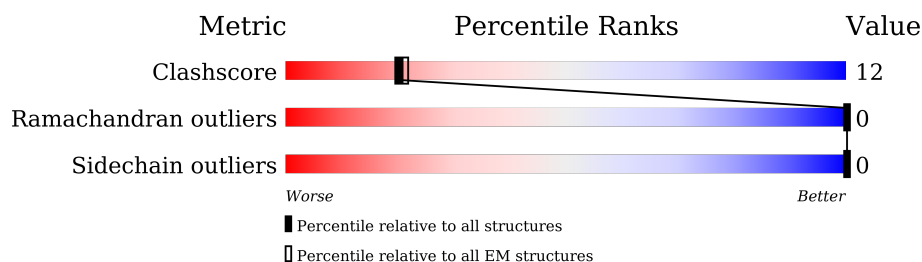
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 3.66 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2547	
1	B	2547	
1	C	2547	
2	D	247	
2	E	247	
2	F	247	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29409 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

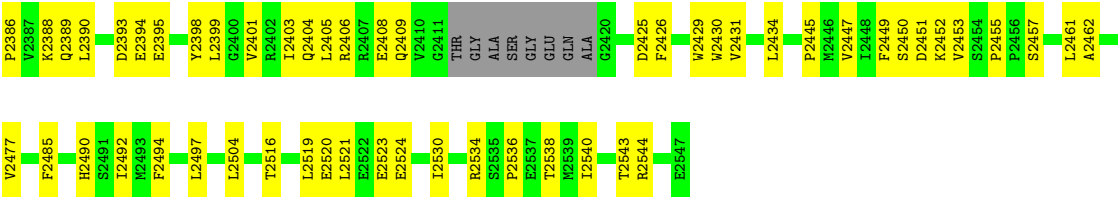
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1223	Total	C	N	O	S	0	0
			9653	6324	1626	1652	51		
1	C	1223	Total	C	N	O	S	0	0
			9653	6324	1626	1652	51		
1	B	1223	Total	C	N	O	S	0	0
			9653	6324	1626	1652	51		

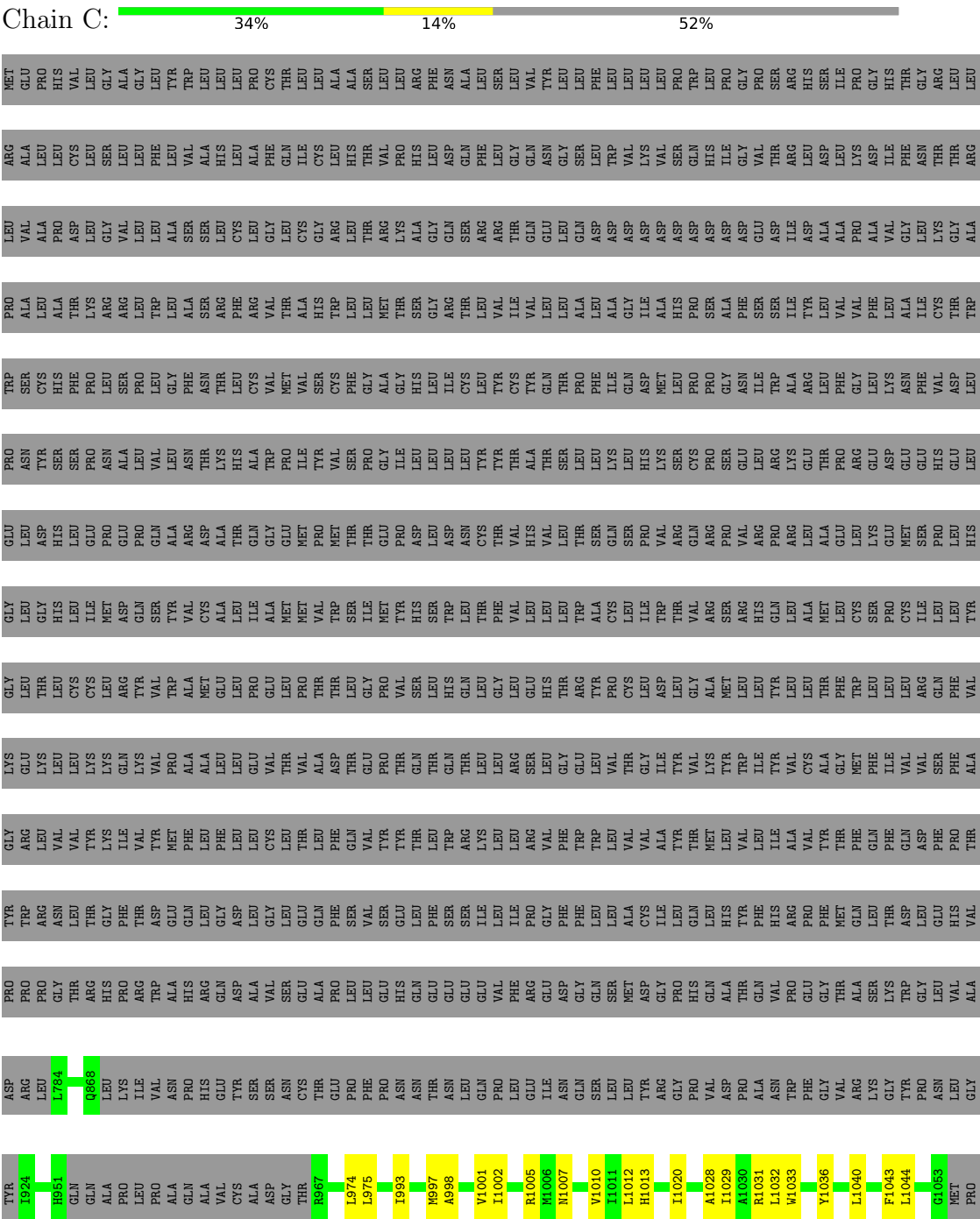
- Molecule 2 is a protein called MyoD family inhibitor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	21	Total	C	N	O	S	0	0
			150	88	21	33	8		
2	E	21	Total	C	N	O	S	0	0
			150	88	21	33	8		
2	F	21	Total	C	N	O	S	0	0
			150	88	21	33	8		





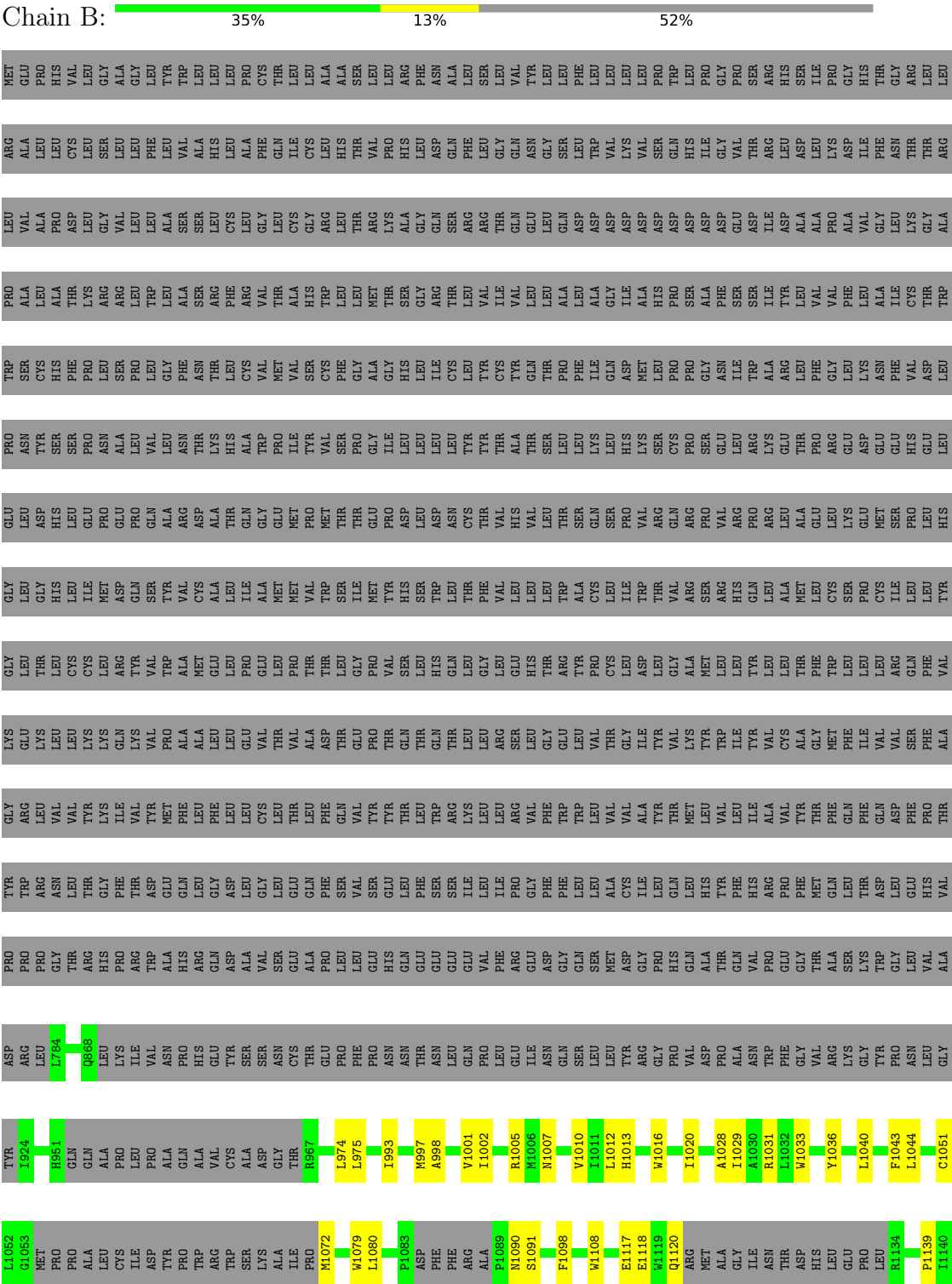
● Molecule 1: Piezo-type mechanosensitive ion channel component 1



E2359	G2360	R2361	Q2362	P2363	S2260	M2153	L2047	ARG	HIS	VAL	F1751	ALA	PRO	GLU	PRO	L1345	VAL	L1150	PRO
G2360	F2263	D2264	P2265	Y2266	F2267	M2153	L2047	LEU	THR	LYS	F1752	ARG	SER	GLU	ALA	K1346	CYS	D1151	ALA
R2361	D2264	V2051	K2162	P2267	K2166	P1753	V2051	GLN	ARG	ASP	P1753	THR	THR	ASP	THR	R1347	THR	M1152	LEU
Q2364	Y2266	H2058	K2166	P2267	K2166	ASP	H2058	PHE	ILE	GLU	ASN	MET	SER	ARG	LYS	R1353	LYS	L1153	CYS
S2365	P2267	M2061	P2178	P2267	K2166	THR	M2061	GLY	ALA	ALA	THR	THR	GLY	PRO	GLY	Y1359	TYR	V1165	ASP
I2368	L2268	P2178	K2179	L2268	P2178	VAL	P2178	ASN	ILE	GLU	VAL	A1645	ALA	ALA	TYR	L1166	TRP	L1166	TRP
P2369	A2269	K2179	K2179	A2269	K2179	GLY	K2179	LYS	PHE	GLU	VAL	A1645	ALA	GLN	ASP	F1170	ARG	F1170	TRP
H2370	M2270	Q2180	Q2181	M2270	Q2180	ALA	Q2180	PRO	ARG	PRO	LEU	L1649	ALA	ALA	ARG	GLY	TRP	I1177	SER
L2371	Q2271	E2070	Q2181	Q2271	E2070	GLU	E2070	GLU	ARG	GLU	ARG	L1650	GLU	ALA	ARG	GLY	TRP	I1178	TRP
F2372	K2182	Q2075	K2182	F2372	Q2075	ALA	Q2075	ALA	ARG	ALA	THR	D1651	GLU	PHE	GLU	GLY	TRP	I1179	LYS
P2373	K2183	Q2075	K2183	P2373	Q2075	LEU	Q2075	LEU	LYS	LEU	THR	R1652	PRO	MET	GLN	GLN	TRP	F1180	ALA
K2374	K2184	Q2075	K2184	K2374	Q2075	GLY	Q2075	GLY	GLU	GLY	GLU	R1652	LEU	THR	SER	LEU	TRP	G1181	PRO
R2377	L2186	V2078	L2186	R2377	V2078	THR	V2078	THR	GLY	GLU	ASN	F1665	LEU	ALA	ALA	ASP	GLY	G1182	PRO
P2382	E2279	A2079	E2279	P2382	A2079	PRO	A2079	PRO	GLY	GLN	LYS	G1670	SER	THR	ALA	GLY	ASP	G1183	PRO
I2381	K2188	Q2080	K2188	I2381	Q2080	GLY	Q2080	SER	THR	GLN	PRO	R1670	THR	MET	GLN	GLY	ASP	G1184	PRO
Y2386	D2280	Y2189	D2280	Y2386	Y2189	LYS	Y2189	THR	LYS	GLY	THR	L1672	ASP	THR	TRP	GLN	ASP	Y1184	PRO
V2387	V2282	Q2190	V2282	V2387	Q2190	THR	Q2190	THR	GLY	THR	PHE	L1673	ASP	THR	TRP	GLN	ASP	Y1184	PRO
K2388	V2283	M2191	V2283	K2388	M2191	GLY	M2191	THR	GLY	THR	THR	R1674	THR	THR	VAL	ASP	CYS	C1188	PRO
Q2389	E2287	G2192	E2287	Q2389	G2192	THR	G2192	SER	THR	THR	VAL	G1775	SER	ASN	GLN	PRO	LEU	C1188	PRO
L2390	S2288	I2195	S2288	L2390	I2195	ALA	I2195	ALA	VAL	HIS	L1776	A1684	SER	SER	GLN	GLY	VAL	L1191	ASP
D2393	G2289	R2097	G2289	D2393	R2097	GLY	R2097	GLY	GLY	GLY	L1776	A1684	PRO	PRO	GLN	GLY	VAL	L1191	ASP
E2394	S2290	R2098	S2290	E2394	R2098	THR	R2098	THR	THR	LYS	T1779	S1687	SER	GLY	VAL	GLY	GLY	G1195	ARG
E2395	A2292	R2104	A2292	E2395	R2104	GLY	R2104	GLY	GLY	PRO	D1780	I1694	SER	GLY	LEU	PRO	ALA	K1201	ALA
Y2398	R2295	I2105	R2295	Y2398	I2105	GLY	I2105	GLY	GLY	PRO	S1781	M1698	THR	GLY	ARG	ASP	GLY	D1202	PRO
L2399	I2296	G2107	L2399	L2399	G2107	LEU	G2107	LEU	LEU	VAL	Y1782	H1699	THR	GLU	GLN	SER	ILE	N1090	PRO
S2297	H2108	N2108	S2297	S2297	H2108	ALA	N2108	HIS	GLY	ALA	K1784	M1700	THR	ARG	ARG	PRO	ILE	Q1206	PRO
G2400	S2109	F2109	G2400	G2400	S2109	GLY	F2109	GLY	GLY	GLY	L1787	Y1701	ARG	GLY	GLY	GLY	GLY	L1213	PRO
V2401	A2113	K2113	V2401	V2401	A2113	THR	K2113	THR	THR	THR	L1787	T1702	SER	GLY	GLY	SER	GLY	L1213	PRO
R2402	T2221	D2225	R2402	R2402	T2221	PRO	D2225	PRO	LYS	PRO	Q1789	A1705	GLY	ALA	ALA	SER	SER	Y1216	PRO
Q2404	N2221	D2225	Q2404	Q2404	N2221	ASP	D2225	ASP	GLY	ARG	V1789	A1706	SER	ARG	ARG	PRO	PRO	N1217	PRO
L2405	E2236	E2236	L2405	L2405	E2236	THR	E2236	THR	THR	THR	H1796	S1707	GLU	GLU	GLN	PRO	PRO	E1117	PRO
R2407	E2237	E2237	R2407	R2407	E2237	ILE	E2237	ILE	GLY	ILE	H1796	L1708	ILE	ARG	ARG	ARG	ARG	E1118	PRO
Q2409	F2237	L2238	Q2409	Q2409	F2237	GLY	L2238	SER	GLY	GLN	Q1799	L1709	VAL	VAL	ARG	GLN	GLN	Y1119	PRO
L2406	L2239	F2239	L2406	L2406	L2239	LYS	F2239	LEU	LYS	LYS	L1800	P1711	THR	THR	ASP	TRP	TRP	Q1120	ARG
R2407	L2240	T2240	R2407	R2407	L2240	ILE	T2240	ASP	ARG	THR	Y1803	V1712	GLY	GLY	PRO	PRO	PRO	ARG	ARG
G2411	K2241	S2242	G2411	G2411	K2241	THR	S2242	ASP	HIS	ARG	G1804	L1713	ASP	ASP	THR	THR	THR	GLY	GLY
THR	S2242	S2242	THR	THR	S2242	GLN	S2242	THR	THR	THR	L1805	L1713	GLY	LEU	GLY	LEU	GLY	VAL	THR
GLY	A2243	Q2244	GLY	GLY	A2243	SER	Q2244	ASP	GLN	ASP	W1806	L1716	LEU	SER	GLY	LEU	GLY	VAL	THR
ALA	Q2244	Q2244	ALA	ALA	Q2244	LYS	Q2244	THR	LYS	ASP	W1806	M1717	GLN	GLY	GLY	GLY	GLY	GLN	ASP
GLY	Q2245	Q2245	GLY	GLY	Q2245	VAL	Q2245	THR	VAL	THR	W1806	M1719	GLY	GLY	ASP	GLY	GLY	GLN	HIS
GLN	S2246	S2247	GLN	GLN	S2246	ILE	S2247	ASP	ILE	GLN	W1806	T1721	SER	THR	ALA	ASN	ASN	GLN	GLY
ALA	P2250	F2251	ALA	ALA	P2250	GLN	F2251	THR	THR	ARG	W1806	T1722	LEU	ASP	PRO	ASP	ASP	ASN	PRO
G2420	T2250	T2252	G2420	G2420	T2250	ARG	T2252	THR	ARG	ASP	W1806	P1723	LEU	THR	VAL	VAL	VAL	PHE	THR
D2425	F2251	T2252	D2425	D2425	F2251	GLY	T2252	THR	GLY	THR	W1806	R1724	GLY	GLY	GLY	GLY	GLY	G1243	THR
F2426	T2252	T2252	F2426	F2426	T2252	PRO	T2252	THR	PRO	PRO	W1806	R1724	GLY	GLY	VAL	VAL	VAL	G1243	THR
Q2353	Q2253	D2144	Q2353	Q2353	Q2253	MET	D2144	ASP	GLY	GLY	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
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Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
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Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	LYS	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
Q2353	Q2253	T2145	Q2353	Q2353	Q2253	ALA	T2145	ASP	ASP	ASP	W1806	K1727	ASP	GLY	GLY	GLY	GLY	G1243	THR
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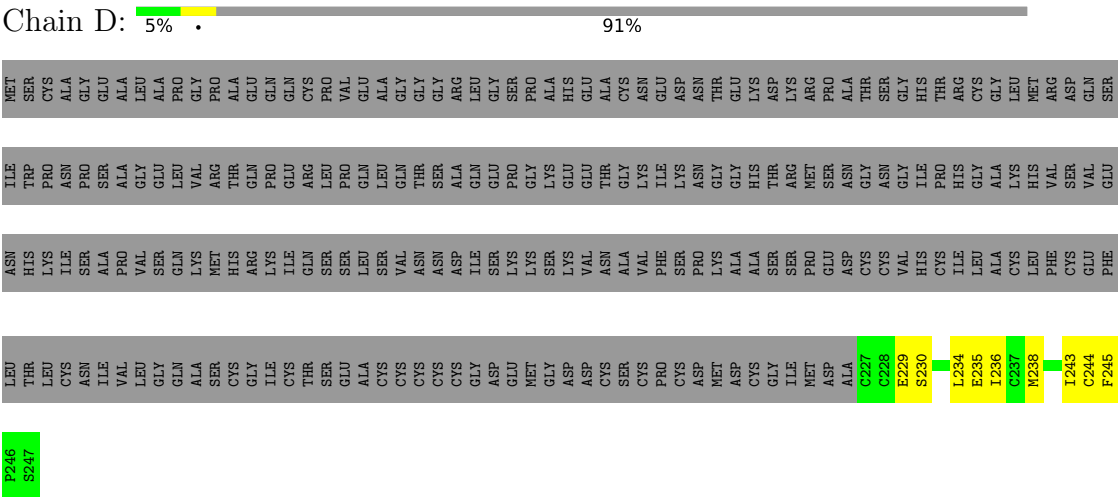


● Molecule 1: Piezo-type mechanosensitive ion channel component 1

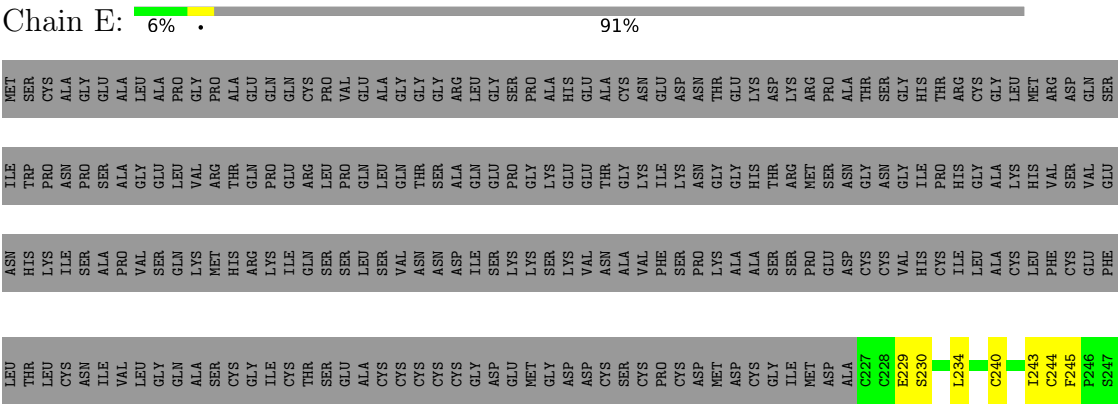


V2447	Q2364	D2264	M2153	V2061	SER	HIS	ARG	TRP	LEU	ARG	GLU	PRO	L1345	S1250	P1141
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F2449	F2267	Y2266	VAL	VAL	CYS	ILE	LYS	TYR	ALA	GLY	ALA	ASP	R1347	CYS	F1143
S2450	L2268	L2267	SER	LEU	SER	PHE	GLU	VAL	ARG	THR	SER	ARG	R1353	THR	D1150
D2451	K2452	A2269	K2179	T2069	LEU	ARG	PRO	VAL	THR	ALA	HIS	ALA	Y1359	VAL	H1151
V2453	L2371	W2270	G2180	E2070	ALA	ARG	GLU	LEU	ARG	MET	MET	ALA	S1365	GLY	H1152
S2454	F2372	Q2271	Q2181	Q2075	GLN	ARG	ALA	ARG	THR	SER	GLY	GLN	S1365	TYR	L1153
P2455	P2373	F2272	K2182	Q2075	SER	LYS	ALA	TYR	ARG	SER	MET	ALA	ARG	TYR	K1154
K2374	K2374	L2273	K2184	Q2075	PHE	GLU	LEU	GLU	THR	GLY	ARG	ALA	GLY	ASP	V1165
S2457	S2274	S2274	K2185	V2078	TYR	THR	GLU	ASN	GLY	GLY	VAL	PHE	GLN	PRO	Y1165
L2461	P2278	P2278	I2186	A2079	GLN	THR	SER	LYS	ALA	ALA	VAL	GLN	LEU	LYS	F1170
A2462	E2279	Q2080	V2187	Q2080	A2079	GLY	GLN	PRO	L1650	GLU	SER	MET	GLN	GLU	F1170
P2382	D2280	W2081	K2188	W2081	PRO	PRO	SER	TYR	D1651	GLU	THR	ALA	SER	MET	I1177
V2477	L2281	Y2189	Y2189	Y2082	LYS	LYS	GLU	PHE	R1652	PRO	MET	TYR	LYS	GLY	S1178
P2386	V2282	G2190	M2191	Y2083	GLY	THR	THR	GLY	F1665	LEU	PHE	GLN	ASP	THR	I1179
V2387	T2283	G2192	G2192	L2092	THR	ALA	THR	L1774	F1665	SER	SER	TRP	GLN	ASP	F1180
K2388	E2287	G2288	I2195	T2097	VAL	VAL	GLY	G1775	G1670	MET	THR	VAL	ASP	ARG	G1181
Q2389	G2288	S2289	I2202	R2098	MET	HIS	PRO	L1776	R1671	THR	THR	THR	PRO	ARG	L1182
L2390	S2289	Y2289	G1994	G1994	GLU	GLU	GLU	G1776	L1672	ASP	ASN	ASN	SER	CYS	G1183
D2393	S2290	G2291	F1988	F1988	THR	HIS	GLU	G1776	L1674	ASP	THR	ALA	GLN	LEU	Y1184
E2395	A2292	G2291	I1988	L2092	GLY	GLY	THR	L1774	R1674	THR	SER	THR	GLU	LEU	C1188
Y2398	R2295	R2295	GLY	T2105	THR	LYS	PRO	L1787	A1684	SER	SER	VAL	PRO	PRO	L1191
G2400	L2296	L2296	LYS	L2106	THR	GLY	GLY	Y1788	G1687	PRO	LEU	GLY	ASP	GLU	G1195
L2401	S2297	S2297	HIS	N2108	GLY	GLY	ALA	Q1789	S1687	LEU	GLY	ARG	ALA	ALA	G1195
R2402	P2298	P2298	SER	F2109	GLY	GLY	GLY	H1796	L1784	SER	SER	GLN	SER	ALA	K1201
L2403	S2299	S2299	ALA	K2113	ALA	LYS	PRO	Q1799	N1698	THR	GLY	ARG	PRO	GLY	I1201
Q2404	S2300	S2300	THR	N2221	THR	GLY	GLY	L1800	H1699	GLY	THR	ARG	GLY	ILE	Q1206
L2405	R2301	R2301	ASP	D2225	ASP	THR	ASP	L1800	M1700	ASN	GLY	ALA	SER	GLY	I1281
E2522	A2302	Q2303	ALA	Y2235	ILE	THR	HIS	Q1799	Y1701	THR	TYR	ALA	PRO	GLY	W1282
E2408	Q2303	Q2303	ALA	N2118	ALA	THR	ILE	H1796	L1702	THR	ASN	ALA	PRO	GLY	L1213
Q2409	W2304	W2304	SER	W2117	SER	ARG	GLN	Q1799	A1705	ARG	GLY	ARG	PRO	GLY	Y1216
Y2410	W2331	W2331	SER	L2121	SER	LYS	LYS	L1800	A1706	GLY	GLY	ARG	PRO	GLY	N1217
G2411	Q2324	Q2324	SER	V2128	SER	ARG	PRO	Y1803	S1707	THR	GLY	ARG	PRO	GLY	Y1218
GLY	GLY	GLY	ASP	F2130	ASP	ARG	SER	G1804	L1708	GLU	GLY	ALA	ARG	GLY	V1287
ALA	V2333	V2333	ASP	L2131	ASP	HIS	ILE	L1805	V1709	GLU	GLY	ALA	ARG	GLY	F1288
SER	E2334	E2334	Q2243	V2132	Q2015	THR	THR	W1806	V1710	ILE	ILE	GLN	ARG	GLY	F1289
GLY	Y2335	Y2335	Q2244	E2133	V2016	GLN	SER	ASP	P1711	VAL	VAL	LEU	ARG	GLY	L1290
GLY	Q2245	Q2245	Q2245	L2134	L2021	LYS	LYS	HIS	Q1716	THR	ASP	ALA	ALA	GLY	I1296
GLN	Q2246	Q2246	S2247	V2137	L2021	SER	ASP	GLU	W1717	ALA	GLY	SER	TERP	GLY	N1225
ALA	S2247	S2247	ALA	N2138	L2024	LYS	VAL	GLU	I1721	GLY	ASP	GLY	LEU	GLY	S1299
A2345	A2345	A2345	P2250	D2139	Q2027	PHE	ILE	ASP	T1721	ASP	VAL	GLY	H1403	VAL	C1232
S2348	S2348	S2348	F2251	W2140	Q2027	ARG	GLN	ARG	I1722	LEU	GLY	LEU	H1403	GLU	V1233
T2349	T2349	T2349	T2252	W2141	T2030	GLU	PRO	TYR	P1723	GLN	GLY	ASN	D1308	GLN	F1234
Q2353	Q2254	Q2254	P2253	W2142	T2030	MET	PRO	LYS	R1724	ALA	ASP	PRO	F1413	MET	VAL
W2429	Q2255	T2143	Q2255	D2143	I2033	LYS	GLU	ASP	Y1745	SER	THR	GLU	D1411	GLN	GLN
W2430	A2255	D2144	A2255	T2145	I2035	ALA	LEU	CYS	Y1745	LEU	THR	PRO	D1418	ASN	ASN
V2431	Y2256	T2145	Q2257	T2146	R2035	GLY	PRO	ARG	Q1748	HIS	SER	VAL	E1421	PHE	C1243
L2434	E2257	L2147	Q2257	L2147	R2040	ARG	ARG	SER	Q1748	GLY	GLY	ASP	GLY	C1243	C1243
L2434	L2358	L2358	S2260	L2149	R2040	ARG	HIS	SER	F1751	SER	PRO	VAL	GLU	I1246	I1246
P2445	E2359	E2359	S2260	L2149	L2047	ARG	THR	VAL	F1752	GLN	GLU	PRO	GLU	Q1247	Q1247
M2446	G2360	G2360	F2263	L2149	L2047	GLN	ARG	ASP	P1753	LEU	THR	ASP	LEU	F1249	F1249

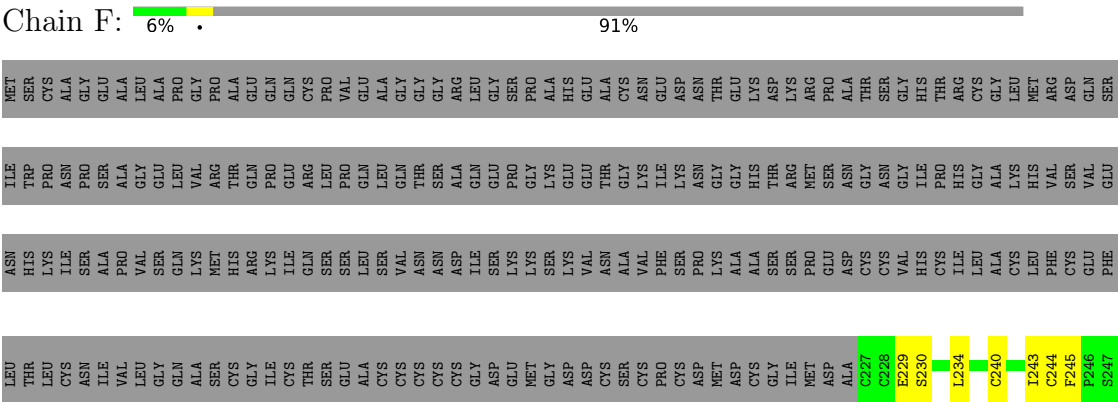
● Molecule 2: MyoD family inhibitor domain-containing protein



● Molecule 2: MyoD family inhibitor domain-containing protein



● Molecule 2: MyoD family inhibitor domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102644	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 ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/9877	0.45	1/13401 (0.0%)
1	B	0.29	0/9877	0.45	1/13401 (0.0%)
1	C	0.29	0/9877	0.45	1/13401 (0.0%)
2	D	0.24	0/151	0.45	0/200
2	E	0.24	0/151	0.45	0/200
2	F	0.24	0/151	0.45	0/200
All	All	0.29	0/30084	0.45	3/40803 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1180	PHE	N-CA-C	-6.65	107.04	114.62
1	B	1180	PHE	N-CA-C	-6.60	107.10	114.62
1	A	1180	PHE	N-CA-C	-6.59	107.11	114.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9653	0	9495	247	0
1	B	9653	0	9495	255	0
1	C	9653	0	9495	254	0
2	D	150	0	132	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	150	0	132	7	0
2	F	150	0	132	5	0
All	All	29409	0	28881	706	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2295:ARG:HD2	1:C:2295:ARG:HH12	1.18	1.05
1:A:2295:ARG:HH12	1:B:2295:ARG:HD2	1.19	1.04
1:C:2295:ARG:HD2	1:B:2295:ARG:HH12	1.19	1.03
1:C:1971:ARG:NE	1:C:2098:ARG:O	2.02	0.92
1:A:1971:ARG:NE	1:A:2098:ARG:O	2.02	0.91
1:B:1971:ARG:NE	1:B:2098:ARG:O	2.02	0.91
1:C:1724:ARG:HH22	1:C:1805:LEU:H	1.20	0.89
1:A:1724:ARG:HH22	1:A:1805:LEU:H	1.20	0.87
1:A:2295:ARG:HH22	1:B:2295:ARG:HB2	1.40	0.85
1:B:1724:ARG:HH22	1:B:1805:LEU:H	1.20	0.85
1:C:2295:ARG:HB2	1:B:2295:ARG:HH22	1.42	0.84
1:C:2292:ALA:HB1	1:B:2295:ARG:HG2	1.60	0.84
1:A:2295:ARG:HB2	1:C:2295:ARG:HH22	1.41	0.83
1:A:2292:ALA:HB1	1:C:2295:ARG:HG2	1.61	0.82
1:A:2295:ARG:HG2	1:B:2292:ALA:HB1	1.63	0.81
1:B:2225:ASP:HB3	1:B:2324:GLN:HB3	1.68	0.76
1:A:2225:ASP:HB3	1:A:2324:GLN:HB3	1.68	0.76
1:C:2225:ASP:HB3	1:C:2324:GLN:HB3	1.68	0.76
1:B:1118:GLU:HB3	1:B:1120:GLN:HG3	1.67	0.76
1:A:2179:LYS:NZ	1:B:1402:ASP:OD1	2.17	0.75
1:C:1118:GLU:HB3	1:C:1120:GLN:HG3	1.67	0.75
1:C:1402:ASP:OD1	1:B:2179:LYS:NZ	2.20	0.74
1:A:1118:GLU:HB3	1:A:1120:GLN:HG3	1.67	0.74
1:A:1402:ASP:OD1	1:C:2179:LYS:NZ	2.19	0.74
1:A:1971:ARG:CD	1:A:2098:ARG:O	2.35	0.74
1:C:1971:ARG:CD	1:C:2098:ARG:O	2.35	0.74
1:C:1702:THR:HB	1:C:1784:LYS:HD2	1.70	0.73
1:B:1971:ARG:CD	1:B:2098:ARG:O	2.35	0.73
1:B:1702:THR:HB	1:B:1784:LYS:HD2	1.70	0.73
1:A:1702:THR:HB	1:A:1784:LYS:HD2	1.70	0.72
1:A:2113:LYS:O	1:A:2118:ASN:ND2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:ILE:HG21	1:B:2477:VAL:HG11	1.72	0.72
1:B:2252:THR:OG1	1:B:2254:GLN:NE2	2.23	0.71
1:A:2252:THR:OG1	1:A:2254:GLN:NE2	2.23	0.71
1:B:2035:ARG:HH12	1:B:2109:PHE:HZ	1.37	0.71
1:A:2035:ARG:HH12	1:A:2109:PHE:HZ	1.36	0.71
1:C:2252:THR:OG1	1:C:2254:GLN:NE2	2.23	0.71
1:C:2270:MET:O	1:C:2274:SER:OG	2.07	0.71
1:B:2113:LYS:O	1:B:2118:ASN:ND2	2.23	0.71
1:C:2202:ILE:HG21	1:C:2477:VAL:HG11	1.72	0.71
1:A:2202:ILE:HG21	1:A:2477:VAL:HG11	1.72	0.70
1:C:2113:LYS:O	1:C:2118:ASN:ND2	2.23	0.70
1:C:2035:ARG:HH12	1:C:2109:PHE:HZ	1.36	0.70
1:B:2069:THR:HG22	1:B:2070:GLU:H	1.57	0.70
1:A:2356:GLN:O	1:A:2359:GLU:HG2	1.92	0.70
1:C:2356:GLN:O	1:C:2359:GLU:HG2	1.92	0.70
1:A:2069:THR:HG22	1:A:2070:GLU:H	1.57	0.70
1:A:2270:MET:O	1:A:2274:SER:OG	2.07	0.70
1:B:2356:GLN:O	1:B:2359:GLU:HG2	1.92	0.70
1:A:2295:ARG:NH1	1:B:2295:ARG:HH11	1.90	0.70
1:C:2069:THR:HG22	1:C:2070:GLU:H	1.57	0.70
1:C:1708:LEU:HD11	1:C:2058:HIS:HB3	1.73	0.69
1:B:1708:LEU:HD11	1:B:2058:HIS:HB3	1.73	0.69
1:B:1010:VAL:HG13	1:B:1225:ASN:HD21	1.58	0.69
1:A:1708:LEU:HD11	1:A:2058:HIS:HB3	1.73	0.69
1:A:1344:GLN:OE1	1:A:1347:ARG:NH2	2.26	0.69
1:A:2295:ARG:HD2	1:C:2295:ARG:NH1	2.02	0.68
1:C:2295:ARG:HH11	1:B:2295:ARG:NH1	1.91	0.68
1:C:1344:GLN:OE1	1:C:1347:ARG:NH2	2.26	0.68
1:B:1344:GLN:OE1	1:B:1347:ARG:NH2	2.26	0.68
1:A:1010:VAL:HG13	1:A:1225:ASN:HD21	1.58	0.68
1:B:2404:GLN:OE1	1:B:2406:ARG:NH2	2.25	0.68
1:A:1994:GLY:HA3	1:A:2078:VAL:HG11	1.76	0.68
1:B:2270:MET:O	1:B:2274:SER:OG	2.07	0.68
1:A:1141:PRO:HB2	1:A:1304:HIS:HB2	1.76	0.68
1:C:1994:GLY:HA3	1:C:2078:VAL:HG11	1.76	0.68
1:C:1010:VAL:HG13	1:C:1225:ASN:HD21	1.58	0.67
1:A:2295:ARG:HH11	1:C:2295:ARG:NH1	1.91	0.67
1:B:2040:ARG:NH2	1:B:2142:TRP:O	2.28	0.67
1:A:1687:SER:OG	1:A:1796:HIS:ND1	2.27	0.67
1:C:1800:LEU:HD22	1:C:1806:TRP:HE3	1.60	0.67
1:C:2040:ARG:NH2	1:C:2142:TRP:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:PRO:HB2	1:B:1304:HIS:HB2	1.76	0.67
1:A:1800:LEU:HD22	1:A:1806:TRP:HE3	1.59	0.66
1:A:1201:LYS:O	1:A:1206:GLN:NE2	2.29	0.66
1:C:2388:LYS:HE3	1:C:2394:GLU:HB2	1.78	0.66
1:A:2295:ARG:NH1	1:B:2295:ARG:HD2	2.03	0.66
1:C:1141:PRO:HB2	1:C:1304:HIS:HB2	1.77	0.66
1:C:1201:LYS:O	1:C:1206:GLN:NE2	2.29	0.66
1:B:1800:LEU:HD22	1:B:1806:TRP:HE3	1.59	0.66
1:A:2040:ARG:NH2	1:A:2142:TRP:O	2.28	0.66
1:A:1671:ARG:HG3	1:A:1672:THR:HG23	1.78	0.66
1:A:2404:GLN:OE1	1:A:2406:ARG:NH2	2.25	0.66
1:B:1994:GLY:HA3	1:B:2078:VAL:HG11	1.76	0.66
1:B:1201:LYS:O	1:B:1206:GLN:NE2	2.29	0.65
1:B:1671:ARG:HG3	1:B:1672:THR:HG23	1.78	0.65
1:C:1671:ARG:HG3	1:C:1672:THR:HG23	1.78	0.65
1:B:1191:LEU:O	1:B:1195:GLY:N	2.29	0.65
1:A:1191:LEU:O	1:A:1195:GLY:N	2.29	0.65
1:A:2388:LYS:HE3	1:A:2394:GLU:HB2	1.78	0.65
1:B:1051:CYS:HG	1:B:1091:SER:HG	1.44	0.65
1:C:1191:LEU:O	1:C:1195:GLY:N	2.29	0.65
1:B:2388:LYS:HE3	1:B:2394:GLU:HB2	1.78	0.65
1:C:2016:VAL:HB	1:C:2069:THR:HG21	1.80	0.64
1:B:2338:GLU:OE2	1:B:2386:PRO:HD3	1.98	0.64
1:A:1699:HIS:ND1	1:A:1707:SER:O	2.31	0.64
1:B:2016:VAL:HB	1:B:2069:THR:HG21	1.80	0.63
1:C:1699:HIS:ND1	1:C:1707:SER:O	2.31	0.63
1:C:2338:GLU:OE2	1:C:2386:PRO:HD3	1.98	0.63
1:B:1699:HIS:ND1	1:B:1707:SER:O	2.31	0.63
1:A:2243:ALA:HB1	1:A:2247:SER:HB3	1.81	0.63
1:C:1118:GLU:OE1	1:C:1120:GLN:NE2	2.30	0.63
1:C:2404:GLN:OE1	1:C:2406:ARG:NH2	2.25	0.63
1:A:2016:VAL:HB	1:A:2069:THR:HG21	1.80	0.62
1:A:2221:ASN:HB2	1:A:2453:VAL:HB	1.81	0.62
1:C:1687:SER:OG	1:C:1796:HIS:ND1	2.27	0.62
1:A:2338:GLU:OE2	1:A:2386:PRO:HD3	1.98	0.62
1:B:2221:ASN:HB2	1:B:2453:VAL:HB	1.81	0.62
1:B:2243:ALA:HB1	1:B:2247:SER:HB3	1.81	0.62
1:A:1988:ILE:HG23	1:A:2024:LEU:HD11	1.82	0.62
1:B:1988:ILE:HG23	1:B:2024:LEU:HD11	1.82	0.62
1:A:1118:GLU:OE1	1:A:1120:GLN:NE2	2.30	0.62
1:A:998:ALA:O	1:A:1002:ILE:HG12	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:CYS:SG	1:B:1233:VAL:N	2.73	0.62
1:B:998:ALA:O	1:B:1002:ILE:HG12	2.00	0.61
1:C:2221:ASN:HB2	1:C:2453:VAL:HB	1.81	0.61
1:C:998:ALA:O	1:C:1002:ILE:HG12	2.00	0.61
1:C:2494:PHE:HD2	1:B:2490:HIS:HD1	1.48	0.61
1:A:1051:CYS:HG	1:A:1091:SER:HG	1.46	0.61
1:A:1232:CYS:SG	1:A:1233:VAL:N	2.73	0.61
1:C:1232:CYS:SG	1:C:1233:VAL:N	2.73	0.61
2:E:240:CYS:HA	1:B:2191:MET:HE1	1.83	0.61
1:C:1988:ILE:HG23	1:C:2024:LEU:HD11	1.82	0.61
1:A:2494:PHE:HD2	1:C:2490:HIS:HD1	1.49	0.61
1:B:1748:GLN:NE2	1:B:1779:THR:O	2.34	0.61
1:C:1748:GLN:NE2	1:C:1779:THR:O	2.34	0.60
1:C:2243:ALA:HB1	1:C:2247:SER:HB3	1.81	0.60
1:C:2497:LEU:HD23	1:C:2543:THR:HG21	1.83	0.60
1:B:1165:VAL:HG22	1:B:1289:PHE:HB3	1.83	0.60
1:A:2497:LEU:HD23	1:A:2543:THR:HG21	1.83	0.60
1:B:1687:SER:OG	1:B:1796:HIS:ND1	2.27	0.60
1:A:1246:ILE:HG13	1:A:1251:LEU:HB2	1.84	0.60
1:B:1118:GLU:OE1	1:B:1120:GLN:NE2	2.30	0.60
1:B:2268:LEU:HD12	1:B:2268:LEU:H	1.67	0.60
1:A:1748:GLN:NE2	1:A:1779:THR:O	2.34	0.60
1:A:2184:LYS:HB2	1:A:2187:VAL:HG12	1.84	0.59
1:A:2268:LEU:HD12	1:A:2268:LEU:H	1.67	0.59
1:B:2184:LYS:HB2	1:B:2187:VAL:HG12	1.84	0.59
1:A:1165:VAL:HG22	1:A:1289:PHE:HB3	1.83	0.59
1:C:1165:VAL:HG22	1:C:1289:PHE:HB3	1.83	0.59
1:A:2408:GLU:OE2	1:A:2409:GLN:N	2.35	0.59
1:B:1246:ILE:HG13	1:B:1251:LEU:HB2	1.84	0.59
1:C:1345:LEU:HD12	1:C:2104:ARG:HH11	1.67	0.59
1:C:2268:LEU:H	1:C:2268:LEU:HD12	1.67	0.59
1:C:2408:GLU:OE2	1:C:2409:GLN:N	2.35	0.59
1:B:2408:GLU:OE2	1:B:2409:GLN:N	2.35	0.59
1:B:2497:LEU:HD23	1:B:2543:THR:HG21	1.83	0.59
1:A:2134:LEU:HB3	1:A:2138:MET:HE2	1.85	0.59
1:A:2182:LYS:HE2	1:B:2144:ASP:HB2	1.85	0.58
1:A:2377:ARG:HA	1:A:2449:PHE:HB2	1.84	0.58
1:C:2377:ARG:HA	1:C:2449:PHE:HB2	1.84	0.58
1:A:2490:HIS:HD1	1:B:2494:PHE:HD2	1.51	0.58
1:C:2184:LYS:HB2	1:C:2187:VAL:HG12	1.84	0.58
1:A:2185:LYS:HD2	1:A:2189:TYR:HE2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2434:LEU:HD11	1:A:2445:PRO:HD2	1.86	0.58
1:B:2058:HIS:NE2	1:B:2083:TYR:OH	2.33	0.58
1:C:2434:LEU:HD11	1:C:2445:PRO:HD2	1.86	0.58
1:B:1345:LEU:HD12	1:B:2104:ARG:HH11	1.67	0.58
1:A:2021:LEU:HD11	1:C:2211:SER:HB3	1.85	0.58
1:B:2185:LYS:HD2	1:B:2189:TYR:HE2	1.69	0.58
1:A:1345:LEU:HD12	1:A:2104:ARG:HH11	1.68	0.58
1:A:2144:ASP:HB2	1:C:2182:LYS:HE2	1.85	0.58
1:C:2021:LEU:HD11	1:B:2211:SER:HB3	1.84	0.58
1:B:2377:ARG:HA	1:B:2449:PHE:HB2	1.84	0.58
1:B:2434:LEU:HD11	1:B:2445:PRO:HD2	1.86	0.58
1:C:2144:ASP:HB2	1:B:2182:LYS:HE2	1.85	0.58
1:C:1213:LEU:HG	1:C:1290:LEU:HD21	1.86	0.57
1:C:1246:ILE:HG13	1:C:1251:LEU:HB2	1.84	0.57
1:B:1705:ALA:HA	1:B:1708:LEU:HB3	1.86	0.57
1:B:2373:PRO:HB3	1:B:2398:TYR:CE1	2.39	0.57
1:A:1213:LEU:HG	1:A:1290:LEU:HD21	1.86	0.57
1:B:1213:LEU:HG	1:B:1290:LEU:HD21	1.86	0.57
1:A:1359:TYR:OH	1:A:1418:ASP:OD2	2.17	0.57
1:A:2058:HIS:NE2	1:A:2083:TYR:OH	2.33	0.57
1:C:2361:ARG:HB3	1:C:2364:GLN:HE21	1.70	0.57
1:A:2361:ARG:HB3	1:A:2364:GLN:HE21	1.70	0.57
1:B:2361:ARG:HB3	1:B:2364:GLN:HE21	1.70	0.57
1:A:1724:ARG:HH22	1:A:1805:LEU:N	1.99	0.57
1:A:2128:VAL:HG11	1:A:2131:LEU:HD12	1.86	0.57
1:B:1184:TYR:OH	1:B:1283:ASP:OD1	2.20	0.57
1:B:2134:LEU:HB3	1:B:2138:MET:HE2	1.85	0.57
1:C:2134:LEU:HB3	1:C:2138:MET:HE2	1.85	0.57
1:B:1541:LEU:HD13	1:B:1555:VAL:HG11	1.87	0.57
1:C:2185:LYS:HD2	1:C:2189:TYR:HE2	1.69	0.57
1:A:1005:ARG:HE	1:A:1007:ASN:ND2	2.03	0.57
1:B:2280:ASP:OD2	1:B:2452:LYS:NZ	2.34	0.56
1:A:2373:PRO:HB3	1:A:2398:TYR:CE1	2.39	0.56
1:C:2058:HIS:NE2	1:C:2083:TYR:OH	2.33	0.56
1:A:1541:LEU:HD13	1:A:1555:VAL:HG11	1.87	0.56
1:A:2211:SER:HB3	1:B:2021:LEU:HD11	1.86	0.56
1:A:2295:ARG:HH11	1:C:2295:ARG:HH12	1.52	0.56
1:C:1705:ALA:HA	1:C:1708:LEU:HB3	1.86	0.56
1:C:2295:ARG:HH11	1:B:2295:ARG:HH12	1.52	0.56
1:B:1005:ARG:HE	1:B:1007:ASN:ND2	2.03	0.56
1:B:2128:VAL:HG11	1:B:2131:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2257:GLU:O	1:A:2260:SER:OG	2.17	0.56
1:C:2295:ARG:HD2	1:B:2295:ARG:NH1	2.04	0.56
1:A:1705:ALA:HA	1:A:1708:LEU:HB3	1.86	0.56
1:C:1005:ARG:HE	1:C:1007:ASN:ND2	2.03	0.56
1:B:2361:ARG:HB3	1:B:2364:GLN:NE2	2.21	0.56
1:C:2373:PRO:HB3	1:C:2398:TYR:CE1	2.40	0.56
1:C:2128:VAL:HG11	1:C:2131:LEU:HD12	1.86	0.55
1:B:2257:GLU:O	1:B:2260:SER:OG	2.17	0.55
1:C:1541:LEU:HD13	1:C:1555:VAL:HG11	1.87	0.55
1:C:2361:ARG:HB3	1:C:2364:GLN:NE2	2.21	0.55
1:A:2108:ASN:OD1	1:A:2109:PHE:N	2.40	0.55
1:A:2425:ASP:HB3	1:A:2426:PHE:HD1	1.72	0.55
1:C:2108:ASN:OD1	1:C:2109:PHE:N	2.40	0.55
1:C:2280:ASP:O	1:C:2450:SER:OG	2.24	0.55
1:A:2280:ASP:O	1:A:2450:SER:OG	2.24	0.55
1:A:2295:ARG:HH12	1:B:2295:ARG:HH11	1.51	0.55
1:C:2368:ILE:HD12	1:C:2403:ILE:HD12	1.89	0.55
1:C:2425:ASP:HB3	1:C:2426:PHE:HD1	1.72	0.55
1:A:2530:ILE:HD12	1:C:2492:ILE:HD11	1.89	0.55
1:C:2104:ARG:HG2	1:C:2104:ARG:HH21	1.72	0.55
1:A:1117:GLU:HG2	1:A:1118:GLU:HG2	1.89	0.55
1:A:1971:ARG:HD2	1:A:2098:ARG:O	2.08	0.55
1:B:1117:GLU:HG2	1:B:1118:GLU:HG2	1.89	0.55
1:B:2368:ILE:HD12	1:B:2403:ILE:HD12	1.89	0.54
1:A:1670:GLY:HA2	1:A:1674:ARG:HG3	1.89	0.54
1:A:2368:ILE:HD12	1:A:2403:ILE:HD12	1.89	0.54
1:C:2530:ILE:HD12	1:B:2492:ILE:HD11	1.89	0.54
1:B:1296:ILE:O	1:B:1299:SER:OG	2.24	0.54
1:B:2104:ARG:HG2	1:B:2104:ARG:HH21	1.71	0.54
1:B:1971:ARG:HD2	1:B:2098:ARG:O	2.07	0.54
1:A:2361:ARG:HB3	1:A:2364:GLN:NE2	2.21	0.54
1:A:2377:ARG:NH1	1:A:2451:ASP:OD2	2.41	0.54
1:C:1670:GLY:HA2	1:C:1674:ARG:HG3	1.89	0.54
1:C:2298:PRO:HG2	1:C:2299:PRO:HD3	1.89	0.54
1:B:2108:ASN:OD1	1:B:2109:PHE:N	2.40	0.54
1:B:2280:ASP:O	1:B:2450:SER:OG	2.24	0.54
1:B:1670:GLY:HA2	1:B:1674:ARG:HG3	1.89	0.54
1:A:1152:MET:HE3	1:A:1665:PHE:HE2	1.72	0.54
1:C:1117:GLU:HG2	1:C:1118:GLU:HG2	1.89	0.54
1:C:1971:ARG:HD2	1:C:2098:ARG:O	2.07	0.54
1:B:1152:MET:HE3	1:B:1665:PHE:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2104:ARG:HG2	1:A:2104:ARG:HH21	1.71	0.54
1:B:2298:PRO:HG2	1:B:2299:PRO:HD3	1.89	0.54
1:A:2298:PRO:HG2	1:A:2299:PRO:HD3	1.89	0.53
1:B:2425:ASP:HB3	1:B:2426:PHE:HD1	1.72	0.53
1:C:1774:LEU:HG	1:C:1776:LEU:HD13	1.91	0.53
1:C:2377:ARG:NH1	1:C:2451:ASP:OD2	2.41	0.53
1:B:2377:ARG:NH1	1:B:2451:ASP:OD2	2.41	0.53
1:C:1152:MET:HE3	1:C:1665:PHE:HE2	1.72	0.53
1:A:1783:ILE:O	1:A:1783:ILE:HG13	2.09	0.53
1:C:1783:ILE:HG13	1:C:1783:ILE:O	2.09	0.53
1:A:1650:LEU:O	1:A:1652:ARG:NH2	2.35	0.53
1:C:2296:ILE:HD11	1:C:2300:SER:OG	2.09	0.53
1:A:1184:TYR:OH	1:A:1283:ASP:OD1	2.20	0.52
1:B:1724:ARG:HH22	1:B:1805:LEU:N	1.99	0.52
1:A:1774:LEU:HG	1:A:1776:LEU:HD13	1.91	0.52
1:C:1217:ASN:HD21	1:C:1287:PHE:HB2	1.74	0.52
1:B:1774:LEU:HG	1:B:1776:LEU:HD13	1.91	0.52
1:A:2116:HIS:CE1	2:D:234:LEU:HD11	2.44	0.52
1:C:2250:PRO:HA	1:C:2282:VAL:HA	1.92	0.52
1:B:1217:ASN:HD21	1:B:1287:PHE:HB2	1.74	0.52
1:C:2272:PHE:HD2	1:C:2389:GLN:OE1	1.92	0.52
1:B:1783:ILE:HG13	1:B:1783:ILE:O	2.09	0.52
1:B:2272:PHE:HD2	1:B:2389:GLN:OE1	1.92	0.52
1:A:2105:ILE:HG13	1:A:2106:LEU:HD12	1.92	0.52
1:C:1002:ILE:HG23	1:C:1225:ASN:HD22	1.75	0.52
1:B:1002:ILE:HG23	1:B:1225:ASN:HD22	1.75	0.52
1:B:2296:ILE:HD11	1:B:2300:SER:OG	2.09	0.52
1:C:2105:ILE:HG13	1:C:2106:LEU:HD12	1.92	0.52
1:A:1002:ILE:HG23	1:A:1225:ASN:HD22	1.75	0.52
1:C:2257:GLU:O	1:C:2260:SER:OG	2.17	0.52
1:B:2105:ILE:HG13	1:B:2106:LEU:HD12	1.92	0.52
1:A:2492:ILE:HD11	1:B:2530:ILE:HD12	1.91	0.52
1:C:1650:LEU:O	1:C:1652:ARG:NH2	2.35	0.52
1:C:2153:MET:HE3	1:B:2485:PHE:CZ	2.45	0.52
1:A:2333:VAL:HG21	1:A:2382:PRO:HD3	1.92	0.52
1:C:1724:ARG:HH22	1:C:1805:LEU:N	1.99	0.52
1:A:1217:ASN:HD21	1:A:1287:PHE:HB2	1.74	0.51
1:A:2153:MET:HE3	1:C:2485:PHE:CE1	2.45	0.51
1:A:2544:ARG:NH1	1:B:1411:ASP:OD1	2.42	0.51
1:C:2272:PHE:HZ	1:C:2377:ARG:HD2	1.76	0.51
1:B:2333:VAL:HG21	1:B:2382:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2333:VAL:HG21	1:C:2382:PRO:HD3	1.93	0.51
1:A:2250:PRO:HA	1:A:2282:VAL:HA	1.92	0.51
1:B:2250:PRO:HA	1:B:2282:VAL:HA	1.92	0.51
1:B:2272:PHE:HZ	1:B:2377:ARG:HD2	1.75	0.51
1:A:2272:PHE:HZ	1:A:2377:ARG:HD2	1.75	0.51
1:A:2290:SER:O	1:A:2290:SER:OG	2.26	0.51
1:C:1411:ASP:OD1	1:B:2544:ARG:NH1	2.43	0.51
1:C:2287:GLU:HG3	1:C:2290:SER:HB3	1.92	0.51
1:B:2287:GLU:HG3	1:B:2290:SER:HB3	1.92	0.51
1:B:2290:SER:O	1:B:2290:SER:OG	2.26	0.51
1:B:2324:GLN:HB2	1:B:2335:TYR:HE1	1.76	0.51
1:A:2153:MET:HE3	1:C:2485:PHE:CZ	2.45	0.50
1:A:2272:PHE:HD2	1:A:2389:GLN:OE1	1.92	0.50
1:C:2405:LEU:HD12	1:C:2430:TRP:CH2	2.47	0.50
1:A:2146:THR:HG23	1:A:2519:LEU:HD22	1.93	0.50
1:A:2296:ILE:HD11	1:A:2300:SER:OG	2.09	0.50
1:A:2406:ARG:HB3	1:A:2429:TRP:CE2	2.46	0.50
1:C:2146:THR:HG23	1:C:2519:LEU:HD22	1.93	0.50
1:C:2153:MET:HE3	1:B:2485:PHE:CE1	2.45	0.50
1:B:1178:SER:HB3	1:B:1250:SER:HB3	1.93	0.50
1:B:2405:LEU:HD12	1:B:2430:TRP:CH2	2.47	0.50
1:A:1411:ASP:OD1	1:C:2544:ARG:NH1	2.43	0.50
1:A:2405:LEU:HD12	1:A:2430:TRP:CH2	2.47	0.50
1:A:2485:PHE:CE1	1:B:2153:MET:HE3	2.46	0.50
1:B:2406:ARG:HB3	1:B:2429:TRP:CE2	2.46	0.50
1:A:1139:PRO:HD2	1:A:1301:TYR:HE1	1.77	0.50
1:A:2324:GLN:HB2	1:A:2335:TYR:HE1	1.77	0.50
1:C:2324:GLN:HB2	1:C:2335:TYR:HE1	1.77	0.50
1:B:2146:THR:HG23	1:B:2519:LEU:HD22	1.94	0.50
1:A:2287:GLU:HG3	1:A:2290:SER:HB3	1.92	0.50
1:C:2290:SER:O	1:C:2290:SER:OG	2.26	0.50
1:A:2485:PHE:CZ	1:B:2153:MET:HE3	2.47	0.50
1:C:1716:LEU:HD21	1:C:2051:VAL:HA	1.94	0.50
1:C:1724:ARG:HH12	1:C:1804:GLY:HA3	1.77	0.50
1:C:2280:ASP:OD2	1:C:2452:LYS:NZ	2.34	0.50
1:A:1178:SER:HB3	1:A:1250:SER:HB3	1.93	0.49
1:C:2406:ARG:HB3	1:C:2429:TRP:CE2	2.46	0.49
1:B:1650:LEU:O	1:B:1652:ARG:NH2	2.35	0.49
2:D:243:ILE:HD11	1:B:2149:LEU:HD23	1.95	0.49
1:C:1178:SER:HB3	1:C:1250:SER:HB3	1.93	0.49
1:A:2280:ASP:OD2	1:A:2452:LYS:NZ	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1139:PRO:HD2	1:C:1301:TYR:HE1	1.77	0.49
1:A:1716:LEU:HD21	1:A:2051:VAL:HA	1.94	0.49
1:B:2183:LYS:HB3	1:B:2188:LYS:HD2	1.95	0.49
1:B:1326:ALA:HA	1:B:1649:LEU:HD21	1.94	0.49
1:B:2345:ALA:O	1:B:2348:SER:OG	2.22	0.49
1:A:1308:ASP:OD1	1:A:1538:ARG:NH1	2.46	0.49
2:D:229:GLU:HG3	2:D:230:SER:H	1.78	0.49
1:B:1359:TYR:OH	1:B:1418:ASP:OD2	2.17	0.49
1:A:1311:ALA:HB2	1:A:1542:THR:HB	1.95	0.49
1:A:1698:ASN:ND2	1:A:1789:GLN:OE1	2.41	0.49
1:A:1724:ARG:HH12	1:A:1804:GLY:HA3	1.77	0.49
2:F:229:GLU:HG3	2:F:230:SER:H	1.78	0.49
2:E:229:GLU:HG3	2:E:230:SER:H	1.78	0.49
1:C:1326:ALA:HA	1:C:1649:LEU:HD21	1.94	0.49
1:B:1139:PRO:HD2	1:B:1301:TYR:HE1	1.77	0.49
1:B:1716:LEU:HD21	1:B:2051:VAL:HA	1.94	0.49
1:A:1326:ALA:HA	1:A:1649:LEU:HD21	1.94	0.48
2:E:243:ILE:HD11	1:C:2149:LEU:HD23	1.95	0.48
1:C:1710:LEU:HB3	1:C:1711:PRO:HD3	1.95	0.48
1:B:2236:GLU:HG2	1:B:2295:ARG:O	2.13	0.48
1:A:1710:LEU:HB3	1:A:1711:PRO:HD3	1.95	0.48
1:A:2236:GLU:HG2	1:A:2295:ARG:O	2.13	0.48
1:B:1311:ALA:HB2	1:B:1542:THR:HB	1.95	0.48
1:A:2371:LEU:HD22	1:A:2401:VAL:HG11	1.96	0.48
1:C:1698:ASN:ND2	1:C:1789:GLN:OE1	2.41	0.48
1:C:2236:GLU:HG2	1:C:2295:ARG:O	2.13	0.48
1:B:1218:VAL:HA	1:B:1221:ILE:HG22	1.96	0.48
1:A:2283:THR:HG22	1:A:2447:VAL:HG22	1.96	0.48
1:C:2283:THR:HG22	1:C:2447:VAL:HG22	1.96	0.48
1:B:1308:ASP:OD1	1:B:1538:ARG:NH1	2.46	0.48
1:C:2183:LYS:HB3	1:C:2188:LYS:HD2	1.95	0.48
1:A:2143:THR:O	1:C:2188:LYS:NZ	2.42	0.48
1:A:2183:LYS:HB3	1:A:2188:LYS:HD2	1.95	0.48
1:C:1559:LEU:HD23	1:C:1559:LEU:H	1.79	0.48
1:A:2162:ILE:HG22	1:A:2504:LEU:HD13	1.96	0.48
1:C:2162:ILE:HG22	1:C:2504:LEU:HD13	1.96	0.48
1:B:1724:ARG:HH12	1:B:1804:GLY:HA3	1.77	0.47
1:C:2137:VAL:O	1:C:2141:VAL:HG23	2.14	0.47
1:A:998:ALA:O	1:A:1001:VAL:HG12	2.14	0.47
1:B:1710:LEU:HB3	1:B:1711:PRO:HD3	1.95	0.47
1:A:1780:ASP:OD1	1:A:1781:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1308:ASP:OD1	1:C:1538:ARG:NH1	2.46	0.47
1:C:1311:ALA:HB2	1:C:1542:THR:HB	1.95	0.47
1:B:998:ALA:O	1:B:1001:VAL:HG12	2.14	0.47
1:C:1334:HIS:HA	1:C:1337:ILE:HG22	1.97	0.47
1:B:2371:LEU:HD22	1:B:2401:VAL:HG11	1.95	0.47
1:A:2264:ASP:O	1:A:2266:TYR:N	2.48	0.47
1:C:1359:TYR:OH	1:C:1418:ASP:OD2	2.17	0.47
1:C:1780:ASP:OD1	1:C:1781:SER:N	2.48	0.47
1:B:1514:ASP:OD1	1:B:1674:ARG:NH2	2.43	0.47
1:B:2162:ILE:HG22	1:B:2504:LEU:HD13	1.96	0.47
1:B:2264:ASP:O	1:B:2266:TYR:N	2.48	0.47
1:A:1218:VAL:HA	1:A:1221:ILE:HG22	1.96	0.47
1:A:1553:ARG:HH11	1:A:1556:LEU:HD11	1.80	0.47
1:C:1044:LEU:HD21	1:C:1098:PHE:CE1	2.50	0.47
1:C:1218:VAL:HA	1:C:1221:ILE:HG22	1.96	0.47
1:B:2137:VAL:O	1:B:2141:VAL:HG23	2.14	0.47
1:A:1334:HIS:HA	1:A:1337:ILE:HG22	1.97	0.47
1:A:1554:GLY:O	1:A:1558:GLN:HB2	2.15	0.47
1:A:2140:TRP:CD1	1:A:2145:THR:HG21	2.50	0.47
1:C:2345:ALA:O	1:C:2348:SER:OG	2.22	0.47
1:C:2371:LEU:HD22	1:C:2401:VAL:HG11	1.95	0.47
1:A:2256:TYR:HB2	1:A:2278:PRO:HB3	1.97	0.47
1:C:2140:TRP:CD1	1:C:2145:THR:HG21	2.50	0.47
1:C:2143:THR:O	1:B:2188:LYS:NZ	2.42	0.47
1:B:2365:SER:OG	1:B:2404:GLN:HG3	2.15	0.47
1:A:2321:TRP:HE1	1:A:2338:GLU:HG2	1.80	0.46
1:C:1184:TYR:OH	1:C:1283:ASP:OD1	2.20	0.46
1:C:2070:GLU:OE1	1:C:2075:GLN:HB2	2.15	0.46
1:B:2283:THR:HG22	1:B:2447:VAL:HG22	1.96	0.46
1:A:2149:LEU:HD23	2:F:243:ILE:HD11	1.96	0.46
1:C:998:ALA:O	1:C:1001:VAL:HG12	2.14	0.46
1:C:2264:ASP:O	1:C:2266:TYR:N	2.48	0.46
1:A:2137:VAL:O	1:A:2141:VAL:HG23	2.14	0.46
1:B:2244:GLN:HG2	1:B:2245:GLN:H	1.80	0.46
1:B:2256:TYR:HB2	1:B:2278:PRO:HB3	1.97	0.46
1:B:1559:LEU:HD23	1:B:1559:LEU:H	1.79	0.46
1:B:2321:TRP:HE1	1:B:2338:GLU:HG2	1.80	0.46
1:A:1044:LEU:HD21	1:A:1098:PHE:CE1	2.50	0.46
1:C:1514:ASP:OD1	1:C:1674:ARG:NH2	2.43	0.46
1:C:1551:VAL:HG22	1:C:1553:ARG:H	1.81	0.46
1:C:2321:TRP:HE1	1:C:2338:GLU:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1780:ASP:OD1	1:B:1781:SER:N	2.48	0.46
1:B:2140:TRP:CD1	1:B:2145:THR:HG21	2.50	0.46
1:A:1179:ILE:HG23	1:A:1179:ILE:O	2.15	0.46
1:A:2070:GLU:OE1	1:A:2075:GLN:HB2	2.15	0.46
1:C:1296:ILE:O	1:C:1299:SER:OG	2.24	0.46
1:C:1553:ARG:HH11	1:C:1556:LEU:HD11	1.80	0.46
1:C:2235:TYR:CD2	1:C:2304:MET:HG3	2.51	0.46
1:C:2289:SER:HA	1:C:2431:VAL:HG22	1.97	0.46
1:B:1334:HIS:HA	1:B:1337:ILE:HG22	1.97	0.46
1:A:2104:ARG:HG2	1:A:2104:ARG:NH2	2.31	0.46
1:A:2365:SER:OG	1:A:2404:GLN:HG3	2.15	0.46
1:C:1554:GLY:O	1:C:1558:GLN:HB2	2.15	0.46
1:C:2365:SER:OG	1:C:2404:GLN:HG3	2.15	0.46
1:B:1179:ILE:HG23	1:B:1179:ILE:O	2.15	0.46
1:B:1353:ARG:HG2	1:B:2521:LEU:HD21	1.98	0.46
1:B:1554:GLY:O	1:B:1558:GLN:HB2	2.15	0.46
1:B:2131:LEU:HD23	1:B:2131:LEU:HA	1.78	0.46
1:B:1553:ARG:HH11	1:B:1556:LEU:HD11	1.80	0.46
1:A:1559:LEU:HD23	1:A:1559:LEU:H	1.79	0.46
1:C:2104:ARG:HG2	1:C:2104:ARG:NH2	2.31	0.46
1:C:2244:GLN:HG2	1:C:2245:GLN:H	1.80	0.46
1:B:2070:GLU:OE1	1:B:2075:GLN:HB2	2.15	0.46
1:A:1170:PHE:CE1	1:A:1787:LEU:HB2	2.51	0.46
1:A:1551:VAL:HG22	1:A:1553:ARG:H	1.81	0.46
1:A:2301:ARG:NH2	1:A:2358:LEU:O	2.33	0.46
1:C:2256:TYR:HB2	1:C:2278:PRO:HB3	1.97	0.46
1:B:2301:ARG:NH2	1:B:2358:LEU:O	2.33	0.46
1:A:2149:LEU:O	1:A:2153:MET:HG2	2.16	0.45
1:C:1179:ILE:O	1:C:1179:ILE:HG23	2.15	0.45
1:B:1044:LEU:HD21	1:B:1098:PHE:CE1	2.50	0.45
1:A:1412:TYR:HD1	1:A:2538:THR:HG21	1.82	0.45
1:A:2406:ARG:HD3	1:A:2406:ARG:HA	1.87	0.45
1:C:2149:LEU:O	1:C:2153:MET:HG2	2.16	0.45
1:B:1170:PHE:CE1	1:B:1787:LEU:HB2	2.51	0.45
1:B:1182:LEU:HB2	1:B:1745:TYR:HE2	1.81	0.45
1:A:2140:TRP:CE3	1:A:2149:LEU:HD13	2.52	0.45
1:A:2188:LYS:NZ	1:B:2143:THR:O	2.43	0.45
1:A:2461:LEU:HD23	1:A:2462:ALA:N	2.32	0.45
1:C:1170:PHE:CE1	1:C:1787:LEU:HB2	2.51	0.45
1:C:1716:LEU:HD22	1:C:2051:VAL:HG22	1.99	0.45
1:B:1412:TYR:HD1	1:B:2538:THR:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2140:TRP:CE3	1:B:2149:LEU:HD13	2.52	0.45
1:B:2149:LEU:O	1:B:2153:MET:HG2	2.16	0.45
1:B:2235:TYR:CD2	1:B:2304:MET:HG3	2.51	0.45
1:A:1716:LEU:HD23	1:A:1716:LEU:HA	1.74	0.45
1:C:1716:LEU:HD23	1:C:1716:LEU:HA	1.74	0.45
1:C:2141:VAL:HG21	1:B:2192:GLY:HA3	1.99	0.45
1:B:2289:SER:HA	1:B:2431:VAL:HG22	1.97	0.45
1:A:2235:TYR:CD2	1:A:2304:MET:HG3	2.51	0.45
1:A:2289:SER:HA	1:A:2431:VAL:HG22	1.97	0.45
1:C:1353:ARG:HG2	1:C:2521:LEU:HD21	1.98	0.45
1:C:2140:TRP:CE3	1:C:2149:LEU:HD13	2.52	0.45
1:B:1150:LEU:O	1:B:1154:LYS:HG2	2.17	0.45
1:A:1514:ASP:OD1	1:A:1674:ARG:NH2	2.43	0.45
1:B:2516:THR:O	1:B:2516:THR:HG22	2.17	0.45
1:A:1007:ASN:HB2	1:A:1079:TRP:O	2.17	0.45
1:A:1411:ASP:HB2	1:A:1413:PHE:CD2	2.52	0.45
1:A:2244:GLN:HG2	1:A:2245:GLN:H	1.80	0.45
1:C:1007:ASN:HB2	1:C:1079:TRP:O	2.17	0.45
1:B:2104:ARG:HG2	1:B:2104:ARG:NH2	2.31	0.45
1:A:1090:ASN:OD1	1:A:1091:SER:N	2.50	0.45
1:A:1150:LEU:O	1:A:1154:LYS:HG2	2.17	0.45
1:A:2141:VAL:HG21	1:C:2192:GLY:HA3	1.99	0.45
1:A:2523:GLU:OE2	1:C:2180:GLY:HA2	2.17	0.45
1:C:1411:ASP:HB2	1:C:1413:PHE:CD2	2.52	0.45
1:C:1412:TYR:HD1	1:C:2538:THR:HG21	1.82	0.45
1:B:2461:LEU:HD23	1:B:2462:ALA:N	2.32	0.45
1:A:1182:LEU:HB2	1:A:1745:TYR:HE2	1.81	0.45
1:A:2349:THR:O	1:A:2353:GLN:HG2	2.17	0.45
1:B:2251:PHE:HE2	1:B:2281:ILE:HG22	1.82	0.45
1:B:2455:PRO:C	1:B:2457:SER:H	2.25	0.45
1:A:1177:ILE:O	1:A:1177:ILE:HG22	2.17	0.44
1:A:2180:GLY:HA2	1:B:2523:GLU:OE2	2.16	0.44
1:A:2516:THR:HG22	1:A:2516:THR:O	2.17	0.44
1:C:1090:ASN:OD1	1:C:1091:SER:N	2.50	0.44
1:C:1182:LEU:HB2	1:C:1745:TYR:HE2	1.81	0.44
1:C:1991:ILE:HD11	1:C:2082:TRP:HE1	1.82	0.44
1:B:1036:TYR:CE2	1:B:1040:LEU:HD11	2.52	0.44
1:A:1353:ARG:HG2	1:A:2521:LEU:HD21	1.98	0.44
1:A:1724:ARG:NH2	1:A:1805:LEU:O	2.50	0.44
1:C:2349:THR:O	1:C:2353:GLN:HG2	2.17	0.44
1:B:2297:SER:O	1:B:2300:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2349:THR:O	1:B:2353:GLN:HG2	2.17	0.44
1:A:2297:SER:O	1:A:2300:SER:N	2.51	0.44
1:C:1036:TYR:CE2	1:C:1040:LEU:HD11	2.53	0.44
1:C:2182:LYS:HB2	1:C:2182:LYS:HE3	1.80	0.44
1:C:2251:PHE:HE2	1:C:2281:ILE:HG22	1.82	0.44
1:B:1698:ASN:ND2	1:B:1789:GLN:OE1	2.41	0.44
1:B:1722:ILE:HG23	1:B:1723:PRO:HD2	2.00	0.44
1:A:2455:PRO:C	1:A:2457:SER:H	2.25	0.44
2:E:243:ILE:HD11	1:B:2195:ILE:HD11	2.00	0.44
1:C:1170:PHE:HB2	1:C:1188:CYS:SG	2.58	0.44
1:C:1177:ILE:HG22	1:C:1177:ILE:O	2.17	0.44
2:E:234:LEU:HD11	1:B:2116:HIS:CE1	2.51	0.44
1:C:2516:THR:HG22	1:C:2516:THR:O	2.17	0.44
1:C:2523:GLU:OE2	1:B:2180:GLY:HA2	2.17	0.44
1:A:2295:ARG:HB2	1:C:2295:ARG:NH2	2.21	0.44
1:C:1150:LEU:O	1:C:1154:LYS:HG2	2.17	0.44
1:C:2301:ARG:NH2	1:C:2358:LEU:O	2.33	0.44
1:B:1090:ASN:OD1	1:B:1091:SER:N	2.50	0.44
1:B:1411:ASP:HB2	1:B:1413:PHE:CD2	2.52	0.44
1:B:1987:ASP:OD1	1:B:2082:TRP:NE1	2.51	0.44
1:C:2461:LEU:HD23	1:C:2462:ALA:N	2.32	0.44
1:B:1551:VAL:HG22	1:B:1553:ARG:H	1.81	0.44
1:B:1716:LEU:HA	1:B:1716:LEU:HD23	1.74	0.44
1:B:2250:PRO:HB3	1:B:2282:VAL:HG12	2.00	0.44
1:A:1036:TYR:CE2	1:A:1040:LEU:HD11	2.52	0.44
1:B:1007:ASN:HB2	1:B:1079:TRP:O	2.17	0.44
1:A:2235:TYR:OH	1:A:2303:GLN:HG2	2.18	0.44
1:B:1716:LEU:HD22	1:B:2051:VAL:HG22	1.99	0.44
1:B:2239:PHE:CE1	1:B:2241:MET:HB2	2.53	0.44
1:A:2250:PRO:HB3	1:A:2282:VAL:HG12	2.00	0.43
1:A:2251:PHE:HE2	1:A:2281:ILE:HG22	1.82	0.43
1:A:2536:PRO:O	1:A:2540:ILE:HG13	2.18	0.43
1:C:1724:ARG:NH2	1:C:1805:LEU:O	2.50	0.43
1:C:2239:PHE:CE1	1:C:2241:MET:HB2	2.53	0.43
1:A:1716:LEU:HD22	1:A:2051:VAL:HG22	1.99	0.43
1:A:2239:PHE:CE1	1:A:2241:MET:HB2	2.53	0.43
1:C:2235:TYR:OH	1:C:2303:GLN:HG2	2.18	0.43
1:C:2297:SER:O	1:C:2300:SER:N	2.51	0.43
1:B:1033:TRP:HD1	1:B:1108:TRP:CD1	2.36	0.43
1:B:1991:ILE:HD11	1:B:2082:TRP:HE1	1.82	0.43
1:B:2235:TYR:OH	1:B:2303:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:TRP:HD1	1:A:1108:TRP:CD1	2.36	0.43
1:A:1170:PHE:HB2	1:A:1188:CYS:SG	2.58	0.43
1:B:1170:PHE:HB2	1:B:1188:CYS:SG	2.57	0.43
1:B:1724:ARG:NH2	1:B:1805:LEU:O	2.50	0.43
1:C:1012:LEU:HD21	1:C:1043:PHE:CE2	2.53	0.43
1:B:1012:LEU:HD21	1:B:1043:PHE:CE2	2.54	0.43
1:B:2148:SER:OG	1:B:2149:LEU:N	2.52	0.43
1:B:2519:LEU:HD23	1:B:2519:LEU:HA	1.88	0.43
1:B:2536:PRO:O	1:B:2540:ILE:HG13	2.18	0.43
1:A:1987:ASP:OD1	1:A:2082:TRP:NE1	2.51	0.43
1:C:1033:TRP:HD1	1:C:1108:TRP:CD1	2.36	0.43
1:C:1713:LEU:HD23	1:C:1713:LEU:HA	1.82	0.43
1:A:1141:PRO:HB2	1:A:1304:HIS:CB	2.47	0.43
1:A:1991:ILE:HD11	1:A:2082:TRP:HE1	1.82	0.43
1:A:2148:SER:OG	1:A:2149:LEU:N	2.52	0.43
1:A:2520:GLU:O	1:A:2524:GLU:HG3	2.19	0.43
1:C:1722:ILE:HG23	1:C:1723:PRO:HD2	2.00	0.43
1:C:2455:PRO:C	1:C:2457:SER:H	2.25	0.43
1:B:1177:ILE:HG22	1:B:1177:ILE:O	2.17	0.43
1:A:1012:LEU:HD21	1:A:1043:PHE:CE2	2.53	0.43
1:A:1233:VAL:HG13	1:A:1233:VAL:O	2.19	0.43
1:A:2192:GLY:HA3	1:B:2141:VAL:HG21	2.01	0.43
1:C:2534:ARG:HG2	1:C:2534:ARG:O	2.19	0.43
1:A:1154:LYS:HA	1:A:1154:LYS:HD2	1.83	0.43
1:A:1248:LEU:HD12	1:A:1751:PHE:CD2	2.54	0.43
1:A:2047:LEU:HA	1:A:2097:ILE:HD13	2.01	0.43
1:C:1166:LEU:HD23	1:C:1166:LEU:HA	1.81	0.43
1:C:2250:PRO:HB3	1:C:2282:VAL:HG12	2.00	0.43
1:C:2116:HIS:CE1	2:F:234:LEU:HD11	2.53	0.43
1:C:2536:PRO:O	1:C:2540:ILE:HG13	2.18	0.43
1:B:2182:LYS:HE3	1:B:2182:LYS:HB2	1.80	0.43
1:B:2520:GLU:O	1:B:2524:GLU:HG3	2.19	0.43
1:A:1722:ILE:HG23	1:A:1723:PRO:HD2	2.00	0.43
1:C:1684:ALA:O	1:C:1799:GLN:NE2	2.52	0.43
1:C:2520:GLU:O	1:C:2524:GLU:HG3	2.19	0.43
1:A:1530:MET:SD	1:A:1803:TYR:CZ	3.12	0.42
1:C:1530:MET:SD	1:C:1803:TYR:CZ	3.12	0.42
1:C:1717:TRP:O	1:C:1721:THR:HG23	2.19	0.42
1:C:1987:ASP:OD1	1:C:2082:TRP:NE1	2.51	0.42
1:C:2525:LEU:HD23	1:C:2525:LEU:HA	1.84	0.42
1:B:2393:ASP:C	1:B:2395:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1530:MET:SD	1:B:1803:TYR:CZ	3.12	0.42
2:E:240:CYS:HA	1:B:2191:MET:CE	2.49	0.42
1:C:1028:ALA:O	1:C:1031:ARG:HG3	2.20	0.42
1:C:1233:VAL:HG13	1:C:1233:VAL:O	2.19	0.42
1:C:2027:GLN:HA	1:C:2030:THR:HG22	2.01	0.42
1:C:2191:MET:HE3	1:C:2195:ILE:HD11	2.01	0.42
1:C:2504:LEU:HD12	1:C:2504:LEU:HA	1.84	0.42
1:B:1700:MET:HE3	1:B:2080:GLN:HB3	2.01	0.42
1:B:2534:ARG:O	1:B:2534:ARG:HG2	2.19	0.42
1:A:1010:VAL:O	1:A:1013:HIS:HB2	2.20	0.42
1:A:1028:ALA:O	1:A:1031:ARG:HG3	2.19	0.42
1:A:1670:GLY:CA	1:A:1674:ARG:HE	2.33	0.42
1:A:2504:LEU:HD12	1:A:2504:LEU:HA	1.84	0.42
1:B:1248:LEU:HD12	1:B:1751:PHE:CD2	2.54	0.42
1:A:1530:MET:SD	1:A:1803:TYR:OH	2.70	0.42
1:A:1717:TRP:O	1:A:1721:THR:HG23	2.19	0.42
1:A:2130:PHE:HA	1:A:2133:GLU:HG3	2.02	0.42
1:C:1010:VAL:O	1:C:1013:HIS:HB2	2.20	0.42
1:C:1178:SER:O	1:C:1745:TYR:OH	2.38	0.42
1:C:1700:MET:HE3	1:C:2080:GLN:HB3	2.01	0.42
1:C:2130:PHE:HA	1:C:2133:GLU:HG3	2.02	0.42
1:B:1010:VAL:O	1:B:1013:HIS:HB2	2.19	0.42
1:B:1670:GLY:CA	1:B:1674:ARG:HE	2.33	0.42
1:B:1684:ALA:O	1:B:1799:GLN:NE2	2.52	0.42
1:B:2092:LEU:HD23	1:B:2092:LEU:HA	1.86	0.42
1:A:1178:SER:O	1:A:1745:TYR:OH	2.38	0.42
1:A:2027:GLN:HA	1:A:2030:THR:HG22	2.01	0.42
1:B:1335:ARG:HH21	1:B:1970:TYR:HB2	1.84	0.42
2:F:244:CYS:HB2	2:F:245:PHE:CD1	2.55	0.42
1:A:2116:HIS:HE1	2:D:234:LEU:HD11	1.84	0.42
1:A:2182:LYS:HB2	1:A:2182:LYS:HE3	1.80	0.42
1:A:2534:ARG:O	1:A:2534:ARG:HG2	2.19	0.42
1:C:1138:ASN:HA	1:C:1139:PRO:HD3	1.89	0.42
1:C:2047:LEU:HA	1:C:2097:ILE:HD13	2.01	0.42
1:C:2295:ARG:HB2	1:B:2295:ARG:NH2	2.23	0.42
1:C:2374:LYS:HE3	1:C:2399:LEU:HD21	2.01	0.42
1:C:2393:ASP:C	1:C:2395:GLU:H	2.27	0.42
1:B:1028:ALA:O	1:B:1031:ARG:HG3	2.19	0.42
1:B:1154:LYS:HA	1:B:1154:LYS:HD2	1.83	0.42
1:B:2027:GLN:HA	1:B:2030:THR:HG22	2.01	0.42
1:B:2191:MET:HE3	1:B:2195:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1183:GLY:HA3	1:A:1216:TYR:OH	2.20	0.42
1:A:2131:LEU:HA	1:A:2131:LEU:HD23	1.78	0.42
1:A:2191:MET:HE3	1:A:2195:ILE:HD11	2.01	0.42
1:C:1782:TYR:CE2	1:C:1783:ILE:HG23	2.55	0.42
1:B:1020:ILE:HG23	1:B:1029:ILE:HD12	2.02	0.42
1:B:1717:TRP:O	1:B:1721:THR:HG23	2.19	0.42
1:A:2171:THR:HG21	2:D:238:MET:HE1	2.01	0.42
1:A:2263:PHE:CZ	1:A:2390:LEU:HD23	2.55	0.42
1:C:974:LEU:HG	1:C:975:LEU:HD12	2.02	0.42
1:B:2121:LEU:HD23	1:B:2121:LEU:HA	1.85	0.42
1:B:2130:PHE:HA	1:B:2133:GLU:HG3	2.02	0.42
1:B:2374:LYS:HE3	1:B:2399:LEU:HD21	2.01	0.42
1:A:1020:ILE:HG23	1:A:1029:ILE:HD12	2.02	0.41
1:A:2272:PHE:CZ	1:A:2377:ARG:HD2	2.54	0.41
1:C:1248:LEU:HD12	1:C:1751:PHE:CD2	2.54	0.41
1:C:2209:PHE:O	1:C:2213:ILE:HG12	2.20	0.41
1:B:1183:GLY:HA3	1:B:1216:TYR:OH	2.20	0.41
1:B:2047:LEU:HA	1:B:2097:ILE:HD13	2.01	0.41
1:A:1335:ARG:HD3	1:A:1335:ARG:HA	1.90	0.41
1:A:2209:PHE:O	1:A:2213:ILE:HG12	2.20	0.41
1:A:2353:GLN:OE1	1:A:2353:GLN:HA	2.20	0.41
1:C:2131:LEU:HA	1:C:2131:LEU:HD23	1.78	0.41
1:C:2148:SER:OG	1:C:2149:LEU:N	2.52	0.41
1:C:2238:LEU:HD23	1:C:2430:TRP:CD2	2.55	0.41
1:C:2519:LEU:HA	1:C:2519:LEU:HD23	1.88	0.41
1:B:974:LEU:HG	1:B:975:LEU:HD12	2.02	0.41
1:B:1233:VAL:HG13	1:B:1233:VAL:O	2.19	0.41
1:B:1782:TYR:CE2	1:B:1783:ILE:HG23	2.55	0.41
1:B:2144:ASP:OD1	1:B:2144:ASP:N	2.54	0.41
2:D:244:CYS:HB2	2:D:245:PHE:CD1	2.55	0.41
1:C:1727:LYS:HG3	1:C:1806:TRP:CZ2	2.56	0.41
1:C:2345:ALA:HB3	1:C:2348:SER:HB3	2.02	0.41
1:A:1335:ARG:HH21	1:A:1970:TYR:HB2	1.85	0.41
1:A:1700:MET:HE3	1:A:2080:GLN:HB3	2.01	0.41
1:B:2033:ILE:HD13	1:B:2033:ILE:HA	1.88	0.41
1:B:2209:PHE:O	1:B:2213:ILE:HG12	2.20	0.41
1:B:2264:ASP:C	1:B:2266:TYR:H	2.29	0.41
1:B:2353:GLN:OE1	1:B:2353:GLN:HA	2.20	0.41
2:E:244:CYS:HB2	2:E:245:PHE:CD1	2.55	0.41
1:B:2263:PHE:CZ	1:B:2390:LEU:HD23	2.55	0.41
1:A:1138:ASN:HA	1:A:1139:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:ALA:O	1:A:1799:GLN:NE2	2.52	0.41
1:A:2393:ASP:C	1:A:2395:GLU:H	2.27	0.41
1:C:1670:GLY:CA	1:C:1674:ARG:HE	2.33	0.41
1:C:2264:ASP:C	1:C:2266:TYR:H	2.29	0.41
1:C:2353:GLN:HA	1:C:2353:GLN:OE1	2.20	0.41
1:B:2238:LEU:HD23	1:B:2430:TRP:CD2	2.55	0.41
1:B:2345:ALA:HB3	1:B:2348:SER:HB3	2.02	0.41
1:A:2178:PRO:O	1:B:1403:HIS:HB2	2.20	0.41
1:C:993:ILE:O	1:C:997:MET:HG2	2.21	0.41
1:A:1782:TYR:CE2	1:A:1783:ILE:HG23	2.55	0.41
1:C:1072:MET:HG3	1:C:1072:MET:O	2.21	0.41
1:C:1717:TRP:CD1	1:C:1717:TRP:C	2.99	0.41
1:B:1036:TYR:O	1:B:1040:LEU:HG	2.21	0.41
1:B:1717:TRP:CD1	1:B:1717:TRP:C	2.99	0.41
1:A:974:LEU:HG	1:A:975:LEU:HD12	2.02	0.41
1:A:1727:LYS:HG3	1:A:1806:TRP:CZ2	2.56	0.41
1:A:2187:VAL:HG11	2:D:235:GLU:OE1	2.21	0.41
1:A:2222:GLN:NE2	1:A:2282:VAL:HG11	2.36	0.41
1:C:1020:ILE:HG23	1:C:1029:ILE:HD12	2.02	0.41
1:C:2263:PHE:CZ	1:C:2390:LEU:HD23	2.55	0.41
1:B:1072:MET:O	1:B:1072:MET:HG3	2.21	0.41
1:B:1178:SER:O	1:B:1745:TYR:OH	2.38	0.41
1:B:1727:LYS:HG3	1:B:1806:TRP:CZ2	2.56	0.41
1:B:2061:MET:HE1	1:B:2079:ALA:HB1	2.03	0.41
1:C:1183:GLY:HA3	1:C:1216:TYR:OH	2.20	0.41
1:C:2033:ILE:HD13	1:C:2033:ILE:HA	1.88	0.41
1:B:2296:ILE:HD12	1:B:2296:ILE:HA	1.97	0.41
1:A:2238:LEU:HD23	1:A:2430:TRP:CD2	2.56	0.40
1:C:1032:LEU:HD12	1:C:1032:LEU:HA	1.91	0.40
1:C:2061:MET:HE1	1:C:2079:ALA:HB1	2.04	0.40
1:B:1016:TRP:HD1	1:B:1036:TYR:CD1	2.40	0.40
1:A:2264:ASP:C	1:A:2266:TYR:H	2.29	0.40
1:C:2368:ILE:HA	1:C:2369:PRO:HD3	1.93	0.40
1:B:1079:TRP:HE3	1:B:1080:LEU:HD12	1.86	0.40
1:B:1143:PHE:HZ	1:B:1301:TYR:CG	2.39	0.40
1:A:1072:MET:O	1:A:1072:MET:HG3	2.21	0.40
1:A:1548:VAL:HG23	1:A:1549:GLY:N	2.36	0.40
1:A:2374:LYS:HE3	1:A:2399:LEU:HD21	2.01	0.40
1:A:2375:TYR:HA	1:A:2447:VAL:O	2.22	0.40
1:C:1143:PHE:HZ	1:C:1301:TYR:CG	2.39	0.40
1:C:1331:ILE:HD13	1:C:1331:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1335:ARG:HH21	1:C:1970:TYR:HB2	1.85	0.40
1:C:2281:ILE:HD13	1:C:2449:PHE:CE1	2.56	0.40
1:A:993:ILE:O	1:A:997:MET:HG2	2.21	0.40
1:A:2187:VAL:HG23	2:D:236:ILE:CG1	2.52	0.40
1:C:1202:ASP:OD1	1:C:1202:ASP:N	2.55	0.40
1:C:1403:HIS:HB2	1:B:2178:PRO:O	2.22	0.40
1:C:1719:MET:HB3	1:C:2094:ALA:HB1	2.04	0.40
1:C:2166:LYS:NZ	1:C:2501:ASP:OD1	2.41	0.40
1:C:2191:MET:HE1	2:F:240:CYS:HA	2.04	0.40
1:B:1141:PRO:HB2	1:B:1304:HIS:CB	2.47	0.40
1:B:1548:VAL:HG23	1:B:1549:GLY:N	2.37	0.40
1:B:2281:ILE:HD13	1:B:2449:PHE:CE1	2.56	0.40
1:A:1403:HIS:HB2	1:C:2178:PRO:O	2.22	0.40
1:A:1717:TRP:CD1	1:A:1717:TRP:C	2.99	0.40
1:C:1152:MET:HE3	1:C:1665:PHE:CE2	2.54	0.40
1:C:1694:ILE:HG21	1:C:1789:GLN:HA	2.04	0.40
1:B:993:ILE:O	1:B:997:MET:HG2	2.21	0.40
1:B:2162:ILE:HD13	1:B:2162:ILE:HA	1.83	0.40
1:B:2525:LEU:HD23	1:B:2525:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1193/2547 (47%)	1107 (93%)	86 (7%)	0	100	100
1	B	1193/2547 (47%)	1108 (93%)	85 (7%)	0	100	100
1	C	1193/2547 (47%)	1107 (93%)	86 (7%)	0	100	100
2	D	19/247 (8%)	18 (95%)	1 (5%)	0	100	100
2	E	19/247 (8%)	18 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	19/247 (8%)	18 (95%)	1 (5%)	0	100	100
All	All	3636/8382 (43%)	3376 (93%)	260 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	983/2246 (44%)	983 (100%)	0	100	100
1	B	983/2246 (44%)	983 (100%)	0	100	100
1	C	983/2246 (44%)	983 (100%)	0	100	100
2	D	20/206 (10%)	20 (100%)	0	100	100
2	E	20/206 (10%)	20 (100%)	0	100	100
2	F	20/206 (10%)	20 (100%)	0	100	100
All	All	3009/7356 (41%)	3009 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1200	GLN
1	A	1217	ASN
1	A	1225	ASN
1	A	1403	HIS
1	A	1408	HIS
1	A	1681	GLN
1	A	2116	HIS
1	A	2254	GLN
1	A	2364	GLN
1	C	1200	GLN
1	C	1217	ASN

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Mol	Chain	Res	Type
1	C	1225	ASN
1	C	1403	HIS
1	C	1408	HIS
1	C	1681	GLN
1	C	2027	GLN
1	C	2116	HIS
1	C	2254	GLN
1	C	2364	GLN
1	B	1200	GLN
1	B	1217	ASN
1	B	1225	ASN
1	B	1403	HIS
1	B	1408	HIS
1	B	1681	GLN
1	B	2116	HIS
1	B	2254	GLN
1	B	2364	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.