



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:15 PM UTC

PDB ID : 6JGZ / pdb_00006jgz
EMDB ID : EMD-9824
Title : Structure of RyR2 (F/P/Ca2+ dataset)
Authors : Chi, X.M.; Gong, D.S.; Ren, K.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Zhou, Q.; Yan, N.
Deposited on : 2019-02-16
Resolution : 4.60 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

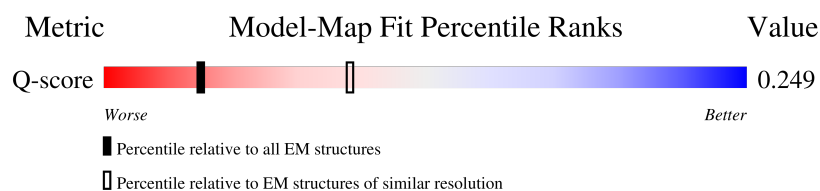
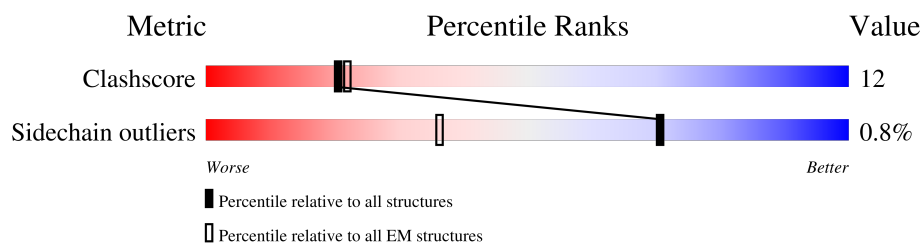
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	108	
1	C	108	
1	E	108	
1	G	108	
2	B	4968	

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Mol	Chain	Length	Quality of chain
2	D	4968	 6% 52% 18% 30%
2	F	4968	 6% 51% 18% 30%
2	H	4968	 5% 51% 18% 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 109824 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	C	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	D	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	F	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		
2	H	3485	Total	C	N	O	S	0	0
			26636	16958	4556	4964	158		

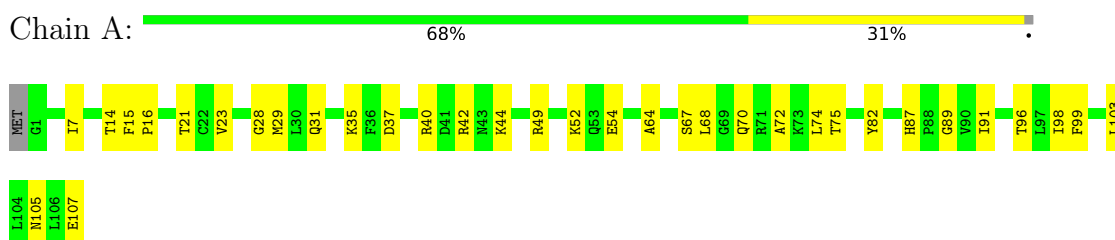
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	H	1	Total	Zn	0
			1	1	

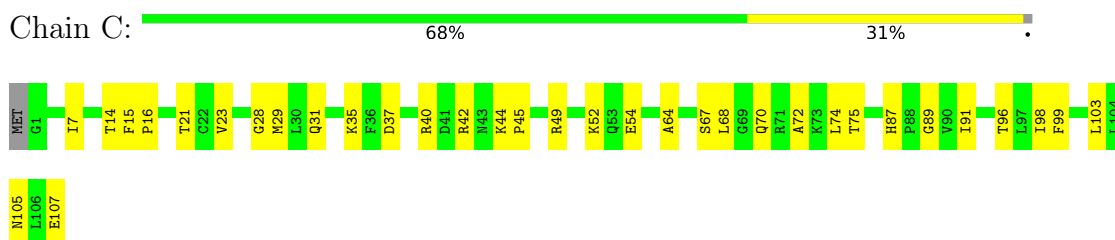
3 Residue-property plots [i](#)

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.

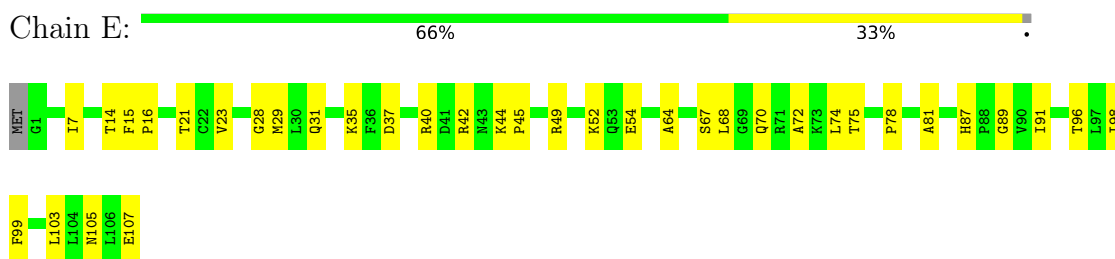
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



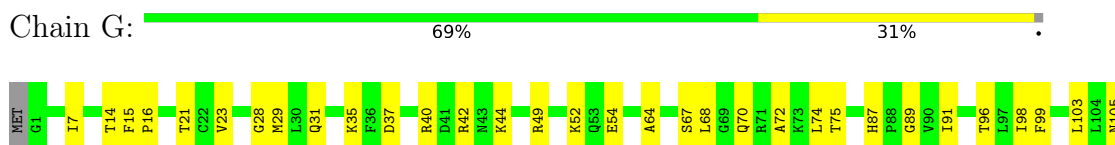
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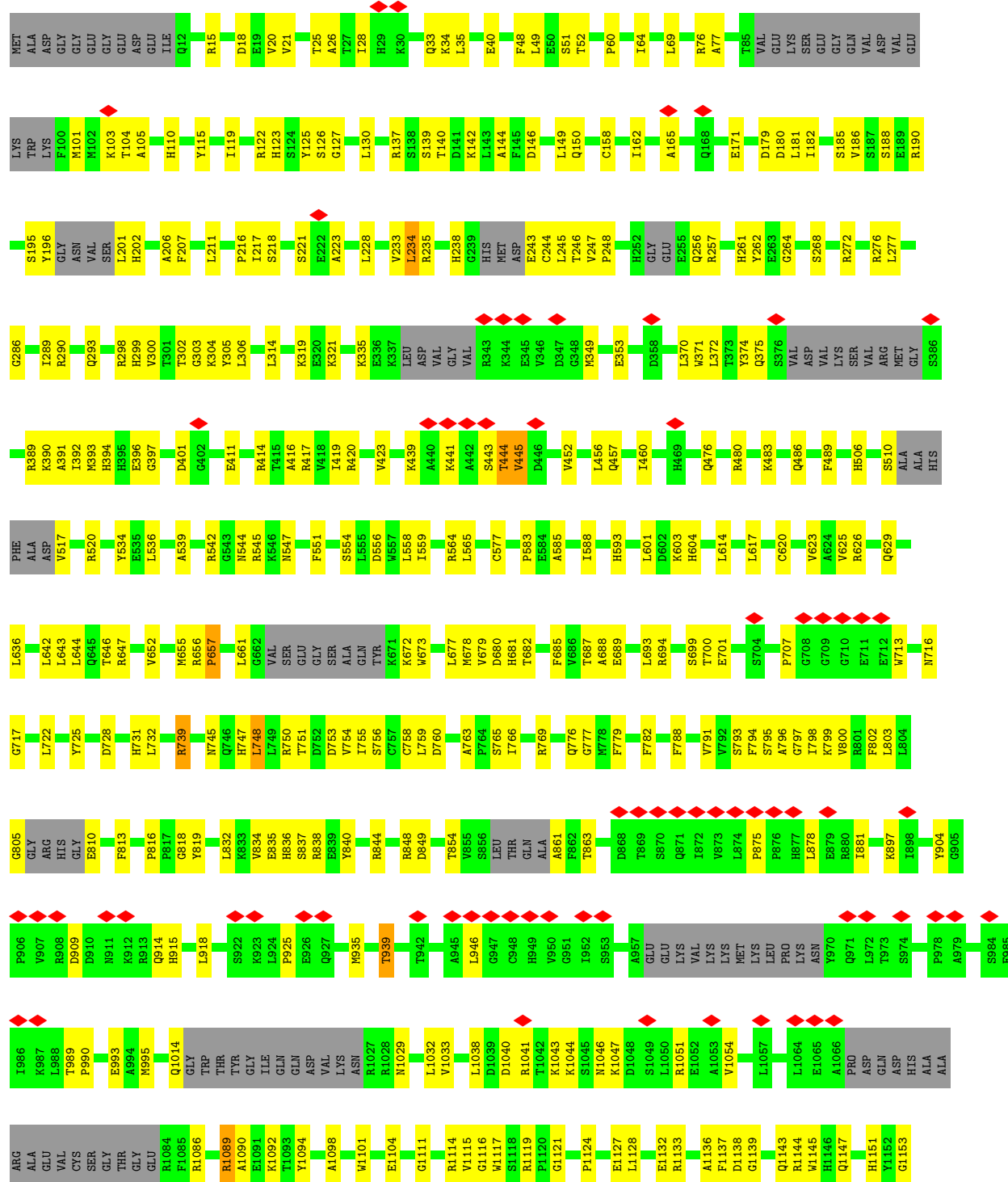


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



L106
E107

• Molecule 2: RyR2



TRP	ASP	Q2060	ASP	LYS	T1716	W1617	V1543	Y1453	LEU	GLY	R1154
ASN	LYS	I2063	LYS	GLU	L1719	Q1620	F1544	L1459	LYS	ALA	S1155
G2296	GLU	M2067	GLU	L1894	L1726	C1621	A1545	ASP	GLN	SER	W1156
Y2299	CYS	A2071	CYS	M1907	E1732	L1622	V1552	VAL	PHE	GLY	Q1157
L2300	PRO	Q2072	PRO	C1908	E1827	F1627	E1556	ARG	LEU	PHE	A1158
D2301	CYS	V2075	CYS	L1909	M1628	S1629	LEU	ARG	PRO	LYS	G1159
R2304	GLU	I2076	GLU	L1910	L1630	T1736	GLY	THR	ASN	ASP	D1160
I2326	ILE	R2083	ILE	Q1912	H1631	T1737	ARG	V1465	THR	ASP	C1164
E2330	THR	A2084	R1994	H1921	H1632	L1738	LYS	V1467	ARG	ASP	M1165
CYS	F2190	M2085	D1995	R1922	P1633	F1739	ASN	G1470	LEU	LYS	T1169
PHE	M2196	L2088	Q1996	R1926	E1634	F1740	VAL	THR	ARG	LYS	H1170
GLY	C2197	R2091	GLU	I1929	E1635	D1741	PRO	K1473	ARG	ASN	L1171
PRO	C2198	Q2092	ASP	F1929	S1638	G1747	LEU	K1474	THR	ASP	T1172
ALA	C2199	I2096	GLY	V1934	D1640	L1841	SER	K1475	THR	ASP	M1173
LEU	F2200	R2100	SER	Q1938	V1639	F1571	GLY	R1482	LEU	ASP	T1176
GLY	C2202	V2100	ASP	R1942	L1642	E1643	GLY	S1483	GLU	VAL	L1177
GLY	C2203	R2101	GLY	R1942	E1648	S1573	GLY	M1487	THR	LEU	G1179
GLY	F2204	A2102	ASN	V1946	L1753	L1651	GLY	C1489	ASP	GLY	E1180
ASN	T2207	L2103	GLN	MET	S1756	H1654	GLY	A1490	ALA	HIS	T1181
G2343	M2211	T2106	ALA	ALA	L1757	Y1655	GLY	G1490	LEU	ASP	L1182
L2344	Q2211	D2116	LEU	LEU	R1758	Y1655	GLY	G1490	LEU	ASP	L1183
M2348	Q2211	T2117	LEU	LEU	M1761	R1659	GLY	G1490	LEU	ASP	D1184
I2354	Y2221	L2118	ASN	ASN	S1761	A1666	GLY	G1490	LEU	ASP	D1185
ALA	L2222	L2121	MET	MET	S1764	L1667	GLY	G1490	LEU	ASP	S1188
GLU	M2225	A2122	SER	SER	S1765	G1668	GLY	G1490	LEU	ASP	E1189
ASP	S2226	S2123	ALA	ALA	T1766	L1669	GLY	G1490	LEU	ASP	L1190
PRO	S2232	Q2126	ALA	ALA	F1768	H1670	GLY	G1490	LEU	ASP	A1191
SER	P2250	I2127	ARG	ARG	M1772	R1671	GLY	G1490	LEU	ASP	K1193
GLY	L2256	V2133	LYS	LYS	C1775	L1676	GLY	G1490	LEU	ASP	D1194
SER	L2256	V2133	LYS	LYS	C1775	E1682	GLY	G1490	LEU	ASP	F1195
THR	C2274	M2135	LYS	LYS	Y1776	P1683	GLY	G1490	LEU	ASP	F1196
SER	LEU	G2136	LYS	LYS	Q1777	Q1684	GLY	G1490	LEU	ASP	V1197
GLY	GLN	L2142	LYS	LYS	Q1778	L1685	GLY	G1490	LEU	ASP	F1201
GLY	CYS	M2143	GLN	GLN	S1779	L1686	GLY	G1490	LEU	ASP	S1206
SER	LEU	I2144	LEU	LEU	A1789	Y1687	GLY	G1490	LEU	ASP	V1209
LYS	VAL	R2145	VAL	VAL	I1689	A1688	GLY	G1490	LEU	ASP	A1210
MET	GLU	G2148	GLU	GLU	K1692	I1692	GLY	G1490	LEU	ASP	Q1211
PRO	VAL	N2152	ASP	ILE	E1797	G1696	GLY	G1490	LEU	ASP	M1215
THR	LYS	N2153	ASP	ASN	A1798	S1699	GLY	G1490	LEU	ASP	N1216
GLY	LYS	K2154	LYS	LEU	V1799	R1699	GLY	G1490	LEU	ASP	F1217
GLY	PRO	Y2157	SER	ASN	S1803	Y1703	GLY	G1490	LEU	ASP	V1221
ASP	ILE	P2160	SER	PHE	R1807	I1709	GLY	G1490	LEU	ASP	L1224
ASP	GLY		ASP	LYS	D1808		GLY	G1490	LEU	ASP	F1227
				ASP	P1809		GLY	G1490	LEU	ASP	T1228
							GLY	G1490	LEU	ASP	L1232

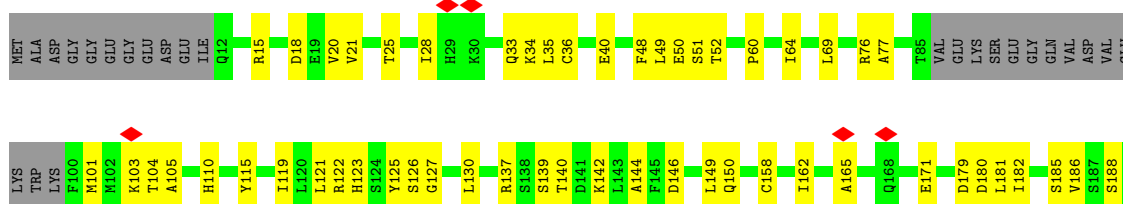


- Molecule 2: RyR2



V2476	ASP	THR	GLY	TRP	Y2157	SER	LYS	GLU	F1816	T1716	I1611	S1536	W1445	ILE	T1238
Y2477	THR	ILE	ASN	ASN	P2160	T2068	SER	G1893	L1817	T1716	S1612	L1539	D1449	PRO	L1232
GLY	ILE	P2293	GLU	L1894	Q2060	Q2068	GLU	L1984	P1820	L1719	E1613	L1539	D1449	GLY	E1237
GLY	THR	G2296	PRO	M1907	L2063	L2067	PRO	C1908	L1821	I1726	Q1615	F1543	Y1453	LEU	N1242
L2488	GLU	Y2299	GLU	L1910	Q2071	Q2076	GLU	L1909	T1827	E1732	Q1620	T1548	L1459	GLY	R1245
L2489	SER	L2300	ILE	Q1912	A2071	A2076	ILE	L1911	I1830	S1735	L1622	V1552	ARG	PRO	R1245
VAL	GLU	D2301	D1995	Q1996	Q2072	L2076	D1998	H1835	H1835	I1736	L1622	V1552	ARG	ASN	M1249
G2492	THR	R2304	Q1996	H1921	V2075	L2076	L1998	L1843	L1846	I1738	F1627	F1566	THR	LEU	L1250
L2503	ILE	T2326	D1997	R1922	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	L1251
ASP	HIS	E2330	L1997	H1921	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	S1252
THR	ALA	E2330	L1997	H1921	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	K1253
ALA	ALA	E2330	L1997	H1921	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	L1254
ALA	ALA	E2330	L1997	H1921	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	L1255
LEU	GLY	E2330	L1997	H1921	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	P1256
SER	GLY	E2330	L1997	H1921	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	Q1257
ALA	ALA	E2330	L1997	H1921	L2076	L2076	L1997	L1843	I1846	F1739	F1627	F1566	THR	LEU	F1258
T2511	ASP	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	V1261
T2523	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	R1272
T2529	THR	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	I1273
THR	ARG	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	D1274
ARG	CYS	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	GLY
ALA	ALA	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
P2534	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ILE
L2535	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
F2536	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	SER
A2537	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	SER
L2549	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	PRO
V2553	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	CYS
TYR	ARG	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	LEU
LEU	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
K2558	SER	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ARG
L2562	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	LYS
S2576	ILE	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	V1285
CYS	GLY	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	M1300
GLN	GLN	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	F1301
R2582	LEU	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	L1302
N2601	GLY	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	L1303
HIS	GLY	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	L1304
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K2605	GLY	R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	M1306
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		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	C1310
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ALA
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	GLU
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	LYS
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		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
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		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
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		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
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		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
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		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	ASP
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	THR
		R2421	S2422	I2423	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	S2426	ASP	VAL
		R2421													

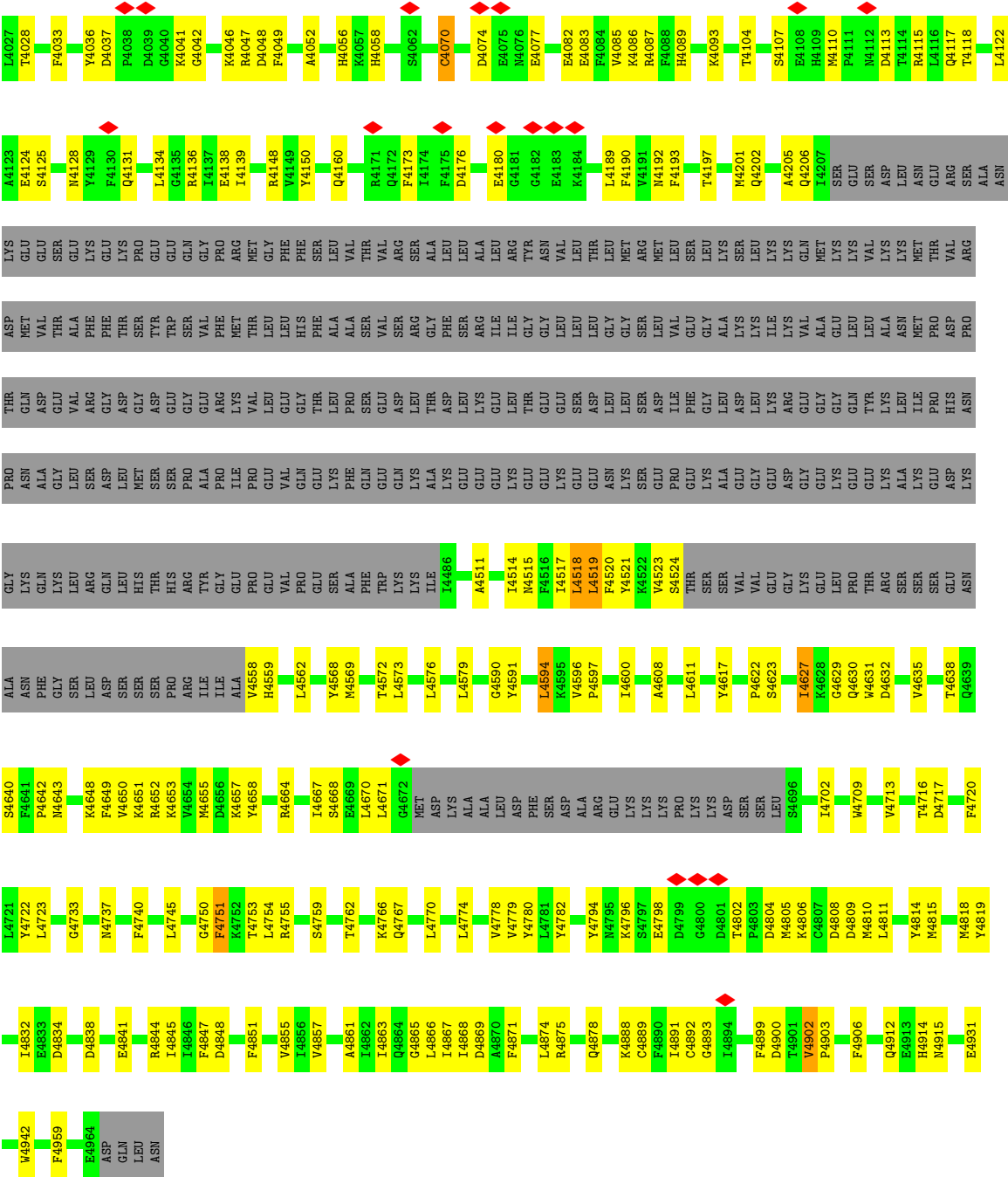




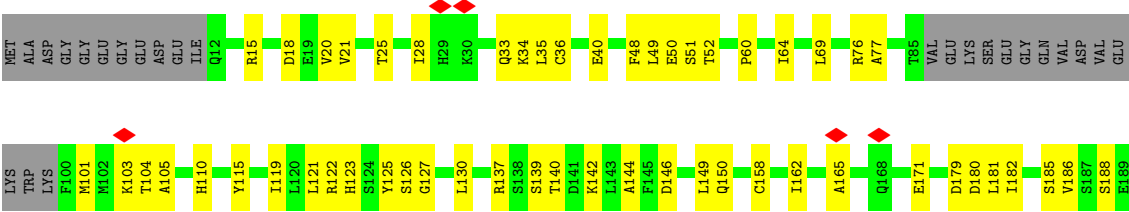








• Molecule 2: RyR2











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	60287	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 ($e^-/\text{\AA}^2$)	48.6	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	0.085	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	522.616, 522.616, 522.616	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	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	0.28	0/835	0.55	0/1123
1	C	0.28	0/835	0.55	0/1123
1	E	0.28	0/835	0.55	0/1123
1	G	0.28	0/835	0.55	0/1123
2	B	0.33	0/27132	0.66	21/36687 (0.1%)
2	D	0.33	0/27132	0.66	21/36687 (0.1%)
2	F	0.33	0/27132	0.66	21/36687 (0.1%)
2	H	0.33	0/27132	0.66	21/36687 (0.1%)
All	All	0.33	0/111868	0.65	84/151240 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	29
2	D	0	29
2	F	0	29
2	H	0	29
All	All	0	116

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2039	TYR	N-CA-C	8.41	123.22	113.38
2	B	2039	TYR	N-CA-C	8.39	123.19	113.38
2	F	2039	TYR	N-CA-C	8.38	123.18	113.38
2	H	2039	TYR	N-CA-C	8.36	123.16	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2039	TYR	CA-C-N	7.22	134.69	121.70
2	D	2039	TYR	C-N-CA	7.22	134.69	121.70
2	F	2039	TYR	CA-C-N	7.20	134.66	121.70
2	F	2039	TYR	C-N-CA	7.20	134.66	121.70
2	B	2039	TYR	CA-C-N	7.20	134.66	121.70
2	B	2039	TYR	C-N-CA	7.20	134.66	121.70
2	F	2022	SER	CA-C-N	7.19	134.64	121.70
2	F	2022	SER	C-N-CA	7.19	134.64	121.70
2	D	2022	SER	CA-C-N	7.17	134.62	121.70
2	D	2022	SER	C-N-CA	7.17	134.62	121.70
2	B	2022	SER	CA-C-N	7.17	134.60	121.70
2	B	2022	SER	C-N-CA	7.17	134.60	121.70
2	H	2022	SER	CA-C-N	7.17	134.60	121.70
2	H	2022	SER	C-N-CA	7.17	134.60	121.70
2	H	2039	TYR	CA-C-N	7.16	134.59	121.70
2	H	2039	TYR	C-N-CA	7.16	134.59	121.70
2	D	139	SER	CA-C-N	7.15	134.56	121.70
2	D	139	SER	C-N-CA	7.15	134.56	121.70
2	B	139	SER	CA-C-N	7.14	134.54	121.70
2	B	139	SER	C-N-CA	7.14	134.54	121.70
2	H	139	SER	CA-C-N	7.13	134.54	121.70
2	H	139	SER	C-N-CA	7.13	134.54	121.70
2	F	139	SER	CA-C-N	7.12	134.51	121.70
2	F	139	SER	C-N-CA	7.12	134.51	121.70
2	D	2133	VAL	CA-C-N	6.54	133.47	121.70
2	D	2133	VAL	C-N-CA	6.54	133.47	121.70
2	B	2133	VAL	CA-C-N	6.53	133.45	121.70
2	B	2133	VAL	C-N-CA	6.53	133.45	121.70
2	F	2133	VAL	CA-C-N	6.52	133.43	121.70
2	F	2133	VAL	C-N-CA	6.52	133.43	121.70
2	H	2133	VAL	CA-C-N	6.51	133.42	121.70
2	H	2133	VAL	C-N-CA	6.51	133.42	121.70
2	D	445	VAL	N-CA-C	-6.20	100.13	108.06
2	B	445	VAL	N-CA-C	-6.17	100.16	108.06
2	F	445	VAL	N-CA-C	-6.17	100.16	108.06
2	H	445	VAL	N-CA-C	-6.16	100.18	108.06
2	B	444	THR	CA-C-N	5.89	130.97	121.95
2	B	444	THR	C-N-CA	5.89	130.97	121.95
2	F	444	THR	CA-C-N	5.89	130.97	121.95
2	F	444	THR	C-N-CA	5.89	130.97	121.95
2	H	444	THR	CA-C-N	5.89	130.97	121.95
2	H	444	THR	C-N-CA	5.89	130.97	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	444	THR	CA-C-N	5.87	130.93	121.95
2	D	444	THR	C-N-CA	5.87	130.93	121.95
2	B	140	THR	CA-C-N	5.70	131.96	121.70
2	B	140	THR	C-N-CA	5.70	131.96	121.70
2	F	140	THR	CA-C-N	5.70	131.96	121.70
2	F	140	THR	C-N-CA	5.70	131.96	121.70
2	D	140	THR	CA-C-N	5.70	131.95	121.70
2	D	140	THR	C-N-CA	5.70	131.95	121.70
2	F	816	PRO	N-CA-C	5.70	117.65	110.70
2	H	140	THR	CA-C-N	5.70	131.95	121.70
2	H	140	THR	C-N-CA	5.70	131.95	121.70
2	B	816	PRO	N-CA-C	5.69	117.64	110.70
2	D	816	PRO	N-CA-C	5.69	117.64	110.70
2	H	816	PRO	N-CA-C	5.68	117.63	110.70
2	B	1997	LEU	CA-C-N	5.58	131.74	121.70
2	B	1997	LEU	C-N-CA	5.58	131.74	121.70
2	D	1997	LEU	CA-C-N	5.58	131.74	121.70
2	D	1997	LEU	C-N-CA	5.58	131.74	121.70
2	H	1997	LEU	CA-C-N	5.58	131.74	121.70
2	H	1997	LEU	C-N-CA	5.58	131.74	121.70
2	F	1997	LEU	CA-C-N	5.57	131.72	121.70
2	F	1997	LEU	C-N-CA	5.57	131.72	121.70
2	D	103	LYS	CA-C-N	5.12	131.32	121.54
2	D	103	LYS	C-N-CA	5.12	131.32	121.54
2	B	103	LYS	CA-C-N	5.09	131.27	121.54
2	B	103	LYS	C-N-CA	5.09	131.27	121.54
2	H	103	LYS	CA-C-N	5.08	131.25	121.54
2	H	103	LYS	C-N-CA	5.08	131.25	121.54
2	F	103	LYS	CA-C-N	5.08	131.24	121.54
2	F	103	LYS	C-N-CA	5.08	131.24	121.54
2	H	2038	THR	CA-C-N	5.05	132.29	123.91
2	H	2038	THR	C-N-CA	5.05	132.29	123.91
2	B	2038	THR	CA-C-N	5.04	132.28	123.91
2	B	2038	THR	C-N-CA	5.04	132.28	123.91
2	D	2038	THR	CA-C-N	5.04	132.28	123.91
2	D	2038	THR	C-N-CA	5.04	132.28	123.91
2	F	2038	THR	CA-C-N	5.03	132.26	123.91
2	F	2038	THR	C-N-CA	5.03	132.26	123.91

There are no chirality outliers.

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	105	ALA	Peptide
2	B	142	LYS	Peptide
2	B	1475	LYS	Peptide
2	B	1579	VAL	Peptide
2	B	1607	ASP	Peptide
2	B	1635	GLU	Peptide
2	B	1756	SER	Peptide
2	B	1758	ARG	Peptide
2	B	1777	GLN	Peptide
2	B	1835	HIS	Peptide
2	B	1847	GLU	Peptide
2	B	2075	VAL	Peptide
2	B	221	SER	Peptide
2	B	2232	SER	Peptide
2	B	2462	CYS	Peptide
2	B	321	LYS	Peptide
2	B	4070	CYS	Peptide
2	B	4074	ASP	Peptide
2	B	4594	LEU	Peptide
2	B	4627	ILE	Peptide
2	B	4751	PHE	Peptide
2	B	657	PRO	Peptide
2	B	728	ASP	Peptide
2	B	739	ARG	Peptide
2	B	748	LEU	Peptide
2	B	777	GLY	Peptide
2	B	818	GLY	Peptide
2	B	819	TYR	Peptide
2	B	838	ARG	Peptide
2	D	105	ALA	Peptide
2	D	142	LYS	Peptide
2	D	1475	LYS	Peptide
2	D	1579	VAL	Peptide
2	D	1607	ASP	Peptide
2	D	1635	GLU	Peptide
2	D	1756	SER	Peptide
2	D	1758	ARG	Peptide
2	D	1777	GLN	Peptide
2	D	1835	HIS	Peptide
2	D	1847	GLU	Peptide
2	D	2075	VAL	Peptide
2	D	221	SER	Peptide
2	D	2232	SER	Peptide

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Mol	Chain	Res	Type	Group
2	D	2462	CYS	Peptide
2	D	321	LYS	Peptide
2	D	4070	CYS	Peptide
2	D	4074	ASP	Peptide
2	D	4594	LEU	Peptide
2	D	4627	ILE	Peptide
2	D	4751	PHE	Peptide
2	D	657	PRO	Peptide
2	D	728	ASP	Peptide
2	D	739	ARG	Peptide
2	D	748	LEU	Peptide
2	D	777	GLY	Peptide
2	D	818	GLY	Peptide
2	D	819	TYR	Peptide
2	D	838	ARG	Peptide
2	F	105	ALA	Peptide
2	F	142	LYS	Peptide
2	F	1475	LYS	Peptide
2	F	1579	VAL	Peptide
2	F	1607	ASP	Peptide
2	F	1635	GLU	Peptide
2	F	1756	SER	Peptide
2	F	1758	ARG	Peptide
2	F	1777	GLN	Peptide
2	F	1835	HIS	Peptide
2	F	1847	GLU	Peptide
2	F	2075	VAL	Peptide
2	F	221	SER	Peptide
2	F	2232	SER	Peptide
2	F	2462	CYS	Peptide
2	F	321	LYS	Peptide
2	F	4070	CYS	Peptide
2	F	4074	ASP	Peptide
2	F	4594	LEU	Peptide
2	F	4627	ILE	Peptide
2	F	4751	PHE	Peptide
2	F	657	PRO	Peptide
2	F	728	ASP	Peptide
2	F	739	ARG	Peptide
2	F	748	LEU	Peptide
2	F	777	GLY	Peptide
2	F	818	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	F	819	TYR	Peptide
2	F	838	ARG	Peptide
2	H	105	ALA	Peptide
2	H	142	LYS	Peptide
2	H	1475	LYS	Peptide
2	H	1579	VAL	Peptide
2	H	1607	ASP	Peptide
2	H	1635	GLU	Peptide
2	H	1756	SER	Peptide
2	H	1758	ARG	Peptide
2	H	1777	GLN	Peptide
2	H	1835	HIS	Peptide
2	H	1847	GLU	Peptide
2	H	2075	VAL	Peptide
2	H	221	SER	Peptide
2	H	2232	SER	Peptide
2	H	2462	CYS	Peptide
2	H	321	LYS	Peptide
2	H	4070	CYS	Peptide
2	H	4074	ASP	Peptide
2	H	4594	LEU	Peptide
2	H	4627	ILE	Peptide
2	H	4751	PHE	Peptide
2	H	657	PRO	Peptide
2	H	728	ASP	Peptide
2	H	739	ARG	Peptide
2	H	748	LEU	Peptide
2	H	777	GLY	Peptide
2	H	818	GLY	Peptide
2	H	819	TYR	Peptide
2	H	838	ARG	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	819	0	824	25	0
1	C	819	0	824	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	819	0	824	26	0
1	G	819	0	824	24	0
2	B	26636	0	25174	691	0
2	D	26636	0	25174	687	0
2	F	26636	0	25174	695	0
2	H	26636	0	25174	703	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	109824	0	103992	2593	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 (2593) 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)
2:F:4520:PHE:CD1	2:F:4562:LEU:HD21	1.50	1.47
2:B:4520:PHE:CD1	2:B:4562:LEU:HD21	1.50	1.47
2:D:4520:PHE:CD1	2:D:4562:LEU:HD21	1.50	1.46
2:H:4520:PHE:CD1	2:H:4562:LEU:HD21	1.50	1.44
2:B:4808:ASP:HB3	2:D:4523:VAL:CG2	1.55	1.36
2:F:207:PHE:CZ	2:H:2326:ILE:HG23	1.60	1.35
2:D:4808:ASP:HB3	2:F:4523:VAL:CG2	1.54	1.35
2:B:2326:ILE:HG23	2:H:207:PHE:CZ	1.61	1.34
2:D:207:PHE:CZ	2:F:2326:ILE:HG23	1.60	1.34
2:B:4523:VAL:CG2	2:H:4808:ASP:HB3	1.57	1.34
2:B:207:PHE:CZ	2:D:2326:ILE:HG23	1.61	1.33
2:F:4808:ASP:HB3	2:H:4523:VAL:CG2	1.58	1.30
2:B:4902:VAL:HG12	2:B:4903:PRO:CD	1.65	1.27
2:H:4902:VAL:HG12	2:H:4903:PRO:CD	1.64	1.25
2:F:4902:VAL:HG12	2:F:4903:PRO:CD	1.64	1.25
2:D:4902:VAL:HG12	2:D:4903:PRO:CD	1.67	1.25
2:H:4779:VAL:HG11	2:H:4818:MET:SD	1.86	1.16
2:B:4808:ASP:CG	2:D:4523:VAL:HG21	1.72	1.15
2:B:4779:VAL:HG11	2:B:4818:MET:SD	1.86	1.15
2:F:4779:VAL:HG11	2:F:4818:MET:SD	1.86	1.14
2:F:4808:ASP:HB3	2:H:4523:VAL:HG23	1.23	1.14
2:B:4523:VAL:HG23	2:H:4808:ASP:HB3	1.19	1.14
2:D:4808:ASP:CG	2:F:4523:VAL:HG21	1.73	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4779:VAL:HG11	2:D:4818:MET:SD	1.86	1.13
2:B:4523:VAL:HG21	2:H:4808:ASP:CG	1.73	1.13
2:B:4808:ASP:HB3	2:D:4523:VAL:HG23	1.18	1.12
2:B:4808:ASP:CB	2:D:4523:VAL:HG21	1.79	1.12
2:D:4808:ASP:CB	2:F:4523:VAL:HG21	1.79	1.12
2:D:4808:ASP:HB3	2:F:4523:VAL:HG23	1.19	1.11
2:D:207:PHE:CE2	2:F:2326:ILE:HG23	1.86	1.10
2:F:207:PHE:CE2	2:H:2326:ILE:HG23	1.85	1.10
2:B:4523:VAL:HG21	2:H:4808:ASP:CB	1.82	1.09
2:D:207:PHE:CE1	2:F:2326:ILE:HG23	1.86	1.09
2:F:207:PHE:CE1	2:H:2326:ILE:HG23	1.87	1.09
2:F:4808:ASP:CG	2:H:4523:VAL:HG21	1.76	1.09
2:B:2326:ILE:HG23	2:H:207:PHE:CE1	1.87	1.08
2:B:207:PHE:CE2	2:D:2326:ILE:HG23	1.89	1.07
2:B:2326:ILE:HG23	2:H:207:PHE:CE2	1.87	1.07
2:B:207:PHE:CE1	2:D:2326:ILE:HG23	1.87	1.07
2:F:4808:ASP:CB	2:H:4523:VAL:HG21	1.83	1.06
2:D:4808:ASP:CB	2:F:4523:VAL:CG2	2.34	1.05
2:B:4774:LEU:CD2	2:D:4754:LEU:HD21	1.86	1.05
2:B:4808:ASP:CB	2:D:4523:VAL:CG2	2.34	1.05
2:B:4754:LEU:HD21	2:H:4774:LEU:CD2	1.87	1.04
2:B:4523:VAL:CG2	2:H:4808:ASP:CB	2.36	1.03
2:D:4774:LEU:CD2	2:F:4754:LEU:HD21	1.89	1.03
2:F:4774:LEU:CD2	2:H:4754:LEU:HD21	1.88	1.03
2:D:4902:VAL:CG1	2:D:4903:PRO:HD2	1.89	1.03
2:H:4902:VAL:CG1	2:H:4903:PRO:HD2	1.89	1.02
2:D:207:PHE:CE1	2:F:2326:ILE:CG2	2.42	1.02
2:B:4902:VAL:CG1	2:B:4903:PRO:HD2	1.89	1.02
2:D:4808:ASP:HB3	2:F:4523:VAL:HG21	1.37	1.02
2:B:2326:ILE:CG2	2:H:207:PHE:CE1	2.43	1.01
2:F:4902:VAL:CG1	2:F:4903:PRO:HD2	1.89	1.01
2:B:207:PHE:CE1	2:D:2326:ILE:CG2	2.44	1.01
2:F:207:PHE:CE1	2:H:2326:ILE:CG2	2.42	1.01
2:H:4902:VAL:HG12	2:H:4903:PRO:HD2	1.00	0.99
2:F:4902:VAL:HG12	2:F:4903:PRO:HD2	0.99	0.99
2:F:4808:ASP:CB	2:H:4523:VAL:CG2	2.38	0.98
2:B:4902:VAL:HG12	2:B:4903:PRO:HD2	0.99	0.98
2:F:4520:PHE:HD1	2:F:4562:LEU:CD2	1.76	0.98
2:B:4774:LEU:HD22	2:D:4754:LEU:CD2	1.93	0.98
2:H:4520:PHE:CD1	2:H:4562:LEU:CD2	2.46	0.98
2:H:4520:PHE:HD1	2:H:4562:LEU:CD2	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4520:PHE:HB3	2:B:4562:LEU:HD23	1.45	0.98
2:B:4754:LEU:CD2	2:H:4774:LEU:HD22	1.93	0.98
2:D:4520:PHE:CD1	2:D:4562:LEU:CD2	2.46	0.98
2:D:4520:PHE:HD1	2:D:4562:LEU:CD2	1.76	0.98
2:D:4774:LEU:HD22	2:F:4754:LEU:HD21	0.99	0.98
2:F:4774:LEU:HD22	2:H:4754:LEU:CD2	1.94	0.97
2:B:4520:PHE:CD1	2:B:4562:LEU:CD2	2.46	0.97
2:D:4902:VAL:HG12	2:D:4903:PRO:HD2	0.97	0.97
2:F:4520:PHE:HB3	2:F:4562:LEU:HD23	1.45	0.97
2:D:207:PHE:CZ	2:F:2326:ILE:HD12	2.00	0.97
2:F:4520:PHE:CD1	2:F:4562:LEU:CD2	2.46	0.97
2:F:4774:LEU:HD22	2:H:4754:LEU:HD21	0.97	0.97
2:H:4520:PHE:HB3	2:H:4562:LEU:HD23	1.45	0.97
2:B:4520:PHE:HD1	2:B:4562:LEU:CD2	1.76	0.97
2:D:207:PHE:CZ	2:F:2326:ILE:CG2	2.48	0.96
2:F:207:PHE:CZ	2:H:2326:ILE:CG2	2.48	0.96
2:F:4808:ASP:HB3	2:H:4523:VAL:HG21	1.40	0.96
2:F:207:PHE:CZ	2:H:2326:ILE:HD12	2.01	0.95
2:B:4754:LEU:HD21	2:H:4774:LEU:HD22	0.96	0.95
2:B:4808:ASP:HB3	2:D:4523:VAL:HG21	1.39	0.95
2:B:2326:ILE:HD12	2:H:207:PHE:CZ	2.02	0.95
2:D:4520:PHE:HB3	2:D:4562:LEU:HD23	1.45	0.95
2:B:207:PHE:CZ	2:D:2326:ILE:CG2	2.50	0.94
2:B:2326:ILE:CG2	2:H:207:PHE:CZ	2.50	0.94
2:B:207:PHE:CZ	2:D:2326:ILE:HD12	2.03	0.94
2:B:4774:LEU:HD22	2:D:4754:LEU:HD21	0.96	0.92
2:D:4865:GLY:HA2	2:F:4868:ILE:HG12	1.54	0.90
2:F:4857:VAL:HG22	2:H:4863:ILE:HG21	1.53	0.90
2:B:4863:ILE:HG21	2:H:4857:VAL:HG22	1.55	0.89
2:B:4865:GLY:HA2	2:D:4868:ILE:HG12	1.55	0.89
2:D:4774:LEU:HD22	2:F:4754:LEU:CD2	1.96	0.89
2:F:4865:GLY:HA2	2:H:4868:ILE:HG12	1.55	0.88
2:B:4868:ILE:HG12	2:H:4865:GLY:HA2	1.56	0.88
2:B:4857:VAL:HG22	2:D:4863:ILE:HG21	1.53	0.88
2:D:4857:VAL:HG22	2:F:4863:ILE:HG21	1.54	0.87
2:F:4902:VAL:CG1	2:F:4903:PRO:CD	2.52	0.86
2:F:4857:VAL:HG13	2:H:4863:ILE:CG2	2.07	0.85
2:B:4902:VAL:CG1	2:B:4903:PRO:CD	2.52	0.85
2:D:4857:VAL:HG13	2:F:4863:ILE:CG2	2.07	0.84
2:H:4902:VAL:CG1	2:H:4903:PRO:CD	2.51	0.84
2:D:76:ARG:CB	2:F:3891:TRP:HB3	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:ARG:CB	2:H:3891:TRP:HB3	2.08	0.83
2:B:4857:VAL:HG13	2:D:4863:ILE:CG2	2.09	0.82
2:B:4863:ILE:CG2	2:H:4857:VAL:HG13	2.10	0.82
2:B:3891:TRP:HB3	2:H:76:ARG:CB	2.10	0.81
2:D:207:PHE:CE2	2:F:2326:ILE:HD12	2.15	0.81
2:F:207:PHE:CE2	2:H:2326:ILE:HD12	2.16	0.80
2:F:4520:PHE:HB3	2:F:4562:LEU:CD2	2.12	0.80
2:H:4520:PHE:HB3	2:H:4562:LEU:CD2	2.12	0.80
2:B:76:ARG:CB	2:D:3891:TRP:HB3	2.11	0.80
2:D:4520:PHE:HB3	2:D:4562:LEU:CD2	2.12	0.79
2:B:4520:PHE:HB3	2:B:4562:LEU:CD2	2.12	0.79
2:F:4779:VAL:CG1	2:F:4818:MET:SD	2.71	0.79
2:B:207:PHE:CE2	2:D:2326:ILE:HD12	2.19	0.78
2:H:4627:ILE:O	2:H:4631:TRP:HB2	1.84	0.78
2:B:4627:ILE:O	2:B:4631:TRP:HB2	1.84	0.78
2:F:4520:PHE:CG	2:F:4562:LEU:HD21	2.17	0.78
2:B:2326:ILE:HD12	2:H:207:PHE:CE2	2.17	0.78
2:H:4520:PHE:CG	2:H:4562:LEU:HD21	2.17	0.78
2:D:4902:VAL:CG1	2:D:4903:PRO:CD	2.54	0.77
2:F:4857:VAL:CG2	2:H:4863:ILE:HG21	2.14	0.77
2:B:4857:VAL:CG2	2:D:4863:ILE:HG21	2.15	0.77
2:F:4627:ILE:O	2:F:4631:TRP:HB2	1.84	0.77
2:H:4779:VAL:CG1	2:H:4818:MET:SD	2.71	0.77
2:F:4857:VAL:HG13	2:H:4863:ILE:HB	1.67	0.77
2:B:4779:VAL:CG1	2:B:4818:MET:SD	2.71	0.76
2:D:4520:PHE:CG	2:D:4562:LEU:HD21	2.17	0.76
2:D:4810:MET:HG2	2:F:4521:TYR:HB2	1.65	0.76
2:B:4810:MET:HG2	2:D:4521:TYR:HB2	1.66	0.76
2:D:4627:ILE:O	2:D:4631:TRP:HB2	1.84	0.76
2:H:4902:VAL:HG12	2:H:4903:PRO:HD3	1.66	0.76
2:D:207:PHE:CD1	2:F:2326:ILE:CG2	2.69	0.75
2:B:4520:PHE:CG	2:B:4562:LEU:HD21	2.17	0.75
2:D:4779:VAL:CG1	2:D:4818:MET:SD	2.71	0.75
2:B:4521:TYR:HB2	2:H:4810:MET:HG2	1.68	0.75
2:D:4857:VAL:CG2	2:F:4863:ILE:HG21	2.16	0.75
2:B:4863:ILE:HG21	2:H:4857:VAL:CG2	2.16	0.74
2:B:4863:ILE:HB	2:H:4857:VAL:HG13	1.70	0.74
2:F:4810:MET:HG2	2:H:4521:TYR:HB2	1.69	0.74
2:B:2326:ILE:CG2	2:H:207:PHE:CD1	2.71	0.73
2:F:76:ARG:CB	2:H:3891:TRP:CB	2.66	0.73
2:B:4857:VAL:HG13	2:D:4863:ILE:HB	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4848:ASP:HB3	2:H:4819:TYR:HE1	1.53	0.73
2:F:4902:VAL:HG12	2:F:4903:PRO:HD3	1.67	0.73
2:B:4814:TYR:CE2	2:B:4815:MET:HE2	2.24	0.73
2:D:4046:LYS:H	2:D:4077:GLU:HB3	1.54	0.73
2:F:207:PHE:CD1	2:H:2326:ILE:CG2	2.70	0.73
2:B:4515:ASN:ND2	2:H:4780:TYR:CE2	2.56	0.73
2:D:190:ARG:NH1	2:F:2423:ILE:HG23	2.04	0.73
2:F:4857:VAL:HG13	2:H:4863:ILE:CB	2.19	0.73
2:B:4902:VAL:HG12	2:B:4903:PRO:HD3	1.68	0.73
2:B:4780:TYR:CE2	2:D:4515:ASN:ND2	2.56	0.73
2:F:4814:TYR:CE2	2:F:4815:MET:HE2	2.24	0.73
2:D:76:ARG:CB	2:F:3891:TRP:CB	2.66	0.72
2:D:4814:TYR:CE2	2:D:4815:MET:HE2	2.23	0.72
2:F:4046:LYS:H	2:F:4077:GLU:HB3	1.54	0.72
2:D:4857:VAL:HG13	2:F:4863:ILE:HB	1.71	0.72
2:F:190:ARG:NH1	2:H:2423:ILE:HG23	2.04	0.72
2:H:4046:LYS:H	2:H:4077:GLU:HB3	1.54	0.72
2:H:4814:TYR:CE2	2:H:4815:MET:HE2	2.24	0.72
2:D:4848:ASP:HB3	2:F:4819:TYR:HE1	1.55	0.72
2:B:3891:TRP:CB	2:H:76:ARG:CB	2.68	0.71
2:B:207:PHE:CD1	2:D:2326:ILE:CG2	2.72	0.71
2:B:4046:LYS:H	2:B:4077:GLU:HB3	1.54	0.71
2:B:4848:ASP:HB3	2:D:4819:TYR:HE1	1.56	0.71
2:D:4851:PHE:O	2:D:4855:VAL:HB	1.91	0.71
2:F:77:ALA:HB2	2:H:3891:TRP:CZ2	2.26	0.71
2:D:77:ALA:HB2	2:F:3891:TRP:CZ2	2.25	0.71
2:F:4851:PHE:O	2:F:4855:VAL:HB	1.91	0.71
2:D:1111:GLY:HA3	2:D:1211:GLN:HE21	1.56	0.71
2:B:76:ARG:CB	2:D:3891:TRP:CB	2.69	0.71
2:D:4865:GLY:HA2	2:F:4868:ILE:CG1	2.20	0.71
2:F:1138:ASP:HB2	2:F:1145:TRP:HE1	1.56	0.71
2:B:2344:LEU:O	2:B:2348:MET:HB2	1.91	0.70
2:B:1111:GLY:HA3	2:B:1211:GLN:HE21	1.56	0.70
2:B:4851:PHE:O	2:B:4855:VAL:HB	1.91	0.70
2:H:1138:ASP:HB2	2:H:1145:TRP:HE1	1.56	0.70
2:B:2423:ILE:HG23	2:H:190:ARG:NH1	2.05	0.70
2:D:4857:VAL:HG13	2:F:4863:ILE:CB	2.22	0.70
2:H:4851:PHE:O	2:H:4855:VAL:HB	1.91	0.70
2:B:4857:VAL:HG13	2:D:4863:ILE:CB	2.21	0.70
2:H:1111:GLY:HA3	2:H:1211:GLN:HE21	1.56	0.70
2:F:4865:GLY:HA2	2:H:4868:ILE:CG1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4863:ILE:CB	2:H:4857:VAL:HG13	2.22	0.70
2:F:4780:TYR:CE2	2:H:4515:ASN:ND2	2.59	0.70
2:B:190:ARG:NH1	2:D:2423:ILE:HG23	2.06	0.70
2:D:4780:TYR:CE2	2:F:4515:ASN:ND2	2.58	0.70
2:F:2344:LEU:O	2:F:2348:MET:HB2	1.91	0.70
2:B:3891:TRP:CZ2	2:H:77:ALA:HB2	2.27	0.69
2:F:1242:ASN:HB3	2:F:1807:ARG:HB2	1.75	0.69
2:D:1138:ASP:HB2	2:D:1145:TRP:HE1	1.56	0.69
2:D:2344:LEU:O	2:D:2348:MET:HB2	1.91	0.69
2:B:1138:ASP:HB2	2:B:1145:TRP:HE1	1.56	0.69
2:H:1242:ASN:HB3	2:H:1807:ARG:HB2	1.74	0.69
2:H:2344:LEU:O	2:H:2348:MET:HB2	1.91	0.69
2:B:4819:TYR:HE1	2:H:4848:ASP:HB3	1.57	0.69
2:B:4861:ALA:HB1	2:D:4867:ILE:HG21	1.75	0.69
2:B:4868:ILE:CG1	2:H:4865:GLY:HA2	2.23	0.69
2:B:77:ALA:HB2	2:D:3891:TRP:CZ2	2.28	0.69
2:F:1111:GLY:HA3	2:F:1211:GLN:HE21	1.56	0.68
2:D:1242:ASN:HB3	2:D:1807:ARG:HB2	1.74	0.68
2:B:1242:ASN:HB3	2:B:1807:ARG:HB2	1.74	0.68
2:F:4857:VAL:CG1	2:H:4863:ILE:CG2	2.70	0.68
2:F:4861:ALA:HB1	2:H:4867:ILE:HG21	1.75	0.68
2:B:4865:GLY:HA2	2:D:4868:ILE:CG1	2.22	0.68
2:B:545:ARG:HH21	2:B:583:PRO:HG3	1.60	0.67
2:D:4857:VAL:CG1	2:F:4863:ILE:CG2	2.72	0.67
2:F:394:HIS:HD2	2:F:397:GLY:H	1.43	0.67
2:B:4867:ILE:HG21	2:H:4861:ALA:HB1	1.77	0.67
2:D:207:PHE:CD2	2:F:2326:ILE:HG23	2.30	0.67
2:D:545:ARG:HH21	2:D:583:PRO:HG3	1.60	0.67
2:B:4857:VAL:CG1	2:D:4863:ILE:CG2	2.73	0.67
2:D:4861:ALA:HB1	2:F:4867:ILE:HG21	1.76	0.67
2:B:262:TYR:HB2	2:B:389:ARG:HB3	1.77	0.67
2:D:394:HIS:HD2	2:D:397:GLY:H	1.43	0.67
2:D:4767:GLN:HG2	2:F:4753:THR:OG1	1.95	0.66
2:H:545:ARG:HH21	2:H:583:PRO:HG3	1.60	0.66
2:B:4863:ILE:CG2	2:H:4857:VAL:CG1	2.73	0.66
2:B:244:CYS:SG	2:B:245:LEU:N	2.69	0.66
2:B:4865:GLY:CA	2:D:4868:ILE:HG12	2.26	0.66
2:D:244:CYS:SG	2:D:245:LEU:N	2.69	0.66
2:D:4902:VAL:HG12	2:D:4903:PRO:HD3	1.75	0.66
2:H:748:LEU:HD13	2:H:750:ARG:HE	1.61	0.66
2:F:545:ARG:HH21	2:F:583:PRO:HG3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4518:LEU:HD13	2:D:4521:TYR:CE2	2.31	0.66
2:F:207:PHE:CD2	2:H:2326:ILE:HG23	2.30	0.66
2:B:1431:ARG:HE	2:B:1505:LEU:HD21	1.60	0.66
2:D:1431:ARG:HE	2:D:1505:LEU:HD21	1.60	0.66
2:F:4518:LEU:HD13	2:F:4521:TYR:CE2	2.31	0.66
2:B:394:HIS:HD2	2:B:397:GLY:H	1.43	0.66
2:B:748:LEU:HD13	2:B:750:ARG:HE	1.61	0.66
2:D:262:TYR:HB2	2:D:389:ARG:HB3	1.77	0.66
2:H:244:CYS:SG	2:H:245:LEU:N	2.69	0.66
2:F:1431:ARG:HE	2:F:1505:LEU:HD21	1.60	0.66
2:F:244:CYS:SG	2:F:245:LEU:N	2.69	0.65
2:B:4767:GLN:HG2	2:D:4753:THR:OG1	1.96	0.65
2:H:262:TYR:HB2	2:H:389:ARG:HB3	1.77	0.65
2:H:1445:TRP:H	2:H:1487:MET:HB2	1.62	0.65
2:B:1445:TRP:H	2:B:1487:MET:HB2	1.62	0.65
2:D:144:ALA:HB1	2:D:206:ALA:HA	1.78	0.65
2:H:1431:ARG:HE	2:H:1505:LEU:HD21	1.60	0.65
2:D:1445:TRP:H	2:D:1487:MET:HB2	1.61	0.65
2:D:1482:ARG:HH11	2:D:1531:TYR:HA	1.61	0.65
2:F:1482:ARG:HH11	2:F:1531:TYR:HA	1.61	0.65
2:H:1117:TRP:HE1	2:H:1164:CYS:HB3	1.62	0.65
2:B:144:ALA:HB1	2:B:206:ALA:HA	1.78	0.65
2:F:1445:TRP:H	2:F:1487:MET:HB2	1.62	0.65
2:D:2891:GLN:HB3	2:D:2895:LYS:HE2	1.79	0.65
2:F:262:TYR:HB2	2:F:389:ARG:HB3	1.77	0.65
2:F:748:LEU:HD13	2:F:750:ARG:HE	1.61	0.65
2:D:3970:LYS:HA	2:D:3973:MET:HE2	1.79	0.65
2:F:144:ALA:HB1	2:F:206:ALA:HA	1.78	0.64
2:D:4810:MET:CG	2:F:4521:TYR:HB2	2.26	0.64
2:H:1703:TYR:HD2	2:H:1820:PRO:HB2	1.63	0.64
2:H:4518:LEU:HD13	2:H:4521:TYR:CE2	2.31	0.64
2:B:4518:LEU:HD13	2:B:4521:TYR:CE2	2.31	0.64
2:B:4753:THR:OG1	2:H:4767:GLN:HG2	1.98	0.64
2:F:4767:GLN:HG2	2:H:4753:THR:OG1	1.98	0.64
2:B:2891:GLN:HB3	2:B:2895:LYS:HE2	1.79	0.64
2:F:1117:TRP:HE1	2:F:1164:CYS:HB3	1.62	0.64
1:G:40:ARG:HH12	2:H:685:PHE:HB3	1.63	0.64
2:D:4511:ALA:HA	2:D:4514:ILE:HD12	1.80	0.64
2:H:1482:ARG:HH11	2:H:1531:TYR:HA	1.61	0.64
2:D:1117:TRP:HE1	2:D:1164:CYS:HB3	1.62	0.64
1:E:40:ARG:HH12	2:F:685:PHE:HB3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:374:TYR:HA	2:F:391:ALA:HA	1.80	0.64
2:H:3970:LYS:HA	2:H:3973:MET:HE2	1.79	0.64
2:B:2770:GLU:HA	2:B:2773:ARG:HB2	1.80	0.64
2:D:748:LEU:HD13	2:D:750:ARG:HE	1.61	0.64
2:F:4511:ALA:HA	2:F:4514:ILE:HD12	1.80	0.64
2:H:144:ALA:HB1	2:H:206:ALA:HA	1.78	0.64
2:D:300:VAL:O	2:D:420:ARG:NH1	2.31	0.64
2:D:2770:GLU:HA	2:D:2773:ARG:HB2	1.80	0.64
2:H:374:TYR:HA	2:H:391:ALA:HA	1.80	0.64
2:B:2326:ILE:HG23	2:H:207:PHE:CD2	2.32	0.63
2:B:4511:ALA:HA	2:B:4514:ILE:HD12	1.80	0.63
2:B:4810:MET:CG	2:D:4521:TYR:HB2	2.28	0.63
2:H:394:HIS:HD2	2:H:397:GLY:H	1.43	0.63
2:B:1165:MET:HB2	2:B:1174:MET:HB2	1.81	0.63
2:B:1482:ARG:HH11	2:B:1531:TYR:HA	1.61	0.63
2:B:1703:TYR:HD2	2:B:1820:PRO:HB2	1.63	0.63
2:F:207:PHE:CD1	2:H:2326:ILE:HG23	2.32	0.63
2:B:4868:ILE:HG12	2:H:4865:GLY:CA	2.27	0.63
2:F:2891:GLN:HB3	2:F:2895:LYS:HE2	1.79	0.63
2:H:1165:MET:HB2	2:H:1174:MET:HB2	1.81	0.63
2:B:3970:LYS:HA	2:B:3973:MET:HE2	1.79	0.63
2:F:1114:ARG:HB2	2:F:1206:SER:HB3	1.81	0.63
2:F:3970:LYS:HA	2:F:3973:MET:HE2	1.79	0.63
2:H:2891:GLN:HB3	2:H:2895:LYS:HE2	1.79	0.63
2:F:1703:TYR:HD2	2:F:1820:PRO:HB2	1.63	0.63
2:H:2770:GLU:HA	2:H:2773:ARG:HB2	1.80	0.63
2:H:4511:ALA:HA	2:H:4514:ILE:HD12	1.80	0.63
1:A:40:ARG:HH12	2:B:685:PHE:HB3	1.63	0.63
1:C:87:HIS:H	1:C:91:ILE:HB	1.64	0.63
2:D:207:PHE:CD1	2:F:2326:ILE:HG23	2.30	0.63
1:G:31:GLN:HB2	1:G:96:THR:HB	1.81	0.63
2:H:4520:PHE:CB	2:H:4562:LEU:CD2	2.77	0.63
2:D:1165:MET:HB2	2:D:1174:MET:HB2	1.81	0.63
2:B:207:PHE:CD2	2:D:2326:ILE:HG23	2.34	0.63
2:B:1117:TRP:HE1	2:B:1164:CYS:HB3	1.62	0.63
1:C:40:ARG:HH12	2:D:685:PHE:HB3	1.63	0.63
2:F:2770:GLU:HA	2:F:2773:ARG:HB2	1.80	0.63
2:F:4520:PHE:CB	2:F:4562:LEU:CD2	2.77	0.63
2:H:300:VAL:O	2:H:420:ARG:NH1	2.31	0.63
2:H:1610:ARG:NH1	2:H:1612:SER:OG	2.32	0.63
1:A:31:GLN:HB2	1:A:96:THR:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:TYR:HA	2:B:391:ALA:HA	1.80	0.62
2:B:1114:ARG:HB2	2:B:1206:SER:HB3	1.81	0.62
2:D:4848:ASP:OD2	2:F:4819:TYR:CE1	2.52	0.62
2:F:4865:GLY:CA	2:H:4868:ILE:HG12	2.25	0.62
1:A:87:HIS:H	1:A:91:ILE:HB	1.64	0.62
2:F:4047:ARG:NH1	2:F:4077:GLU:OE2	2.33	0.62
2:B:300:VAL:O	2:B:420:ARG:NH1	2.31	0.62
2:B:4047:ARG:NH1	2:B:4077:GLU:OE2	2.33	0.62
2:D:374:TYR:HA	2:D:391:ALA:HA	1.80	0.62
2:B:1610:ARG:NH1	2:B:1612:SER:OG	2.32	0.62
1:E:87:HIS:H	1:E:91:ILE:HB	1.64	0.62
2:F:1165:MET:HB2	2:F:1174:MET:HB2	1.81	0.62
2:D:4865:GLY:CA	2:F:4868:ILE:HG12	2.25	0.62
2:F:1137:PHE:HA	2:F:1144:ARG:HA	1.82	0.62
2:D:1137:PHE:HA	2:D:1144:ARG:HA	1.82	0.62
2:H:4047:ARG:NH1	2:H:4077:GLU:OE2	2.33	0.62
2:D:1114:ARG:HB2	2:D:1206:SER:HB3	1.81	0.62
2:B:4521:TYR:HB2	2:H:4810:MET:CG	2.29	0.62
1:C:31:GLN:HB2	1:C:96:THR:HB	1.81	0.62
2:D:1703:TYR:HD2	2:D:1820:PRO:HB2	1.63	0.62
1:E:31:GLN:HB2	1:E:96:THR:HB	1.81	0.62
2:H:1114:ARG:HB2	2:H:1206:SER:HB3	1.81	0.62
2:H:1137:PHE:HA	2:H:1144:ARG:HA	1.82	0.62
2:D:1153:GLY:HA3	2:D:1182:LEU:HB3	1.82	0.62
2:D:4520:PHE:CB	2:D:4562:LEU:CD2	2.77	0.62
2:F:677:LEU:HB2	2:F:755:ILE:HB	1.82	0.62
2:F:1610:ARG:NH1	2:F:1612:SER:OG	2.32	0.62
2:F:4810:MET:CG	2:H:4521:TYR:HB2	2.30	0.62
2:F:1153:GLY:HA3	2:F:1182:LEU:HB3	1.82	0.61
2:D:677:LEU:HB2	2:D:755:ILE:HB	1.82	0.61
2:D:4047:ARG:NH1	2:D:4077:GLU:OE2	2.33	0.61
2:D:4874:LEU:O	2:D:4878:GLN:NE2	2.33	0.61
2:B:1153:GLY:HA3	2:B:1182:LEU:HB3	1.82	0.61
2:D:1250:TRP:HE1	2:D:1643:GLU:HG3	1.65	0.61
2:F:1670:HIS:ND1	2:F:1778:TYR:O	2.34	0.61
2:F:4148:ARG:NH2	2:F:4150:TYR:OH	2.33	0.61
2:F:4874:LEU:O	2:F:4878:GLN:NE2	2.33	0.61
2:H:1153:GLY:HA3	2:H:1182:LEU:HB3	1.82	0.61
2:D:4148:ARG:NH2	2:D:4150:TYR:OH	2.33	0.61
2:B:1101:TRP:HA	2:B:1237:GLU:HB2	1.82	0.61
2:D:1670:HIS:ND1	2:D:1778:TYR:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2127:ILE:HD11	2:H:2143:MET:HG3	1.83	0.61
2:B:1137:PHE:HA	2:B:1144:ARG:HA	1.82	0.61
2:B:2326:ILE:HG23	2:H:207:PHE:CD1	2.32	0.61
1:G:87:HIS:H	1:G:91:ILE:HB	1.64	0.61
2:B:1761:MET:SD	2:B:1761:MET:N	2.73	0.61
2:B:4520:PHE:CB	2:B:4562:LEU:CD2	2.77	0.61
2:D:1610:ARG:NH1	2:D:1612:SER:OG	2.32	0.61
2:F:300:VAL:O	2:F:420:ARG:NH1	2.31	0.61
2:B:4874:LEU:O	2:B:4878:GLN:NE2	2.33	0.61
2:H:677:LEU:HB2	2:H:755:ILE:HB	1.82	0.61
2:H:1250:TRP:HE1	2:H:1643:GLU:HG3	1.65	0.61
2:B:2127:ILE:HD11	2:B:2143:MET:HG3	1.83	0.61
2:F:4848:ASP:OD2	2:H:4819:TYR:CE1	2.54	0.61
2:B:1427:TYR:HA	2:B:1509:CYS:HA	1.83	0.61
2:H:4874:LEU:O	2:H:4878:GLN:NE2	2.33	0.61
2:D:1427:TYR:HA	2:D:1509:CYS:HA	1.83	0.60
2:F:1250:TRP:HE1	2:F:1643:GLU:HG3	1.65	0.60
2:B:1250:TRP:HE1	2:B:1643:GLU:HG3	1.65	0.60
2:B:4517:ILE:O	2:B:4519:LEU:N	2.32	0.60
2:F:1427:TYR:HA	2:F:1509:CYS:HA	1.83	0.60
2:B:1670:HIS:ND1	2:B:1778:TYR:O	2.34	0.60
2:D:1258:PHE:HB2	2:D:1593:HIS:HB3	1.83	0.60
2:H:1116:GLY:HA3	2:H:1136:ALA:HA	1.84	0.60
2:D:1101:TRP:HA	2:D:1237:GLU:HB2	1.83	0.60
2:B:1116:GLY:HA3	2:B:1136:ALA:HA	1.84	0.60
2:B:4814:TYR:HE2	2:B:4815:MET:HE2	1.66	0.60
2:D:188:SER:HB2	2:D:190:ARG:HH21	1.67	0.60
2:F:1258:PHE:HB2	2:F:1593:HIS:HB3	1.83	0.60
2:H:1670:HIS:ND1	2:H:1778:TYR:O	2.34	0.60
2:B:677:LEU:HB2	2:B:755:ILE:HB	1.82	0.60
2:B:4148:ARG:NH2	2:B:4150:TYR:OH	2.33	0.60
2:D:1116:GLY:HA3	2:D:1136:ALA:HA	1.84	0.60
2:D:1726:ILE:HD11	2:D:2121:LEU:HD11	1.84	0.60
2:F:1124:PRO:HB2	2:F:1252:SER:HB3	1.83	0.60
2:H:1258:PHE:HB2	2:H:1593:HIS:HB3	1.83	0.60
2:H:1427:TYR:HA	2:H:1509:CYS:HA	1.83	0.60
2:H:1761:MET:SD	2:H:1761:MET:N	2.73	0.60
1:E:21:THR:H	1:E:107:GLU:HB2	1.67	0.60
2:F:2127:ILE:HD11	2:F:2143:MET:HG3	1.83	0.60
2:B:4848:ASP:OD2	2:D:4819:TYR:CE1	2.55	0.60
2:D:629:GLN:OE1	2:D:1669:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1124:PRO:HB2	2:D:1252:SER:HB3	1.83	0.60
2:H:1101:TRP:HA	2:H:1237:GLU:HB2	1.82	0.60
2:B:1726:ILE:HD11	2:B:2121:LEU:HD11	1.84	0.60
2:B:188:SER:HB2	2:B:190:ARG:HH21	1.67	0.59
2:D:2470:VAL:HG11	2:D:2523:THR:HG23	1.84	0.59
2:F:1116:GLY:HA3	2:F:1136:ALA:HA	1.84	0.59
1:G:21:THR:H	1:G:107:GLU:HB2	1.67	0.59
2:B:1258:PHE:HB2	2:B:1593:HIS:HB3	1.83	0.59
2:D:4814:TYR:HE2	2:D:4815:MET:HE2	1.66	0.59
2:F:756:SER:HB3	2:F:769:ARG:HB2	1.84	0.59
2:D:2127:ILE:HD11	2:D:2143:MET:HG3	1.83	0.59
2:F:298:ARG:HE	2:F:303:GLY:HA2	1.68	0.59
2:F:1809:PRO:HB3	2:F:1817:LEU:HB2	1.84	0.59
2:F:2470:VAL:HG11	2:F:2523:THR:HG23	1.85	0.59
2:F:4814:TYR:HE2	2:F:4815:MET:HE2	1.66	0.59
2:H:4517:ILE:O	2:H:4519:LEU:N	2.32	0.59
2:B:2470:VAL:HG11	2:B:2523:THR:HG23	1.85	0.59
2:F:636:LEU:HD21	2:F:643:LEU:HD21	1.85	0.59
2:F:4517:ILE:O	2:F:4519:LEU:N	2.32	0.59
2:H:4148:ARG:NH2	2:H:4150:TYR:OH	2.33	0.59
2:H:4814:TYR:HE2	2:H:4815:MET:HE2	1.66	0.59
2:D:4608:ALA:HB1	2:D:4650:VAL:HG11	1.84	0.59
2:H:629:GLN:OE1	2:H:1669:ASN:ND2	2.35	0.59
2:H:2470:VAL:HG11	2:H:2523:THR:HG23	1.84	0.59
2:H:4608:ALA:HB1	2:H:4650:VAL:HG11	1.84	0.59
2:B:4608:ALA:HB1	2:B:4650:VAL:HG11	1.84	0.59
2:F:4751:PHE:O	2:F:4755:ARG:NH1	2.36	0.59
2:F:247:VAL:O	2:F:272:ARG:NH1	2.36	0.59
2:F:1726:ILE:HD11	2:F:2121:LEU:HD11	1.84	0.59
2:H:247:VAL:O	2:H:272:ARG:NH1	2.36	0.59
2:H:1124:PRO:HB2	2:H:1252:SER:HB3	1.83	0.59
2:D:4866:LEU:HD12	2:F:4871:PHE:HE2	1.68	0.59
2:F:629:GLN:OE1	2:F:1669:ASN:ND2	2.35	0.59
2:F:1101:TRP:HA	2:F:1237:GLU:HB2	1.83	0.59
2:B:247:VAL:O	2:B:272:ARG:NH1	2.36	0.59
2:B:4819:TYR:CE1	2:H:4848:ASP:OD2	2.56	0.59
2:D:832:LEU:O	2:D:1614:ARG:NH1	2.36	0.59
2:D:1809:PRO:HB3	2:D:1817:LEU:HB2	1.84	0.59
2:F:4608:ALA:HB1	2:F:4650:VAL:HG11	1.84	0.59
2:F:4845:ILE:HG23	2:H:4819:TYR:CD1	2.38	0.59
2:H:756:SER:HB3	2:H:769:ARG:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1726:ILE:HD11	2:H:2121:LEU:HD11	1.84	0.59
2:B:1124:PRO:HB2	2:B:1252:SER:HB3	1.83	0.58
2:D:247:VAL:O	2:D:272:ARG:NH1	2.36	0.58
2:D:636:LEU:HD21	2:D:643:LEU:HD21	1.85	0.58
2:H:188:SER:HB2	2:H:190:ARG:HH21	1.67	0.58
2:H:298:ARG:HE	2:H:303:GLY:HA2	1.67	0.58
2:H:636:LEU:HD21	2:H:643:LEU:HD21	1.85	0.58
2:H:1809:PRO:HB3	2:H:1817:LEU:HB2	1.84	0.58
2:B:832:LEU:O	2:B:1614:ARG:NH1	2.36	0.58
1:C:21:THR:H	1:C:107:GLU:HB2	1.67	0.58
2:D:4751:PHE:O	2:D:4755:ARG:NH1	2.36	0.58
2:F:188:SER:HB2	2:F:190:ARG:HH21	1.67	0.58
2:H:4751:PHE:O	2:H:4755:ARG:NH1	2.36	0.58
2:B:150:GLN:NE2	2:B:158:CYS:SG	2.76	0.58
2:D:298:ARG:HE	2:D:303:GLY:HA2	1.68	0.58
2:F:832:LEU:O	2:F:1614:ARG:NH1	2.36	0.58
2:B:693:LEU:HD21	2:B:798:ILE:HG21	1.86	0.58
2:F:1121:GLY:O	2:F:1133:ARG:NH1	2.36	0.58
2:H:1589:GLN:NE2	2:H:1634:GLU:OE1	2.37	0.58
2:B:298:ARG:HE	2:B:303:GLY:HA2	1.68	0.58
2:B:629:GLN:OE1	2:B:1669:ASN:ND2	2.35	0.58
2:F:1589:GLN:NE2	2:F:1634:GLU:OE1	2.37	0.58
2:H:832:LEU:O	2:H:1614:ARG:NH1	2.36	0.58
2:H:248:PRO:O	2:H:257:ARG:NH2	2.37	0.58
1:A:21:THR:H	1:A:107:GLU:HB2	1.67	0.58
2:B:1809:PRO:HB3	2:B:1817:LEU:HB2	1.84	0.58
2:B:4751:PHE:O	2:B:4755:ARG:NH1	2.36	0.58
2:D:758:CYS:SG	2:D:759:LEU:N	2.77	0.58
2:F:4866:LEU:HD12	2:H:4871:PHE:HE2	1.69	0.58
2:B:248:PRO:O	2:B:257:ARG:NH2	2.37	0.58
2:H:693:LEU:HD21	2:H:798:ILE:HG21	1.86	0.58
2:F:802:PHE:HB2	2:F:1617:TRP:HB2	1.85	0.58
2:F:2142:LEU:HD23	2:F:2145:ARG:HD2	1.86	0.58
2:H:2142:LEU:HD23	2:H:2145:ARG:HD2	1.86	0.58
2:B:476:GLN:NE2	2:B:3679:GLU:OE1	2.37	0.58
2:B:2718:LEU:HD13	2:B:2780:LEU:HB3	1.86	0.58
2:B:4866:LEU:HD12	2:D:4871:PHE:HE2	1.69	0.58
2:D:2535:LEU:HD12	2:D:2537:ALA:H	1.69	0.58
2:F:2535:LEU:HD12	2:F:2537:ALA:H	1.69	0.58
2:B:4819:TYR:CD1	2:H:4845:ILE:HG23	2.39	0.57
2:D:248:PRO:O	2:D:257:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:756:SER:HB3	2:D:769:ARG:HB2	1.84	0.57
2:F:758:CYS:SG	2:F:759:LEU:N	2.77	0.57
2:D:1589:GLN:NE2	2:D:1634:GLU:OE1	2.37	0.57
2:B:636:LEU:HD21	2:B:643:LEU:HD21	1.85	0.57
2:H:4640:SER:O	2:H:4643:ASN:ND2	2.38	0.57
2:B:758:CYS:SG	2:B:759:LEU:N	2.77	0.57
2:B:1089:ARG:HH21	2:B:1600:PRO:HG3	1.70	0.57
2:D:476:GLN:NE2	2:D:3679:GLU:OE1	2.37	0.57
2:D:2142:LEU:HD23	2:D:2145:ARG:HD2	1.86	0.57
2:D:2718:LEU:HD13	2:D:2780:LEU:HB3	1.86	0.57
2:D:3996:ILE:HG12	2:D:4000:MET:HE3	1.86	0.57
2:D:4640:SER:O	2:D:4643:ASN:ND2	2.38	0.57
2:F:4865:GLY:HA2	2:H:4868:ILE:CD1	2.34	0.57
2:H:1089:ARG:HH21	2:H:1600:PRO:HG3	1.70	0.57
2:H:2718:LEU:HD13	2:H:2780:LEU:HB3	1.86	0.57
2:B:756:SER:HB3	2:B:769:ARG:HB2	1.84	0.57
2:B:1589:GLN:NE2	2:B:1634:GLU:OE1	2.37	0.57
2:D:693:LEU:HD21	2:D:798:ILE:HG21	1.86	0.57
2:H:758:CYS:SG	2:H:759:LEU:N	2.77	0.57
2:B:1631:HIS:HA	2:B:1638:SER:HA	1.87	0.57
2:B:2060:GLN:NE2	2:B:2092:GLN:O	2.38	0.57
2:B:2535:LEU:HD12	2:B:2537:ALA:H	1.69	0.57
2:F:4838:ASP:HB3	2:F:4841:GLU:HB2	1.87	0.57
2:H:476:GLN:NE2	2:H:3679:GLU:OE1	2.37	0.57
2:H:1121:GLY:O	2:H:1133:ARG:NH1	2.36	0.57
2:H:3808:ALA:HA	2:H:3811:ARG:HD3	1.87	0.57
2:H:3996:ILE:HG12	2:H:4000:MET:HE3	1.86	0.57
2:B:3808:ALA:HA	2:B:3811:ARG:HD3	1.87	0.57
2:D:1631:HIS:HA	2:D:1638:SER:HA	1.87	0.57
2:D:1761:MET:N	2:D:1761:MET:SD	2.73	0.57
2:F:1089:ARG:HH21	2:F:1600:PRO:HG3	1.70	0.57
2:H:1043:LYS:HD3	2:H:1047:LYS:HE3	1.87	0.57
2:B:1121:GLY:O	2:B:1133:ARG:NH1	2.36	0.57
2:D:207:PHE:CE2	2:F:2326:ILE:CD1	2.88	0.57
2:F:248:PRO:O	2:F:257:ARG:NH2	2.37	0.57
2:F:476:GLN:NE2	2:F:3679:GLU:OE1	2.37	0.57
2:B:4838:ASP:HB3	2:B:4841:GLU:HB2	1.87	0.57
2:B:2142:LEU:HD23	2:B:2145:ARG:HD2	1.86	0.57
2:B:3996:ILE:HG12	2:B:4000:MET:HE3	1.86	0.57
2:D:1089:ARG:HH21	2:D:1600:PRO:HG3	1.70	0.57
2:D:4517:ILE:O	2:D:4519:LEU:N	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:HIS:NE2	2:F:1774:GLU:OE2	2.38	0.57
2:F:693:LEU:HD21	2:F:798:ILE:HG21	1.86	0.57
2:F:2060:GLN:NE2	2:F:2092:GLN:O	2.38	0.57
2:F:3996:ILE:HG12	2:F:4000:MET:HE3	1.86	0.57
2:F:4857:VAL:CG1	2:H:4863:ILE:HG22	2.35	0.57
1:G:87:HIS:NE2	2:H:1774:GLU:OE2	2.38	0.57
2:H:150:GLN:NE2	2:H:158:CYS:SG	2.76	0.57
2:H:4838:ASP:HB3	2:H:4841:GLU:HB2	1.87	0.57
2:B:657:PRO:HB3	2:B:834:VAL:HG22	1.87	0.56
2:B:4640:SER:O	2:B:4643:ASN:ND2	2.38	0.56
2:D:655:MET:HG2	2:D:836:HIS:HA	1.87	0.56
2:D:657:PRO:HB3	2:D:834:VAL:HG22	1.87	0.56
2:F:4138:GLU:OE2	2:F:4148:ARG:NH1	2.38	0.56
2:H:2535:LEU:HD12	2:H:2537:ALA:H	1.69	0.56
2:B:4138:GLU:OE2	2:B:4148:ARG:NH1	2.38	0.56
2:D:802:PHE:HB2	2:D:1617:TRP:HB2	1.85	0.56
2:F:2296:GLY:HA2	2:F:2299:TYR:HD2	1.70	0.56
2:H:802:PHE:HB2	2:H:1617:TRP:HB2	1.85	0.56
2:H:1631:HIS:HA	2:H:1638:SER:HA	1.87	0.56
1:A:87:HIS:NE2	2:B:1774:GLU:OE2	2.38	0.56
2:B:797:GLY:HA2	2:B:1622:LEU:HA	1.87	0.56
2:B:4871:PHE:HE2	2:H:4866:LEU:HD12	1.70	0.56
2:B:4888:LYS:HB3	2:B:4893:GLY:HA2	1.86	0.56
2:D:1043:LYS:HD3	2:D:1047:LYS:HE3	1.87	0.56
2:D:2060:GLN:NE2	2:D:2092:GLN:O	2.38	0.56
2:F:76:ARG:CB	2:H:3891:TRP:CG	2.88	0.56
2:F:1631:HIS:HA	2:F:1638:SER:HA	1.87	0.56
2:F:2421:ARG:NH2	2:F:2476:VAL:O	2.39	0.56
2:F:4520:PHE:HD1	2:F:4562:LEU:HD21	0.84	0.56
2:H:797:GLY:HA2	2:H:1622:LEU:HA	1.87	0.56
2:H:2060:GLN:NE2	2:H:2092:GLN:O	2.38	0.56
2:H:4138:GLU:OE2	2:H:4148:ARG:NH1	2.39	0.56
2:B:207:PHE:CD1	2:D:2326:ILE:HG23	2.33	0.56
2:B:802:PHE:HB2	2:B:1617:TRP:HB2	1.85	0.56
2:B:4845:ILE:HG23	2:D:4819:TYR:CD1	2.39	0.56
2:D:3808:ALA:HA	2:D:3811:ARG:HD3	1.87	0.56
2:D:4888:LYS:HB3	2:D:4893:GLY:HA2	1.86	0.56
2:F:2718:LEU:HD13	2:F:2780:LEU:HB3	1.86	0.56
2:H:655:MET:HG2	2:H:836:HIS:HA	1.87	0.56
2:H:4722:TYR:OH	2:H:4745:LEU:O	2.24	0.56
2:H:4888:LYS:HB3	2:H:4893:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1043:LYS:HD3	2:B:1047:LYS:HE3	1.87	0.56
2:B:4520:PHE:HD1	2:B:4562:LEU:HD21	0.84	0.56
2:D:2296:GLY:HA2	2:D:2299:TYR:HD2	1.70	0.56
2:D:2421:ARG:NH2	2:D:2476:VAL:O	2.39	0.56
2:D:4865:GLY:HA2	2:F:4868:ILE:CD1	2.35	0.56
2:F:150:GLN:NE2	2:F:158:CYS:SG	2.76	0.56
2:F:655:MET:HG2	2:F:836:HIS:HA	1.87	0.56
2:F:4888:LYS:HB3	2:F:4893:GLY:HA2	1.86	0.56
2:H:4136:ARG:NH2	2:H:4150:TYR:OH	2.38	0.56
2:D:15:ARG:HB3	2:D:110:HIS:HB3	1.88	0.56
2:F:15:ARG:HB3	2:F:110:HIS:HB3	1.88	0.56
2:F:1043:LYS:HD3	2:F:1047:LYS:HE3	1.87	0.56
2:F:4640:SER:O	2:F:4643:ASN:ND2	2.38	0.56
2:F:4722:TYR:OH	2:F:4745:LEU:O	2.24	0.56
2:D:4138:GLU:OE2	2:D:4148:ARG:NH1	2.38	0.56
2:H:15:ARG:HB3	2:H:110:HIS:HB3	1.88	0.56
2:B:2157:TYR:HH	2:B:2203:TYR:HH	1.52	0.56
2:B:4865:GLY:HA2	2:D:4868:ILE:CD1	2.36	0.56
2:D:4838:ASP:HB3	2:D:4841:GLU:HB2	1.87	0.56
2:B:15:ARG:HB3	2:B:110:HIS:HB3	1.88	0.56
2:B:2421:ARG:NH2	2:B:2476:VAL:O	2.39	0.56
2:D:4056:HIS:O	2:D:4058:HIS:ND1	2.39	0.56
2:F:3808:ALA:HA	2:F:3811:ARG:HD3	1.87	0.56
1:C:87:HIS:NE2	2:D:1774:GLU:OE2	2.38	0.56
2:D:2157:TYR:HH	2:D:2203:TYR:HH	1.54	0.56
2:F:2728:HIS:NE2	2:F:2829:MET:SD	2.79	0.56
2:H:2421:ARG:NH2	2:H:2476:VAL:O	2.39	0.56
2:B:2296:GLY:HA2	2:B:2299:TYR:HD2	1.70	0.55
2:B:4622:PRO:O	2:B:4630:GLN:NE2	2.39	0.55
2:F:657:PRO:HB3	2:F:834:VAL:HG22	1.87	0.55
2:B:4912:GLN:O	2:B:4915:ASN:ND2	2.40	0.55
2:D:517:VAL:HG23	2:D:520:ARG:HE	1.71	0.55
2:F:3917:VAL:O	2:F:3920:THR:OG1	2.24	0.55
2:H:2296:GLY:HA2	2:H:2299:TYR:HD2	1.70	0.55
2:H:2728:HIS:NE2	2:H:2829:MET:SD	2.79	0.55
2:B:243:GLU:HA	2:B:264:GLY:HA2	1.88	0.55
2:B:4814:TYR:CD2	2:B:4815:MET:HE2	2.41	0.55
2:F:207:PHE:CE2	2:H:2326:ILE:CD1	2.89	0.55
2:H:4056:HIS:O	2:H:4058:HIS:ND1	2.39	0.55
2:B:1128:LEU:HD13	2:B:1206:SER:HB2	1.89	0.55
2:B:1304:LEU:HG	2:B:1591:LEU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4056:HIS:O	2:B:4058:HIS:ND1	2.39	0.55
2:B:4868:ILE:CD1	2:H:4865:GLY:HA2	2.37	0.55
2:D:150:GLN:NE2	2:D:158:CYS:SG	2.76	0.55
2:F:4524:SER:HG	2:F:4558:VAL:N	2.05	0.55
2:H:243:GLU:HA	2:H:264:GLY:HA2	1.88	0.55
2:H:1827:THR:HA	2:H:1830:ILE:HD12	1.89	0.55
2:H:4912:GLN:O	2:H:4915:ASN:ND2	2.40	0.55
2:B:655:MET:HG2	2:B:836:HIS:HA	1.87	0.55
2:D:76:ARG:CB	2:F:3891:TRP:CG	2.89	0.55
2:D:1827:THR:HA	2:D:1830:ILE:HD12	1.89	0.55
2:D:2718:LEU:HB3	2:D:2780:LEU:HD13	1.89	0.55
2:F:1304:LEU:HG	2:F:1591:LEU:H	1.72	0.55
2:F:4622:PRO:O	2:F:4630:GLN:NE2	2.39	0.55
2:H:4622:PRO:O	2:H:4630:GLN:NE2	2.39	0.55
2:H:4814:TYR:CD2	2:H:4815:MET:HE2	2.41	0.55
2:B:1827:THR:HA	2:B:1830:ILE:HD12	1.89	0.55
2:F:1827:THR:HA	2:F:1830:ILE:HD12	1.89	0.55
2:F:2718:LEU:HB3	2:F:2780:LEU:HD13	1.89	0.55
2:B:517:VAL:HG23	2:B:520:ARG:HE	1.71	0.55
2:D:1128:LEU:HD13	2:D:1206:SER:HB2	1.89	0.55
2:D:4845:ILE:HG23	2:F:4819:TYR:CD1	2.41	0.55
2:F:4056:HIS:O	2:F:4058:HIS:ND1	2.39	0.55
2:F:4814:TYR:CD2	2:F:4815:MET:HE2	2.41	0.55
2:H:1257:GLN:O	2:H:1596:TRP:N	2.40	0.55
2:B:4722:TYR:OH	2:B:4745:LEU:O	2.24	0.55
2:H:4524:SER:HG	2:H:4558:VAL:N	2.04	0.55
2:D:797:GLY:HA2	2:D:1622:LEU:HA	1.87	0.55
2:D:1121:GLY:O	2:D:1133:ARG:NH1	2.36	0.55
2:D:1304:LEU:HG	2:D:1591:LEU:H	1.72	0.55
2:D:3917:VAL:O	2:D:3920:THR:OG1	2.24	0.55
2:D:4857:VAL:CG1	2:F:4863:ILE:HG22	2.36	0.55
2:F:4912:GLN:O	2:F:4915:ASN:ND2	2.40	0.55
2:H:299:HIS:HD2	2:H:302:THR:H	1.55	0.55
2:B:4002:ASP:OD1	2:B:4115:ARG:NH1	2.40	0.55
2:B:4857:VAL:CG1	2:D:4863:ILE:HG22	2.37	0.55
2:D:1014:GLN:HB3	2:D:1032:LEU:HD21	1.89	0.55
2:D:2072:GLN:NE2	2:D:3647:LYS:O	2.40	0.55
2:D:3771:ASN:ND2	2:D:3773:THR:OG1	2.40	0.55
2:D:4622:PRO:O	2:D:4630:GLN:NE2	2.39	0.55
2:D:4627:ILE:O	2:D:4631:TRP:CB	2.55	0.55
2:D:4722:TYR:OH	2:D:4745:LEU:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4814:TYR:CD2	2:D:4815:MET:HE2	2.41	0.55
2:F:797:GLY:HA2	2:F:1622:LEU:HA	1.87	0.55
2:H:657:PRO:HB3	2:H:834:VAL:HG22	1.87	0.55
2:H:1304:LEU:HG	2:H:1591:LEU:H	1.72	0.55
2:H:4002:ASP:OD1	2:H:4115:ARG:NH1	2.40	0.55
2:B:2072:GLN:NE2	2:B:3647:LYS:O	2.40	0.54
2:D:1160:ASP:OD1	2:D:1178:ASN:ND2	2.40	0.54
2:D:1257:GLN:O	2:D:1596:TRP:N	2.40	0.54
2:D:4912:GLN:O	2:D:4915:ASN:ND2	2.40	0.54
2:F:299:HIS:HD2	2:F:302:THR:H	1.55	0.54
2:F:687:THR:HG22	2:F:689:GLU:H	1.72	0.54
2:F:3771:ASN:ND2	2:F:3773:THR:OG1	2.40	0.54
2:H:2024:LEU:HD23	2:H:2026:ILE:H	1.73	0.54
2:H:2718:LEU:HB3	2:H:2780:LEU:HD13	1.89	0.54
2:D:556:ASP:HA	2:D:559:ILE:HD12	1.90	0.54
2:D:4002:ASP:OD1	2:D:4115:ARG:NH1	2.40	0.54
2:F:28:ILE:HD12	2:F:33:GLN:HG2	1.90	0.54
2:F:444:THR:OG1	2:F:445:VAL:N	2.40	0.54
2:F:4655:MET:HA	2:F:4667:ILE:HD12	1.90	0.54
2:F:1128:LEU:HD13	2:F:1206:SER:HB2	1.89	0.54
2:F:1154:ARG:NH2	2:F:1180:GLU:OE1	2.41	0.54
2:H:2072:GLN:NE2	2:H:3647:LYS:O	2.40	0.54
2:H:4520:PHE:HD1	2:H:4562:LEU:HD21	0.84	0.54
2:B:2718:LEU:HB3	2:B:2780:LEU:HD13	1.89	0.54
2:D:4524:SER:HG	2:D:4558:VAL:N	2.04	0.54
2:F:1160:ASP:OD1	2:F:1178:ASN:ND2	2.40	0.54
2:H:115:TYR:OH	2:H:179:ASP:OD2	2.26	0.54
2:H:3771:ASN:ND2	2:H:3773:THR:OG1	2.40	0.54
2:B:115:TYR:OH	2:B:179:ASP:OD2	2.26	0.54
2:B:3891:TRP:CG	2:H:76:ARG:CB	2.91	0.54
2:D:115:TYR:OH	2:D:179:ASP:OD2	2.26	0.54
2:H:1014:GLN:HB3	2:H:1032:LEU:HD21	1.89	0.54
2:H:1907:MET:HA	2:H:1910:LEU:HD23	1.90	0.54
2:H:4655:MET:HA	2:H:4667:ILE:HD12	1.90	0.54
2:B:1014:GLN:HB3	2:B:1032:LEU:HD21	1.89	0.54
2:B:1160:ASP:OD1	2:B:1178:ASN:ND2	2.40	0.54
2:B:2024:LEU:HD23	2:B:2026:ILE:H	1.72	0.54
1:C:7:ILE:H	1:C:72:ALA:HA	1.73	0.54
2:D:946:LEU:HB2	2:D:995:MET:HE3	1.90	0.54
2:D:2024:LEU:HD23	2:D:2026:ILE:H	1.72	0.54
2:F:115:TYR:OH	2:F:179:ASP:OD2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:681:HIS:HB2	2:F:799:LYS:HG2	1.90	0.54
2:F:3628:SER:HG	2:F:3629:TRP:CD1	2.25	0.54
2:F:3767:LEU:HD21	2:F:3774:VAL:HB	1.90	0.54
2:H:1086:ARG:HH22	2:H:1254:ARG:HD3	1.73	0.54
2:H:3767:LEU:HD21	2:H:3774:VAL:HB	1.90	0.54
2:B:1272:ARG:NH2	2:B:1590:PHE:O	2.41	0.54
2:D:444:THR:OG1	2:D:445:VAL:N	2.40	0.54
2:D:1154:ARG:NH2	2:D:1180:GLU:OE1	2.41	0.54
2:F:517:VAL:HG23	2:F:520:ARG:HE	1.71	0.54
2:F:1602:GLN:HE22	2:F:1642:LEU:HB3	1.73	0.54
2:H:28:ILE:HD12	2:H:33:GLN:HG2	1.90	0.54
2:H:517:VAL:HG23	2:H:520:ARG:HE	1.71	0.54
2:H:1160:ASP:OD1	2:H:1178:ASN:ND2	2.40	0.54
2:H:1272:ARG:NH2	2:H:1590:PHE:O	2.41	0.54
2:H:1922:ARG:NH1	2:H:2038:THR:O	2.39	0.54
1:A:7:ILE:H	1:A:72:ALA:HA	1.73	0.54
2:B:946:LEU:HB2	2:B:995:MET:HE3	1.90	0.54
2:B:1257:GLN:O	2:B:1596:TRP:N	2.40	0.54
2:B:1907:MET:HA	2:B:1910:LEU:HD23	1.90	0.54
2:B:3771:ASN:ND2	2:B:3773:THR:OG1	2.40	0.54
2:B:4524:SER:HG	2:B:4558:VAL:N	2.04	0.54
2:D:28:ILE:HD12	2:D:33:GLN:HG2	1.90	0.54
2:D:243:GLU:HA	2:D:264:GLY:HA2	1.88	0.54
2:D:687:THR:HG22	2:D:689:GLU:H	1.72	0.54
2:D:4814:TYR:HE2	2:D:4815:MET:CE	2.21	0.54
2:F:243:GLU:HA	2:F:264:GLY:HA2	1.88	0.54
2:F:371:TRP:N	2:F:394:HIS:O	2.38	0.54
2:F:1257:GLN:O	2:F:1596:TRP:N	2.40	0.54
2:F:2072:GLN:NE2	2:F:3647:LYS:O	2.40	0.54
2:F:4002:ASP:OD1	2:F:4115:ARG:NH1	2.40	0.54
2:F:4627:ILE:O	2:F:4631:TRP:CB	2.55	0.54
2:H:444:THR:OG1	2:H:445:VAL:N	2.40	0.54
2:B:1154:ARG:NH2	2:B:1180:GLU:OE1	2.41	0.54
2:B:4627:ILE:O	2:B:4631:TRP:CB	2.55	0.54
2:D:371:TRP:N	2:D:394:HIS:O	2.38	0.54
2:F:1014:GLN:HB3	2:F:1032:LEU:HD21	1.89	0.54
2:H:1128:LEU:HD13	2:H:1206:SER:HB2	1.89	0.54
2:B:444:THR:OG1	2:B:445:VAL:N	2.40	0.54
2:B:4863:ILE:HG22	2:H:4857:VAL:CG1	2.38	0.54
2:D:480:ARG:NH2	2:D:3679:GLU:OE2	2.41	0.54
2:D:4655:MET:HA	2:D:4667:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4814:TYR:HE2	2:F:4815:MET:CE	2.21	0.54
2:H:235:ARG:NH2	2:H:268:SER:O	2.41	0.54
2:H:506:HIS:NE2	2:H:534:TYR:OH	2.40	0.54
2:H:4627:ILE:O	2:H:4631:TRP:CB	2.55	0.54
2:B:25:THR:HG22	2:B:34:LYS:HG2	1.90	0.53
2:B:371:TRP:N	2:B:394:HIS:O	2.38	0.53
2:B:375:GLN:N	2:B:390:LYS:O	2.41	0.53
2:B:687:THR:HG22	2:B:689:GLU:H	1.72	0.53
2:D:1224:LEU:HD13	2:D:1227:PHE:HD2	1.74	0.53
2:D:1907:MET:HA	2:D:1910:LEU:HD23	1.90	0.53
2:F:2840:ALA:HB3	2:F:2906:ARG:HD3	1.91	0.53
2:H:646:THR:HA	2:H:1630:LEU:HA	1.91	0.53
2:B:4136:ARG:NH2	2:B:4150:TYR:OH	2.38	0.53
2:D:246:THR:OG1	2:D:272:ARG:NH1	2.42	0.53
2:D:1029:ASN:HB3	2:D:1032:LEU:HG	1.91	0.53
2:D:1922:ARG:NH1	2:D:2038:THR:O	2.39	0.53
2:D:2728:HIS:NE2	2:D:2829:MET:SD	2.79	0.53
2:D:3919:ASN:O	2:D:3922:THR:OG1	2.27	0.53
2:D:4037:ASP:OD2	2:D:4042:GLY:N	2.41	0.53
2:F:15:ARG:N	2:F:18:ASP:OD2	2.40	0.53
2:F:1907:MET:HA	2:F:1910:LEU:HD23	1.90	0.53
2:F:2024:LEU:HD23	2:F:2026:ILE:H	1.72	0.53
2:H:681:HIS:HB2	2:H:799:LYS:HG2	1.90	0.53
2:B:207:PHE:CE2	2:D:2326:ILE:CD1	2.91	0.53
2:B:1245:ARG:NH2	2:B:1797:GLU:OE2	2.42	0.53
2:B:2326:ILE:CD1	2:H:207:PHE:CE2	2.90	0.53
2:D:235:ARG:NH2	2:D:268:SER:O	2.41	0.53
2:D:1245:ARG:NH2	2:D:1797:GLU:OE2	2.42	0.53
2:D:1272:ARG:NH2	2:D:1590:PHE:O	2.41	0.53
2:D:1570:LEU:O	2:D:1573:SER:OG	2.27	0.53
2:D:3805:ASP:OD2	2:D:3808:ALA:N	2.41	0.53
2:D:4136:ARG:NH2	2:D:4150:TYR:OH	2.38	0.53
2:F:506:HIS:NE2	2:F:534:TYR:OH	2.40	0.53
2:F:646:THR:HA	2:F:1630:LEU:HA	1.90	0.53
2:F:1224:LEU:HD13	2:F:1227:PHE:HD2	1.74	0.53
2:B:246:THR:OG1	2:B:272:ARG:NH1	2.42	0.53
2:B:1086:ARG:HH22	2:B:1254:ARG:HD3	1.73	0.53
2:D:207:PHE:CD1	2:F:2326:ILE:HG22	2.42	0.53
2:D:646:THR:HA	2:D:1630:LEU:HA	1.90	0.53
2:D:1602:GLN:HE22	2:D:1642:LEU:HB3	1.72	0.53
2:D:2760:PRO:HD2	2:D:2763:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2840:ALA:HB3	2:D:2906:ARG:HD3	1.91	0.53
2:F:1272:ARG:NH2	2:F:1590:PHE:O	2.41	0.53
2:F:4037:ASP:OD2	2:F:4042:GLY:N	2.41	0.53
2:H:1245:ARG:NH2	2:H:1797:GLU:OE2	2.42	0.53
2:H:3805:ASP:OD2	2:H:3808:ALA:N	2.40	0.53
2:H:4782:TYR:OH	2:H:4847:PHE:O	2.27	0.53
2:B:28:ILE:HD12	2:B:33:GLN:HG2	1.90	0.53
2:B:299:HIS:HD2	2:B:302:THR:H	1.55	0.53
2:B:556:ASP:HA	2:B:559:ILE:HD12	1.90	0.53
2:D:299:HIS:HD2	2:D:302:THR:H	1.55	0.53
2:D:565:LEU:HD11	2:D:603:LYS:HG2	1.91	0.53
2:D:1938:GLN:OE1	2:D:1942:ARG:NH1	2.42	0.53
2:F:556:ASP:HA	2:F:559:ILE:HD12	1.90	0.53
2:F:946:LEU:HB2	2:F:995:MET:HE3	1.90	0.53
2:F:1938:GLN:OE1	2:F:1942:ARG:NH1	2.42	0.53
2:F:3919:ASN:O	2:F:3922:THR:OG1	2.27	0.53
2:H:480:ARG:NH2	2:H:3679:GLU:OE2	2.41	0.53
2:H:1154:ARG:NH2	2:H:1180:GLU:OE1	2.41	0.53
2:H:1308:ILE:HD12	2:H:1539:LEU:HB2	1.90	0.53
2:H:1912:GLN:OE1	2:H:2091:ARG:NH1	2.42	0.53
2:B:196:TYR:O	2:B:201:LEU:N	2.42	0.53
2:B:1602:GLN:HE22	2:B:1642:LEU:HB3	1.73	0.53
2:B:4655:MET:HA	2:B:4667:ILE:HD12	1.90	0.53
2:D:25:THR:HG22	2:D:34:LYS:HG2	1.90	0.53
2:D:1912:GLN:OE1	2:D:2091:ARG:NH1	2.42	0.53
2:D:3904:GLN:NE2	2:D:3965:GLN:OE1	2.41	0.53
2:F:4782:TYR:OH	2:F:4847:PHE:O	2.27	0.53
1:G:7:ILE:H	1:G:72:ALA:HA	1.73	0.53
2:H:3904:GLN:NE2	2:H:3965:GLN:OE1	2.41	0.53
2:B:235:ARG:NH2	2:B:268:SER:O	2.41	0.53
2:D:681:HIS:HB2	2:D:799:LYS:HG2	1.90	0.53
2:D:3767:LEU:HD21	2:D:3774:VAL:HB	1.90	0.53
2:D:4866:LEU:HD12	2:F:4871:PHE:CE2	2.44	0.53
2:F:196:TYR:O	2:F:201:LEU:N	2.42	0.53
2:F:1086:ARG:HH22	2:F:1254:ARG:HD3	1.73	0.53
2:F:1487:MET:HE1	2:F:1531:TYR:HD2	1.73	0.53
2:F:1640:ASP:OD1	2:F:1640:ASP:N	2.41	0.53
2:F:1908:CYS:HB2	2:F:2088:LEU:HD11	1.91	0.53
2:F:2157:TYR:HH	2:F:2203:TYR:HH	1.55	0.53
2:H:196:TYR:O	2:H:201:LEU:N	2.42	0.53
2:B:678:MET:HG3	2:B:754:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1092:LYS:H	2:B:1250:TRP:HZ3	1.56	0.53
2:B:2728:HIS:NE2	2:B:2829:MET:SD	2.79	0.53
2:B:2760:PRO:HD2	2:B:2763:LEU:HD12	1.91	0.53
2:B:3628:SER:HG	2:B:3629:TRP:CD1	2.26	0.53
2:B:3919:ASN:O	2:B:3922:THR:OG1	2.27	0.53
2:D:1092:LYS:H	2:D:1250:TRP:HZ3	1.56	0.53
2:F:246:THR:OG1	2:F:272:ARG:NH1	2.42	0.53
2:H:556:ASP:HA	2:H:559:ILE:HD12	1.90	0.53
2:H:678:MET:HG3	2:H:754:VAL:HG22	1.91	0.53
2:H:1640:ASP:N	2:H:1640:ASP:OD1	2.41	0.53
2:B:480:ARG:NH2	2:B:3679:GLU:OE2	2.41	0.53
2:B:601:LEU:HB3	2:B:642:LEU:HD21	1.91	0.53
2:B:1029:ASN:HB3	2:B:1032:LEU:HG	1.91	0.53
2:B:4782:TYR:OH	2:B:4847:PHE:O	2.27	0.53
2:D:15:ARG:N	2:D:18:ASP:OD2	2.40	0.53
2:D:196:TYR:O	2:D:201:LEU:N	2.42	0.53
2:D:4640:SER:HB3	2:D:4643:ASN:HD21	1.74	0.53
2:F:207:PHE:CE1	2:H:2326:ILE:HG21	2.40	0.53
2:F:480:ARG:NH2	2:F:3679:GLU:OE2	2.41	0.53
2:F:601:LEU:HB3	2:F:642:LEU:HD21	1.91	0.53
2:F:3805:ASP:OD2	2:F:3808:ALA:N	2.40	0.53
2:H:1173:MET:HB3	2:H:1192:PHE:HB2	1.91	0.53
2:H:2840:ALA:HB3	2:H:2906:ARG:HD3	1.91	0.53
2:B:76:ARG:CB	2:D:3891:TRP:CG	2.91	0.53
2:B:3805:ASP:OD2	2:B:3808:ALA:N	2.40	0.53
2:B:3904:GLN:NE2	2:B:3965:GLN:OE1	2.41	0.53
2:B:3983:LEU:O	2:B:3987:LEU:HB2	2.10	0.53
2:D:601:LEU:HB3	2:D:642:LEU:HD21	1.91	0.53
2:F:1308:ILE:HD12	2:F:1539:LEU:HB2	1.90	0.53
2:F:1761:MET:SD	2:F:1761:MET:N	2.73	0.53
2:F:3904:GLN:NE2	2:F:3965:GLN:OE1	2.41	0.53
2:F:4640:SER:HB3	2:F:4643:ASN:HD21	1.74	0.53
2:H:687:THR:HG22	2:H:689:GLU:H	1.72	0.53
2:H:1487:MET:HE1	2:H:1531:TYR:HD2	1.73	0.53
2:H:4037:ASP:OD2	2:H:4042:GLY:N	2.41	0.53
2:B:1487:MET:HE1	2:B:1531:TYR:HD2	1.73	0.52
2:B:1938:GLN:OE1	2:B:1942:ARG:NH1	2.42	0.52
2:B:2840:ALA:HB3	2:B:2906:ARG:HD3	1.91	0.52
2:B:4640:SER:HB3	2:B:4643:ASN:HD21	1.74	0.52
2:D:1086:ARG:HH22	2:D:1254:ARG:HD3	1.73	0.52
2:D:2204:PHE:O	2:D:2211:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:PHE:CD1	2:H:2326:ILE:HG22	2.43	0.52
2:F:235:ARG:NH2	2:F:268:SER:O	2.41	0.52
2:F:1029:ASN:HB3	2:F:1032:LEU:HG	1.91	0.52
2:F:2204:PHE:O	2:F:2211:ASN:ND2	2.42	0.52
2:F:2760:PRO:HD2	2:F:2763:LEU:HD12	1.91	0.52
2:F:3960:SER:HG	2:F:4070:CYS:HG	1.56	0.52
2:H:4640:SER:HB3	2:H:4643:ASN:HD21	1.74	0.52
2:H:4655:MET:O	2:H:4664:ARG:NH2	2.39	0.52
2:H:4814:TYR:HE2	2:H:4815:MET:CE	2.21	0.52
2:B:679:VAL:HA	2:B:800:VAL:HG12	1.92	0.52
2:B:681:HIS:HB2	2:B:799:LYS:HG2	1.90	0.52
2:B:1224:LEU:HD13	2:B:1227:PHE:HD2	1.74	0.52
2:B:1912:GLN:OE1	2:B:2091:ARG:NH1	2.42	0.52
2:B:3767:LEU:HD21	2:B:3774:VAL:HB	1.90	0.52
2:D:375:GLN:N	2:D:390:LYS:O	2.41	0.52
2:F:25:THR:HG22	2:F:34:LYS:HG2	1.90	0.52
2:F:565:LEU:HD11	2:F:603:LYS:HG2	1.91	0.52
2:F:4028:THR:HA	2:F:4033:PHE:HD2	1.75	0.52
2:F:4148:ARG:HH11	2:F:4959:PHE:HB3	1.75	0.52
2:F:4655:MET:O	2:F:4664:ARG:NH2	2.39	0.52
2:H:601:LEU:HB3	2:H:642:LEU:HD21	1.91	0.52
2:H:1938:GLN:OE1	2:H:1942:ARG:NH1	2.42	0.52
2:H:3983:LEU:O	2:H:3987:LEU:HB2	2.10	0.52
2:H:4597:PRO:HA	2:H:4600:ILE:HG22	1.91	0.52
2:B:1308:ILE:HD12	2:B:1539:LEU:HB2	1.90	0.52
2:B:1996:GLN:HA	2:B:1997:LEU:HD23	1.92	0.52
2:D:678:MET:HG3	2:D:754:VAL:HG22	1.91	0.52
2:D:1640:ASP:OD1	2:D:1640:ASP:N	2.41	0.52
1:E:7:ILE:H	1:E:72:ALA:HA	1.73	0.52
2:F:1132:GLU:HB3	2:F:1147:GLN:HE21	1.74	0.52
2:F:1245:ARG:NH2	2:F:1797:GLU:OE2	2.42	0.52
2:H:371:TRP:N	2:H:394:HIS:O	2.38	0.52
2:H:946:LEU:HB2	2:H:995:MET:HE3	1.90	0.52
2:H:1132:GLU:HB3	2:H:1147:GLN:HE21	1.74	0.52
2:H:1908:CYS:HB2	2:H:2088:LEU:HD11	1.91	0.52
2:H:4028:THR:HA	2:H:4033:PHE:HD2	1.75	0.52
2:B:646:THR:HA	2:B:1630:LEU:HA	1.90	0.52
2:B:1119:ARG:NH2	2:B:1196:ASP:O	2.39	0.52
2:B:2204:PHE:O	2:B:2211:ASN:ND2	2.42	0.52
2:D:4655:MET:O	2:D:4664:ARG:NH2	2.39	0.52
2:F:246:THR:N	2:F:261:HIS:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1092:LYS:H	2:F:1250:TRP:HZ3	1.56	0.52
2:B:1640:ASP:N	2:B:1640:ASP:OD1	2.41	0.52
2:B:2326:ILE:HG22	2:H:207:PHE:CD1	2.44	0.52
2:B:4037:ASP:OD2	2:B:4042:GLY:N	2.41	0.52
2:D:1301:PHE:HE2	2:D:1453:TYR:HA	1.75	0.52
2:D:1487:MET:HE1	2:D:1531:TYR:HD2	1.73	0.52
2:F:805:GLY:O	2:F:810:GLU:N	2.43	0.52
2:F:1173:MET:HB3	2:F:1192:PHE:HB2	1.91	0.52
2:F:1301:PHE:HE2	2:F:1453:TYR:HA	1.75	0.52
2:F:2857:LYS:HE3	2:F:2861:LEU:HD11	1.92	0.52
2:F:3983:LEU:O	2:F:3987:LEU:HB2	2.10	0.52
2:F:4136:ARG:NH2	2:F:4150:TYR:OH	2.38	0.52
2:F:4722:TYR:HD2	2:F:4723:LEU:HD12	1.75	0.52
2:F:4848:ASP:HB3	2:H:4819:TYR:CE1	2.39	0.52
2:H:679:VAL:HA	2:H:800:VAL:HG12	1.92	0.52
2:B:15:ARG:N	2:B:18:ASP:OD2	2.40	0.52
2:B:233:VAL:HG13	2:B:300:VAL:HG21	1.92	0.52
2:B:1922:ARG:NH1	2:B:2038:THR:O	2.39	0.52
2:B:3683:LEU:HD22	2:B:3748:SER:HB3	1.92	0.52
2:D:1173:MET:HB3	2:D:1192:PHE:HB2	1.91	0.52
2:D:4148:ARG:HH11	2:D:4959:PHE:HB3	1.75	0.52
2:F:375:GLN:N	2:F:390:LYS:O	2.41	0.52
2:F:1094:TYR:OH	2:F:1808:ASP:OD1	2.27	0.52
2:F:4597:PRO:HA	2:F:4600:ILE:HG22	1.91	0.52
2:H:15:ARG:N	2:H:18:ASP:OD2	2.40	0.52
2:H:25:THR:HG22	2:H:34:LYS:HG2	1.90	0.52
2:H:246:THR:N	2:H:261:HIS:O	2.42	0.52
2:H:1092:LYS:H	2:H:1250:TRP:HZ3	1.56	0.52
2:H:1301:PHE:HE2	2:H:1453:TYR:HA	1.75	0.52
2:H:2760:PRO:HD2	2:H:2763:LEU:HD12	1.91	0.52
2:B:4814:TYR:HE2	2:B:4815:MET:CE	2.21	0.52
2:D:805:GLY:O	2:D:810:GLU:N	2.43	0.52
2:D:1251:LEU:O	2:D:1601:ASN:N	2.43	0.52
2:D:1996:GLN:HA	2:D:1997:LEU:HD23	1.92	0.52
2:D:4782:TYR:OH	2:D:4847:PHE:O	2.27	0.52
2:F:748:LEU:HB2	2:F:750:ARG:HG3	1.92	0.52
2:F:1922:ARG:NH1	2:F:2038:THR:O	2.39	0.52
2:F:3683:LEU:HD22	2:F:3748:SER:HB3	1.92	0.52
2:F:3803:VAL:HG21	2:F:3881:ARG:HD2	1.92	0.52
2:H:246:THR:OG1	2:H:272:ARG:NH1	2.42	0.52
2:H:565:LEU:HD11	2:H:603:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PRO:HD2	1:A:64:ALA:HA	1.92	0.52
2:B:207:PHE:CD1	2:D:2326:ILE:HG22	2.45	0.52
2:B:1301:PHE:HE2	2:B:1453:TYR:HA	1.75	0.52
2:B:3803:VAL:HG21	2:B:3881:ARG:HD2	1.92	0.52
2:B:4028:THR:HA	2:B:4033:PHE:HD2	1.75	0.52
2:B:4082:GLU:HA	2:B:4086:LYS:HD2	1.92	0.52
2:B:4617:TYR:OH	2:B:4629:GLY:O	2.28	0.52
2:D:1908:CYS:HB2	2:D:2088:LEU:HD11	1.91	0.52
2:D:2116:ASP:OD1	2:D:2153:ASN:ND2	2.43	0.52
2:D:3983:LEU:O	2:D:3987:LEU:HB2	2.10	0.52
2:D:4722:TYR:HD2	2:D:4723:LEU:HD12	1.75	0.52
2:F:2116:ASP:OD1	2:F:2153:ASN:ND2	2.43	0.52
2:F:4617:TYR:OH	2:F:4629:GLY:O	2.28	0.52
2:H:1224:LEU:HD13	2:H:1227:PHE:HD2	1.74	0.52
2:H:3683:LEU:HD22	2:H:3748:SER:HB3	1.92	0.52
2:B:1094:TYR:OH	2:B:1808:ASP:OD1	2.27	0.52
2:B:1570:LEU:O	2:B:1573:SER:OG	2.27	0.52
2:B:4597:PRO:HA	2:B:4600:ILE:HG22	1.91	0.52
2:D:486:GLN:NE2	2:D:539:ALA:O	2.43	0.52
2:D:1132:GLU:HB3	2:D:1147:GLN:HE21	1.74	0.52
2:D:3683:LEU:HD22	2:D:3748:SER:HB3	1.92	0.52
2:D:4597:PRO:HA	2:D:4600:ILE:HG22	1.91	0.52
1:E:16:PRO:HD2	1:E:64:ALA:HA	1.92	0.52
2:F:679:VAL:HA	2:F:800:VAL:HG12	1.92	0.52
2:F:4866:LEU:HD12	2:H:4871:PHE:CE2	2.45	0.52
2:H:375:GLN:N	2:H:390:LYS:O	2.41	0.52
2:H:1602:GLN:HE22	2:H:1642:LEU:HB3	1.73	0.52
2:B:565:LEU:HD11	2:B:603:LYS:HG2	1.91	0.52
2:B:909:ASP:HB2	2:B:914:GLN:HB2	1.91	0.52
2:B:1098:ALA:O	2:B:1101:TRP:NE1	2.42	0.52
2:B:4568:TYR:O	2:B:4572:THR:OG1	2.22	0.52
1:C:16:PRO:HD2	1:C:64:ALA:HA	1.92	0.52
2:D:748:LEU:HB2	2:D:750:ARG:HG3	1.92	0.52
2:D:4518:LEU:N	2:D:4518:LEU:CD2	2.73	0.52
2:F:909:ASP:HB2	2:F:914:GLN:HB2	1.91	0.52
2:F:1912:GLN:OE1	2:F:2091:ARG:NH1	2.42	0.52
2:H:486:GLN:NE2	2:H:539:ALA:O	2.43	0.52
2:H:725:TYR:HA	2:H:732:LEU:HA	1.92	0.52
2:H:4617:TYR:OH	2:H:4629:GLY:O	2.28	0.52
2:B:1132:GLU:HB3	2:B:1147:GLN:HE21	1.74	0.51
2:B:2160:PRO:HB3	2:B:2207:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2857:LYS:HE3	2:B:2861:LEU:HD11	1.92	0.51
2:B:4572:THR:O	2:B:4576:LEU:HB2	2.10	0.51
2:D:3803:VAL:HG21	2:D:3881:ARG:HD2	1.92	0.51
2:F:657:PRO:HA	2:F:834:VAL:HA	1.92	0.51
2:F:678:MET:HG3	2:F:754:VAL:HG22	1.91	0.51
2:F:3848:CYS:HB3	2:F:3856:GLN:HE21	1.76	0.51
2:H:162:ILE:HG23	2:H:181:LEU:HD13	1.92	0.51
2:H:657:PRO:HA	2:H:834:VAL:HA	1.92	0.51
2:H:805:GLY:O	2:H:810:GLU:N	2.43	0.51
2:H:1098:ALA:O	2:H:1101:TRP:NE1	2.42	0.51
2:B:748:LEU:HB2	2:B:750:ARG:HG3	1.92	0.51
2:B:2221:TYR:O	2:B:2225:ASN:ND2	2.44	0.51
2:B:4148:ARG:HH11	2:B:4959:PHE:HB3	1.75	0.51
2:B:4655:MET:O	2:B:4664:ARG:NH2	2.39	0.51
2:D:1308:ILE:HD12	2:D:1539:LEU:HB2	1.90	0.51
2:D:4572:THR:O	2:D:4576:LEU:HB2	2.10	0.51
2:D:4617:TYR:OH	2:D:4629:GLY:O	2.28	0.51
1:G:16:PRO:HD2	1:G:64:ALA:HA	1.92	0.51
2:H:233:VAL:HG13	2:H:300:VAL:HG21	1.92	0.51
2:H:1029:ASN:HB3	2:H:1032:LEU:HG	1.91	0.51
2:H:2160:PRO:HB3	2:H:2207:ILE:HD12	1.91	0.51
2:D:909:ASP:HB2	2:D:914:GLN:HB2	1.91	0.51
2:D:1094:TYR:OH	2:D:1808:ASP:OD1	2.27	0.51
2:D:2096:ILE:O	2:D:2100:VAL:N	2.43	0.51
2:D:2221:TYR:O	2:D:2225:ASN:ND2	2.44	0.51
2:D:3848:CYS:HB3	2:D:3856:GLN:HE21	1.76	0.51
2:F:162:ILE:HG23	2:F:181:LEU:HD13	1.93	0.51
2:F:725:TYR:HA	2:F:732:LEU:HA	1.92	0.51
2:F:2157:TYR:OH	2:F:2203:TYR:OH	2.26	0.51
2:H:483:LYS:O	2:H:544:ASN:ND2	2.38	0.51
2:H:3803:VAL:HG21	2:H:3881:ARG:HD2	1.92	0.51
2:H:3897:ASP:OD1	2:H:3958:LYS:NZ	2.40	0.51
2:B:506:HIS:NE2	2:B:534:TYR:OH	2.40	0.51
2:B:1251:LEU:O	2:B:1601:ASN:N	2.43	0.51
2:B:1908:CYS:HB2	2:B:2088:LEU:HD11	1.91	0.51
2:B:3848:CYS:HB3	2:B:3856:GLN:HE21	1.76	0.51
2:B:3917:VAL:O	2:B:3920:THR:OG1	2.24	0.51
2:B:4518:LEU:CD2	2:B:4518:LEU:N	2.73	0.51
2:B:4866:LEU:HD12	2:D:4871:PHE:CE2	2.44	0.51
2:D:1098:ALA:O	2:D:1101:TRP:NE1	2.42	0.51
2:D:4891:ILE:HD13	2:D:4914:HIS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2221:TYR:O	2:H:2225:ASN:ND2	2.44	0.51
2:H:2857:LYS:HE3	2:H:2861:LEU:HD11	1.92	0.51
2:B:1799:VAL:HG22	2:B:1894:LEU:HD13	1.93	0.51
1:C:42:ARG:NH2	2:D:1766:PRO:O	2.44	0.51
2:D:679:VAL:HA	2:D:800:VAL:HG12	1.92	0.51
2:D:1799:VAL:HG22	2:D:1894:LEU:HD13	1.93	0.51
1:E:28:GLY:N	1:E:37:ASP:O	2.37	0.51
2:F:1666:ALA:N	2:F:1669:ASN:OD1	2.41	0.51
2:F:4798:GLU:O	2:F:4802:THR:OG1	2.27	0.51
2:H:1996:GLN:HA	2:H:1997:LEU:HD23	1.92	0.51
2:H:3848:CYS:HB3	2:H:3856:GLN:HE21	1.76	0.51
2:H:4148:ARG:HH11	2:H:4959:PHE:HB3	1.75	0.51
2:B:486:GLN:NE2	2:B:539:ALA:O	2.43	0.51
2:B:776:GLN:HB3	2:B:1470:GLY:HA3	1.93	0.51
2:D:40:GLU:HB2	2:D:48:PHE:HE1	1.76	0.51
2:D:233:VAL:HG13	2:D:300:VAL:HG21	1.92	0.51
2:D:646:THR:OG1	2:D:1684:GLN:NE2	2.44	0.51
2:D:4118:THR:O	2:D:4122:LEU:HB2	2.11	0.51
2:F:1119:ARG:NH2	2:F:1196:ASP:O	2.39	0.51
2:F:1799:VAL:HG22	2:F:1894:LEU:HD13	1.93	0.51
2:F:4082:GLU:HA	2:F:4086:LYS:HD2	1.92	0.51
2:F:4118:THR:O	2:F:4122:LEU:HB2	2.11	0.51
2:F:4891:ILE:HD13	2:F:4914:HIS:HB3	1.92	0.51
2:H:40:GLU:HB2	2:H:48:PHE:HE1	1.76	0.51
2:H:2116:ASP:OD1	2:H:2153:ASN:ND2	2.43	0.51
2:B:805:GLY:O	2:B:810:GLU:N	2.43	0.51
2:D:4082:GLU:HA	2:D:4086:LYS:HD2	1.92	0.51
2:F:486:GLN:NE2	2:F:539:ALA:O	2.43	0.51
2:F:1300:MET:HB2	2:F:1545:ALA:HB3	1.93	0.51
2:F:4572:THR:O	2:F:4576:LEU:HB2	2.10	0.51
2:H:1300:MET:HB2	2:H:1545:ALA:HB3	1.93	0.51
2:H:2083:ARG:NH2	2:H:3686:ASP:OD1	2.43	0.51
2:H:4572:THR:O	2:H:4576:LEU:HB2	2.10	0.51
2:H:4794:TYR:HB2	2:H:4806:LYS:HD2	1.93	0.51
2:B:300:VAL:HG12	2:B:420:ARG:HH22	1.76	0.51
2:B:1173:MET:HB3	2:B:1192:PHE:HB2	1.91	0.51
2:B:2222:LEU:O	2:B:2226:SER:N	2.35	0.51
2:B:4085:VAL:O	2:B:4089:HIS:N	2.44	0.51
2:B:4871:PHE:CE2	2:H:4866:LEU:HD12	2.46	0.51
2:B:4891:ILE:HD13	2:B:4914:HIS:HB3	1.92	0.51
2:D:510:SER:O	2:D:520:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2160:PRO:HB3	2:D:2207:ILE:HD12	1.91	0.51
2:F:290:ARG:HG2	2:F:353:GLU:HB2	1.93	0.51
2:F:510:SER:O	2:F:520:ARG:NH2	2.44	0.51
2:F:4124:GLU:HG3	2:F:4128:ASN:HD21	1.76	0.51
2:H:165:ALA:HB2	2:H:182:ILE:HG12	1.93	0.51
2:H:2558:LYS:O	2:H:2562:LEU:N	2.44	0.51
2:H:4085:VAL:O	2:H:4089:HIS:N	2.44	0.51
2:H:4722:TYR:HD2	2:H:4723:LEU:HD12	1.75	0.51
2:B:246:THR:N	2:B:261:HIS:O	2.42	0.51
2:B:646:THR:OG1	2:B:1684:GLN:NE2	2.44	0.51
2:D:2083:ARG:NH2	2:D:3686:ASP:OD1	2.43	0.51
2:D:4028:THR:HA	2:D:4033:PHE:HD2	1.75	0.51
2:F:1098:ALA:O	2:F:1101:TRP:NE1	2.42	0.51
2:F:1996:GLN:HA	2:F:1997:LEU:HD23	1.92	0.51
1:G:42:ARG:NH2	2:H:1766:PRO:O	2.44	0.51
2:H:646:THR:OG1	2:H:1684:GLN:NE2	2.44	0.51
2:H:776:GLN:HB3	2:H:1470:GLY:HA3	1.93	0.51
2:H:909:ASP:HB2	2:H:914:GLN:HB2	1.91	0.51
2:H:3919:ASN:O	2:H:3922:THR:OG1	2.27	0.51
2:H:4518:LEU:CD2	2:H:4518:LEU:N	2.73	0.51
2:D:1252:SER:HB2	2:D:1598:ARG:HB2	1.93	0.51
1:E:42:ARG:NH2	2:F:1766:PRO:O	2.44	0.51
2:F:40:GLU:HB2	2:F:48:PHE:HE1	1.76	0.51
2:F:2096:ILE:O	2:F:2100:VAL:N	2.43	0.51
2:F:2193:MET:HA	2:F:2196:ASN:HD22	1.76	0.51
2:H:694:ARG:O	2:H:793:SER:N	2.42	0.51
2:H:2204:PHE:O	2:H:2211:ASN:ND2	2.42	0.51
2:H:3806:LEU:O	2:H:3810:GLU:N	2.43	0.51
2:B:40:GLU:HB2	2:B:48:PHE:HE1	1.76	0.50
2:B:694:ARG:O	2:B:793:SER:N	2.42	0.50
2:B:2773:ARG:HA	2:B:2776:ILE:HD12	1.93	0.50
2:B:4124:GLU:HG3	2:B:4128:ASN:HD21	1.76	0.50
2:B:4722:TYR:HD2	2:B:4723:LEU:HD12	1.75	0.50
2:D:1119:ARG:NH2	2:D:1196:ASP:O	2.39	0.50
2:D:1171:HIS:O	2:D:1194:ASP:N	2.44	0.50
2:D:4848:ASP:HB3	2:F:4819:TYR:CE1	2.41	0.50
2:F:233:VAL:HG13	2:F:300:VAL:HG21	1.92	0.50
2:F:2221:TYR:O	2:F:2225:ASN:ND2	2.44	0.50
2:F:4018:PHE:O	2:F:4022:LEU:HB2	2.11	0.50
2:F:4794:TYR:HB2	2:F:4806:LYS:HD2	1.93	0.50
2:H:4568:TYR:O	2:H:4572:THR:OG1	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4651:LYS:NZ	2:H:4670:LEU:O	2.45	0.50
1:A:42:ARG:NH2	2:B:1766:PRO:O	2.44	0.50
2:B:207:PHE:CE1	2:D:2326:ILE:HG21	2.42	0.50
2:B:2083:ARG:NH2	2:B:3686:ASP:OD1	2.43	0.50
2:B:4591:TYR:OH	2:B:4717:ASP:OD2	2.29	0.50
2:B:4798:GLU:O	2:B:4802:THR:OG1	2.27	0.50
2:D:2193:MET:HA	2:D:2196:ASN:HD22	1.76	0.50
2:D:4590:GLY:O	2:D:4594:LEU:N	2.44	0.50
2:D:4794:TYR:HB2	2:D:4806:LYS:HD2	1.93	0.50
2:F:1171:HIS:O	2:F:1194:ASP:N	2.44	0.50
2:F:2160:PRO:HB3	2:F:2207:ILE:HD12	1.91	0.50
2:F:3810:GLU:O	2:F:3814:LYS:HB2	2.12	0.50
2:F:4518:LEU:N	2:F:4518:LEU:CD2	2.74	0.50
2:H:748:LEU:HB2	2:H:750:ARG:HG3	1.92	0.50
2:H:1094:TYR:OH	2:H:1808:ASP:OD1	2.27	0.50
2:H:1666:ALA:N	2:H:1669:ASN:OD1	2.41	0.50
2:B:2116:ASP:OD1	2:B:2153:ASN:ND2	2.43	0.50
2:D:2773:ARG:HA	2:D:2776:ILE:HD12	1.93	0.50
2:F:165:ALA:HB2	2:F:182:ILE:HG12	1.93	0.50
2:F:2083:ARG:NH2	2:F:3686:ASP:OD1	2.44	0.50
2:F:4085:VAL:O	2:F:4089:HIS:N	2.44	0.50
2:F:4651:LYS:NZ	2:F:4670:LEU:O	2.45	0.50
2:H:300:VAL:HG12	2:H:420:ARG:HH22	1.76	0.50
2:B:657:PRO:HA	2:B:834:VAL:HA	1.92	0.50
2:B:1799:VAL:O	2:B:1803:SER:CB	2.60	0.50
2:D:162:ILE:HG23	2:D:181:LEU:HD13	1.93	0.50
2:D:657:PRO:HA	2:D:834:VAL:HA	1.92	0.50
2:D:4085:VAL:O	2:D:4089:HIS:N	2.44	0.50
2:D:4520:PHE:HD1	2:D:4562:LEU:HD21	0.84	0.50
1:E:89:GLY:HA3	2:F:1671:ARG:HH12	1.76	0.50
2:F:646:THR:OG1	2:F:1684:GLN:NE2	2.44	0.50
2:H:290:ARG:HG2	2:H:353:GLU:HB2	1.93	0.50
2:H:904:TYR:HB2	2:H:918:LEU:HB2	1.93	0.50
2:H:2193:MET:HA	2:H:2196:ASN:HD22	1.76	0.50
2:H:4082:GLU:HA	2:H:4086:LYS:HD2	1.92	0.50
2:H:4891:ILE:HD13	2:H:4914:HIS:HB3	1.92	0.50
2:B:165:ALA:HB2	2:B:182:ILE:HG12	1.93	0.50
2:B:1611:ILE:HB	2:B:1620:GLN:HB3	1.94	0.50
2:B:2193:MET:HA	2:B:2196:ASN:HD22	1.76	0.50
2:B:4118:THR:O	2:B:4122:LEU:HB2	2.11	0.50
2:D:776:GLN:HB3	2:D:1470:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:300:VAL:HG12	2:F:420:ARG:HH22	1.76	0.50
2:F:802:PHE:N	2:F:1616:GLY:O	2.45	0.50
2:H:802:PHE:N	2:H:1616:GLY:O	2.45	0.50
1:A:89:GLY:HA3	2:B:1671:ARG:HH12	1.76	0.50
2:B:620:CYS:N	2:B:623:VAL:O	2.39	0.50
2:D:207:PHE:CD2	2:F:2326:ILE:O	2.65	0.50
2:D:290:ARG:HG2	2:D:353:GLU:HB2	1.93	0.50
2:H:4118:THR:O	2:H:4122:LEU:HB2	2.11	0.50
2:B:1666:ALA:N	2:B:1669:ASN:OD1	2.41	0.50
2:B:4794:TYR:HB2	2:B:4806:LYS:HD2	1.93	0.50
2:D:300:VAL:HG12	2:D:420:ARG:HH22	1.76	0.50
2:F:1184:ASP:OD2	2:F:1188:SER:OG	2.30	0.50
2:F:1252:SER:HB2	2:F:1598:ARG:HB2	1.93	0.50
2:F:2773:ARG:HA	2:F:2776:ILE:HD12	1.93	0.50
2:F:4568:TYR:O	2:F:4572:THR:OG1	2.22	0.50
2:H:559:ILE:HD13	2:H:593:HIS:HB3	1.94	0.50
2:H:1611:ILE:HB	2:H:1620:GLN:HB3	1.94	0.50
2:B:289:ILE:HA	2:B:293:GLN:HE22	1.77	0.50
2:B:652:VAL:HA	2:B:795:SER:HB2	1.94	0.50
2:B:694:ARG:HB2	2:B:793:SER:HB2	1.94	0.50
2:B:725:TYR:HA	2:B:732:LEU:HA	1.92	0.50
2:B:3810:GLU:O	2:B:3814:LYS:HB2	2.12	0.50
2:D:289:ILE:HA	2:D:293:GLN:HE22	1.77	0.50
2:D:2857:LYS:HE3	2:D:2861:LEU:HD11	1.92	0.50
2:D:4651:LYS:NZ	2:D:4670:LEU:O	2.45	0.50
1:E:75:THR:HG23	1:E:98:ILE:HG12	1.94	0.50
2:H:1682:GLU:HA	2:H:1685:LEU:HD13	1.93	0.50
2:H:3810:GLU:O	2:H:3814:LYS:HB2	2.12	0.50
2:B:510:SER:O	2:B:520:ARG:NH2	2.44	0.50
2:B:559:ILE:HD13	2:B:593:HIS:HB3	1.94	0.50
2:B:2071:ALA:HA	2:B:2076:ILE:HD11	1.94	0.50
2:B:4523:VAL:CG2	2:H:4808:ASP:CG	2.62	0.50
2:B:4651:LYS:NZ	2:B:4670:LEU:O	2.45	0.50
1:C:75:THR:HG23	1:C:98:ILE:HG12	1.94	0.50
2:D:904:TYR:HB2	2:D:918:LEU:HB2	1.93	0.50
2:D:3810:GLU:O	2:D:3814:LYS:HB2	2.12	0.50
2:D:4931:GLU:OE2	2:D:4942:TRP:NE1	2.45	0.50
2:H:510:SER:O	2:H:520:ARG:NH2	2.44	0.50
2:H:1799:VAL:O	2:H:1803:SER:CB	2.60	0.50
2:H:4018:PHE:O	2:H:4022:LEU:HB2	2.11	0.50
2:B:802:PHE:N	2:B:1616:GLY:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1682:GLU:HA	2:B:1685:LEU:HD13	1.94	0.49
2:B:4515:ASN:HA	2:H:4780:TYR:OH	2.12	0.49
2:B:4931:GLU:OE2	2:B:4942:TRP:NE1	2.45	0.49
2:D:694:ARG:O	2:D:793:SER:N	2.42	0.49
2:D:725:TYR:HA	2:D:732:LEU:HA	1.92	0.49
2:D:1611:ILE:HB	2:D:1620:GLN:HB3	1.94	0.49
2:D:4018:PHE:O	2:D:4022:LEU:HB2	2.11	0.49
2:F:776:GLN:HB3	2:F:1470:GLY:HA3	1.93	0.49
2:F:4931:GLU:OE2	2:F:4942:TRP:NE1	2.45	0.49
2:H:652:VAL:HA	2:H:795:SER:HB2	1.94	0.49
2:H:1171:HIS:O	2:H:1194:ASP:N	2.44	0.49
2:H:1799:VAL:HG22	2:H:1894:LEU:HD13	1.93	0.49
2:H:4931:GLU:OE2	2:H:4942:TRP:NE1	2.45	0.49
2:B:162:ILE:HG23	2:B:181:LEU:HD13	1.92	0.49
2:B:1252:SER:HB2	2:B:1598:ARG:HB2	1.93	0.49
2:D:375:GLN:HE21	2:D:392:ILE:HD13	1.77	0.49
2:D:3810:GLU:O	2:D:3814:LYS:CB	2.60	0.49
1:E:54:GLU:OE1	2:F:1772:ASN:ND2	2.45	0.49
2:F:904:TYR:HB2	2:F:918:LEU:HB2	1.93	0.49
2:F:1251:LEU:O	2:F:1601:ASN:N	2.43	0.49
2:H:3763:GLY:HA2	2:H:3766:ILE:HD12	1.94	0.49
2:H:4590:GLY:O	2:H:4594:LEU:N	2.44	0.49
2:B:3856:GLN:NE2	2:B:3923:GLU:O	2.45	0.49
2:D:1682:GLU:HA	2:D:1685:LEU:HD13	1.93	0.49
2:D:2026:ILE:HG23	2:D:2030:LEU:HD12	1.94	0.49
2:D:2301:ASP:OD1	2:D:2304:ARG:NH2	2.46	0.49
2:D:3806:LEU:O	2:D:3810:GLU:N	2.43	0.49
2:D:4124:GLU:HG3	2:D:4128:ASN:HD21	1.76	0.49
2:F:2558:LYS:O	2:F:2562:LEU:N	2.44	0.49
2:F:3810:GLU:O	2:F:3814:LYS:CB	2.60	0.49
2:H:707:PRO:HD3	2:H:840:TYR:HE1	1.78	0.49
2:H:1443:VAL:O	2:H:1489:CYS:N	2.43	0.49
2:H:2773:ARG:HA	2:H:2776:ILE:HD12	1.93	0.49
2:H:4124:GLU:HG3	2:H:4128:ASN:HD21	1.76	0.49
2:B:1041:ARG:HA	2:B:1044:LYS:HG3	1.94	0.49
2:B:3763:GLY:HA2	2:B:3766:ILE:HD12	1.94	0.49
2:B:3810:GLU:O	2:B:3814:LYS:CB	2.60	0.49
2:B:4523:VAL:HG22	2:B:4559:HIS:HE1	1.78	0.49
1:C:89:GLY:HA3	2:D:1671:ARG:HH12	1.76	0.49
2:D:165:ALA:HB2	2:D:182:ILE:HG12	1.93	0.49
2:D:1300:MET:HB2	2:D:1545:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4523:VAL:HG22	2:D:4559:HIS:HE1	1.78	0.49
2:F:375:GLN:HE21	2:F:392:ILE:HD13	1.77	0.49
2:F:559:ILE:HD13	2:F:593:HIS:HB3	1.94	0.49
2:F:1041:ARG:HA	2:F:1044:LYS:HG3	1.94	0.49
2:F:3806:LEU:O	2:F:3810:GLU:N	2.43	0.49
1:G:75:THR:HG23	1:G:98:ILE:HG12	1.94	0.49
1:G:89:GLY:HA3	2:H:1671:ARG:HH12	1.76	0.49
2:H:4176:ASP:HA	2:H:4180:GLU:HB3	1.95	0.49
1:A:54:GLU:OE1	2:B:1772:ASN:ND2	2.45	0.49
1:A:75:THR:HG23	1:A:98:ILE:HG12	1.94	0.49
2:B:904:TYR:HB2	2:B:918:LEU:HB2	1.93	0.49
2:B:2026:ILE:HG23	2:B:2030:LEU:HD12	1.94	0.49
2:B:2301:ASP:OD1	2:B:2304:ARG:NH2	2.46	0.49
1:C:54:GLU:OE1	2:D:1772:ASN:ND2	2.46	0.49
2:D:1666:ALA:N	2:D:1669:ASN:OD1	2.41	0.49
2:D:4796:LYS:HD2	2:D:4805:MET:HB3	1.95	0.49
2:H:1252:SER:HB2	2:H:1598:ARG:HB2	1.93	0.49
2:B:290:ARG:HG2	2:B:353:GLU:HB2	1.93	0.49
2:B:542:ARG:NE	2:B:577:CYS:SG	2.85	0.49
2:B:4176:ASP:HA	2:B:4180:GLU:HB3	1.95	0.49
2:D:4176:ASP:HA	2:D:4180:GLU:HB3	1.95	0.49
2:F:1682:GLU:HA	2:F:1685:LEU:HD13	1.94	0.49
2:F:1799:VAL:O	2:F:1803:SER:CB	2.60	0.49
2:F:3763:GLY:HA2	2:F:3766:ILE:HD12	1.94	0.49
2:F:4523:VAL:HG22	2:F:4559:HIS:HE1	1.78	0.49
2:F:4713:VAL:O	2:F:4716:THR:OG1	2.27	0.49
2:H:289:ILE:HA	2:H:293:GLN:HE22	1.77	0.49
2:B:207:PHE:CD2	2:D:2326:ILE:O	2.66	0.49
2:B:655:MET:HE2	2:B:834:VAL:HG12	1.95	0.49
2:B:4018:PHE:O	2:B:4022:LEU:HB2	2.12	0.49
2:D:207:PHE:CE1	2:F:2326:ILE:HG21	2.39	0.49
2:D:4520:PHE:CB	2:D:4562:LEU:HD21	2.43	0.49
2:F:1611:ILE:HB	2:F:1620:GLN:HB3	1.94	0.49
2:F:4759:SER:HA	2:F:4762:THR:HG22	1.95	0.49
2:H:620:CYS:N	2:H:623:VAL:O	2.39	0.49
2:H:2096:ILE:O	2:H:2100:VAL:N	2.43	0.49
2:H:2301:ASP:OD1	2:H:2304:ARG:NH2	2.46	0.49
2:H:3921:LEU:HD23	2:H:3924:TYR:HD2	1.78	0.49
2:H:4798:GLU:O	2:H:4802:THR:OG1	2.27	0.49
2:B:2096:ILE:O	2:B:2100:VAL:N	2.43	0.49
2:B:2326:ILE:O	2:H:207:PHE:CD2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3806:LEU:O	2:B:3810:GLU:N	2.43	0.49
1:C:28:GLY:N	1:C:37:ASP:O	2.37	0.49
2:D:506:HIS:NE2	2:D:534:TYR:OH	2.40	0.49
2:D:559:ILE:HD13	2:D:593:HIS:HB3	1.94	0.49
2:D:802:PHE:N	2:D:1616:GLY:O	2.45	0.49
2:D:1799:VAL:O	2:D:1803:SER:CB	2.60	0.49
2:D:3763:GLY:HA2	2:D:3766:ILE:HD12	1.94	0.49
2:D:4798:GLU:O	2:D:4802:THR:OG1	2.27	0.49
2:D:4857:VAL:HG13	2:F:4863:ILE:HG21	1.93	0.49
2:F:207:PHE:CD2	2:H:2326:ILE:O	2.65	0.49
2:F:289:ILE:HA	2:F:293:GLN:HE22	1.77	0.49
2:F:694:ARG:HB2	2:F:793:SER:HB2	1.94	0.49
2:F:4590:GLY:O	2:F:4594:LEU:N	2.44	0.49
2:F:4796:LYS:HD2	2:F:4805:MET:HB3	1.95	0.49
2:B:694:ARG:HB3	2:B:716:ASN:HB3	1.94	0.49
2:B:3682:LYS:HZ3	2:B:3684:GLU:HG2	1.77	0.49
2:B:4193:PHE:O	2:B:4197:THR:OG1	2.25	0.49
2:B:4796:LYS:HD2	2:B:4805:MET:HB3	1.95	0.49
2:B:4819:TYR:CE1	2:H:4848:ASP:HB3	2.42	0.49
2:B:4848:ASP:HB3	2:D:4819:TYR:CE1	2.42	0.49
2:D:694:ARG:HB2	2:D:793:SER:HB2	1.94	0.49
2:D:1041:ARG:HA	2:D:1044:LYS:HG3	1.94	0.49
2:F:2738:LEU:HD13	2:F:2819:ALA:HB3	1.95	0.49
2:F:2835:SER:H	2:F:2838:LEU:HB2	1.78	0.49
1:G:54:GLU:OE1	2:H:1772:ASN:ND2	2.45	0.49
2:H:375:GLN:HE21	2:H:392:ILE:HD13	1.77	0.49
2:H:750:ARG:N	2:H:753:ASP:OD2	2.46	0.49
2:H:1926:ILE:HD11	2:H:2034:VAL:HG22	1.95	0.49
2:B:1300:MET:HB2	2:B:1545:ALA:HB3	1.93	0.49
2:B:2326:ILE:HG21	2:H:207:PHE:CE1	2.41	0.49
2:B:2835:SER:H	2:B:2838:LEU:HB2	1.78	0.49
2:D:655:MET:HE2	2:D:834:VAL:HG12	1.95	0.49
2:F:228:LEU:HB3	2:F:289:ILE:HB	1.95	0.49
2:F:655:MET:HE2	2:F:834:VAL:HG12	1.95	0.49
2:F:1926:ILE:HD11	2:F:2034:VAL:HG22	1.95	0.49
2:F:2071:ALA:HA	2:F:2076:ILE:HD11	1.94	0.49
2:F:3856:GLN:NE2	2:F:3923:GLU:O	2.45	0.49
2:F:4569:MET:O	2:F:4573:LEU:HB2	2.13	0.49
2:F:4591:TYR:OH	2:F:4717:ASP:OD2	2.29	0.49
2:H:655:MET:HE2	2:H:834:VAL:HG12	1.95	0.49
2:H:1041:ARG:HA	2:H:1044:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2738:LEU:HD13	2:H:2819:ALA:HB3	1.95	0.49
2:B:483:LYS:O	2:B:544:ASN:ND2	2.38	0.48
2:B:2558:LYS:O	2:B:2562:LEU:N	2.44	0.48
2:B:4780:TYR:OH	2:D:4515:ASN:HA	2.12	0.48
2:D:207:PHE:HB3	2:F:2326:ILE:O	2.13	0.48
2:D:246:THR:N	2:D:261:HIS:O	2.42	0.48
2:D:483:LYS:O	2:D:544:ASN:ND2	2.38	0.48
2:D:707:PRO:HD3	2:D:840:TYR:HE1	1.78	0.48
2:D:2835:SER:H	2:D:2838:LEU:HB2	1.78	0.48
2:D:3856:GLN:NE2	2:D:3923:GLU:O	2.45	0.48
2:F:1570:LEU:O	2:F:1573:SER:OG	2.27	0.48
2:F:4176:ASP:HA	2:F:4180:GLU:HB3	1.95	0.48
2:H:1184:ASP:OD2	2:H:1188:SER:OG	2.30	0.48
2:H:2835:SER:H	2:H:2838:LEU:HB2	1.78	0.48
2:H:4759:SER:HA	2:H:4762:THR:HG22	1.95	0.48
2:B:707:PRO:HD3	2:B:840:TYR:HE1	1.78	0.48
2:B:803:LEU:HD13	2:B:813:PHE:H	1.78	0.48
2:B:4520:PHE:CB	2:B:4562:LEU:HD21	2.43	0.48
2:D:228:LEU:HB3	2:D:289:ILE:HB	1.95	0.48
2:D:335:LYS:NZ	2:D:401:ASP:OD2	2.46	0.48
2:F:542:ARG:NE	2:F:577:CYS:SG	2.85	0.48
2:F:3921:LEU:HD23	2:F:3924:TYR:HD2	1.78	0.48
2:F:4899:PHE:HB2	2:F:4906:PHE:HD1	1.78	0.48
2:H:3810:GLU:O	2:H:3814:LYS:CB	2.61	0.48
2:H:3917:VAL:O	2:H:3920:THR:OG1	2.24	0.48
2:B:375:GLN:HE21	2:B:392:ILE:HD13	1.77	0.48
2:B:556:ASP:N	2:B:556:ASP:OD1	2.46	0.48
2:D:652:VAL:HA	2:D:795:SER:HB2	1.94	0.48
2:D:694:ARG:HB3	2:D:716:ASN:HB3	1.94	0.48
2:D:2837:ASP:OD1	2:D:2906:ARG:NE	2.42	0.48
2:F:707:PRO:HD3	2:F:840:TYR:HE1	1.78	0.48
1:A:42:ARG:HG3	1:A:44:LYS:HB3	1.95	0.48
2:B:506:HIS:HE2	2:B:534:TYR:HH	1.59	0.48
2:B:699:SER:OG	2:B:701:GLU:O	2.31	0.48
2:B:750:ARG:N	2:B:753:ASP:OD2	2.46	0.48
2:B:2425:ARG:HG3	2:B:2477:TYR:CE1	2.48	0.48
2:B:2738:LEU:HD13	2:B:2819:ALA:HB3	1.95	0.48
2:B:4759:SER:HA	2:B:4762:THR:HG22	1.95	0.48
2:B:4899:PHE:HB2	2:B:4906:PHE:HD1	1.78	0.48
2:D:803:LEU:HD13	2:D:813:PHE:H	1.78	0.48
2:D:4569:MET:O	2:D:4573:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:652:VAL:HA	2:F:795:SER:HB2	1.94	0.48
2:H:457:GLN:HA	2:H:460:ILE:HD12	1.95	0.48
2:H:694:ARG:HB3	2:H:716:ASN:HB3	1.94	0.48
2:H:4523:VAL:HG22	2:H:4559:HIS:HE1	1.78	0.48
2:B:122:ARG:HE	2:B:127:GLY:HA2	1.79	0.48
2:B:457:GLN:HA	2:B:460:ILE:HD12	1.95	0.48
2:D:207:PHE:HZ	2:F:2326:ILE:HD12	1.70	0.48
2:F:434:ASP:O	2:F:438:LYS:NZ	2.43	0.48
2:F:1443:VAL:O	2:F:1489:CYS:N	2.43	0.48
2:F:3682:LYS:HZ3	2:F:3684:GLU:HG2	1.79	0.48
2:F:4520:PHE:CB	2:F:4562:LEU:HD21	2.43	0.48
1:G:74:LEU:HB2	1:G:99:PHE:HB2	1.95	0.48
2:H:542:ARG:NE	2:H:577:CYS:SG	2.85	0.48
2:H:694:ARG:HB2	2:H:793:SER:HB2	1.94	0.48
2:H:2026:ILE:HG23	2:H:2030:LEU:HD12	1.94	0.48
2:H:2071:ALA:HA	2:H:2076:ILE:HD11	1.94	0.48
2:H:2731:ASP:OD1	2:H:2822:TYR:OH	2.30	0.48
2:H:4569:MET:O	2:H:4573:LEU:HB2	2.13	0.48
2:H:4649:PHE:HB3	2:H:4653:LYS:HE3	1.96	0.48
2:H:4796:LYS:HD2	2:H:4805:MET:HB3	1.95	0.48
1:C:23:VAL:HB	1:C:105:ASN:H	1.79	0.48
2:D:2071:ALA:HA	2:D:2076:ILE:HD11	1.94	0.48
2:D:2222:LEU:O	2:D:2226:SER:N	2.35	0.48
2:D:4568:TYR:O	2:D:4572:THR:OG1	2.22	0.48
2:D:4649:PHE:HB3	2:D:4653:LYS:HE3	1.96	0.48
2:F:122:ARG:HE	2:F:127:GLY:HA2	1.79	0.48
2:F:750:ARG:N	2:F:753:ASP:OD2	2.46	0.48
2:F:2026:ILE:HG23	2:F:2030:LEU:HD12	1.94	0.48
2:F:2301:ASP:OD1	2:F:2304:ARG:NH2	2.46	0.48
2:H:122:ARG:HE	2:H:127:GLY:HA2	1.79	0.48
2:H:1119:ARG:NH2	2:H:1196:ASP:O	2.39	0.48
2:B:4089:HIS:O	2:B:4093:LYS:N	2.44	0.48
2:D:4759:SER:HA	2:D:4762:THR:HG22	1.95	0.48
2:H:3856:GLN:NE2	2:H:3923:GLU:O	2.45	0.48
2:H:4814:TYR:CE2	2:H:4815:MET:CE	2.95	0.48
2:B:4569:MET:O	2:B:4573:LEU:HB2	2.13	0.48
2:D:2738:LEU:HD13	2:D:2819:ALA:HB3	1.95	0.48
2:F:803:LEU:HD13	2:F:813:PHE:H	1.78	0.48
2:H:1570:LEU:O	2:H:1573:SER:OG	2.27	0.48
2:H:4089:HIS:O	2:H:4093:LYS:N	2.44	0.48
2:B:4668:SER:HA	2:B:4671:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:SER:OG	2:D:186:VAL:N	2.47	0.48
2:D:1197:VAL:HA	2:D:1201:PHE:HE2	1.79	0.48
2:D:1209:VAL:N	2:D:1211:GLN:OE1	2.47	0.48
1:E:42:ARG:HG3	1:E:44:LYS:HB3	1.95	0.48
2:F:694:ARG:O	2:F:793:SER:N	2.42	0.48
2:F:1209:VAL:N	2:F:1211:GLN:OE1	2.47	0.48
2:F:1799:VAL:O	2:F:1803:SER:OG	2.30	0.48
2:H:803:LEU:HD13	2:H:813:PHE:H	1.78	0.48
1:C:74:LEU:HB2	1:C:99:PHE:HB2	1.95	0.48
2:D:122:ARG:HE	2:D:127:GLY:HA2	1.79	0.48
2:D:1310:CYS:HB2	2:D:1536:SER:HA	1.95	0.48
2:D:1799:VAL:O	2:D:1803:SER:OG	2.30	0.48
2:D:2558:LYS:O	2:D:2562:LEU:N	2.44	0.48
2:F:185:SER:OG	2:F:186:VAL:N	2.47	0.48
2:F:1197:VAL:HA	2:F:1201:PHE:HE2	1.79	0.48
2:H:434:ASP:O	2:H:438:LYS:NZ	2.43	0.48
2:H:656:ARG:HH12	2:H:700:THR:HG22	1.79	0.48
2:H:699:SER:OG	2:H:701:GLU:O	2.31	0.48
2:H:1799:VAL:O	2:H:1803:SER:OG	2.30	0.48
2:H:2135:MET:HA	2:H:2136:GLY:HA3	1.68	0.48
2:H:4520:PHE:CB	2:H:4562:LEU:HD21	2.43	0.48
2:B:1184:ASP:OD2	2:B:1188:SER:OG	2.30	0.47
2:B:1926:ILE:HD11	2:B:2034:VAL:HG22	1.95	0.47
2:D:750:ARG:N	2:D:753:ASP:OD2	2.46	0.47
2:D:1443:VAL:O	2:D:1489:CYS:N	2.43	0.47
2:D:1926:ILE:HD11	2:D:2034:VAL:HG22	1.95	0.47
2:D:4642:PRO:HG2	2:D:4648:LYS:HD2	1.96	0.47
2:F:228:LEU:HB3	2:F:289:ILE:HD12	1.96	0.47
2:F:457:GLN:HA	2:F:460:ILE:HD12	1.95	0.47
2:F:694:ARG:HB3	2:F:716:ASN:HB3	1.94	0.47
2:F:2835:SER:O	2:F:2839:HIS:N	2.38	0.47
2:F:4594:LEU:O	2:F:4596:VAL:N	2.47	0.47
2:B:656:ARG:HH12	2:B:700:THR:HG22	1.79	0.47
2:B:4594:LEU:O	2:B:4596:VAL:N	2.47	0.47
2:D:457:GLN:HA	2:D:460:ILE:HD12	1.95	0.47
2:D:1302:TYR:HB2	2:D:1543:VAL:HB	1.96	0.47
2:D:4193:PHE:O	2:D:4197:THR:OG1	2.25	0.47
2:D:4627:ILE:HA	2:D:4630:GLN:HB2	1.96	0.47
1:E:74:LEU:HB2	1:E:99:PHE:HB2	1.95	0.47
2:F:4857:VAL:HG13	2:H:4863:ILE:HG21	1.93	0.47
2:B:443:SER:HA	2:B:444:THR:HA	1.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1171:HIS:O	2:B:1194:ASP:N	2.44	0.47
2:B:1310:CYS:HB2	2:B:1536:SER:HA	1.96	0.47
2:B:1648:GLU:HA	2:B:1651:LEU:HB3	1.97	0.47
2:D:2038:THR:OG1	2:D:2039:TYR:N	2.47	0.47
1:E:23:VAL:HB	1:E:105:ASN:H	1.79	0.47
2:F:443:SER:HA	2:F:444:THR:HA	1.64	0.47
2:H:228:LEU:HB3	2:H:289:ILE:HB	1.95	0.47
2:H:443:SER:HA	2:H:444:THR:HA	1.64	0.47
2:H:4804:ASP:N	2:H:4804:ASP:OD1	2.47	0.47
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.95	0.47
2:B:101:MET:HE3	2:B:104:THR:HA	1.97	0.47
2:B:228:LEU:HB3	2:B:289:ILE:HB	1.95	0.47
2:B:420:ARG:HE	2:B:420:ARG:H	1.63	0.47
2:B:3921:LEU:HD23	2:B:3924:TYR:HD2	1.78	0.47
2:D:542:ARG:NE	2:D:577:CYS:SG	2.85	0.47
2:D:2256:LEU:HD11	2:D:3815:ALA:HB3	1.97	0.47
2:D:4899:PHE:HB2	2:D:4906:PHE:HD1	1.78	0.47
2:F:1043:LYS:HA	2:F:1046:ASN:HB2	1.97	0.47
2:H:101:MET:HE3	2:H:104:THR:HA	1.97	0.47
2:H:125:TYR:CZ	2:H:417:ARG:HB3	2.50	0.47
2:H:3682:LYS:HZ3	2:H:3684:GLU:HG2	1.79	0.47
2:B:2256:LEU:HD11	2:B:3815:ALA:HB3	1.97	0.47
2:B:4627:ILE:HA	2:B:4630:GLN:HB2	1.96	0.47
2:D:1689:ILE:HG12	2:D:1703:TYR:HE1	1.80	0.47
2:D:4594:LEU:O	2:D:4596:VAL:N	2.47	0.47
2:F:218:SER:HB3	2:F:286:GLY:HA3	1.96	0.47
2:F:223:ALA:HB2	2:F:349:MET:HE2	1.96	0.47
2:H:1043:LYS:HA	2:H:1046:ASN:HB2	1.97	0.47
2:H:1209:VAL:N	2:H:1211:GLN:OE1	2.47	0.47
2:H:1251:LEU:O	2:H:1601:ASN:N	2.43	0.47
2:H:4899:PHE:HB2	2:H:4906:PHE:HD1	1.78	0.47
2:B:228:LEU:HB3	2:B:289:ILE:HD12	1.96	0.47
2:B:1197:VAL:HA	2:B:1201:PHE:HE2	1.79	0.47
2:B:1209:VAL:N	2:B:1211:GLN:OE1	2.47	0.47
2:B:1302:TYR:HB2	2:B:1543:VAL:HB	1.96	0.47
2:B:1689:ILE:HG12	2:B:1703:TYR:HE1	1.80	0.47
2:B:2425:ARG:HG3	2:B:2477:TYR:HE1	1.79	0.47
2:D:228:LEU:HB3	2:D:289:ILE:HD12	1.96	0.47
2:D:656:ARG:HH12	2:D:700:THR:HG22	1.79	0.47
2:D:3956:GLN:HE21	2:D:3976:GLN:HE22	1.63	0.47
2:D:4780:TYR:OH	2:F:4515:ASN:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2256:LEU:HD11	2:F:3815:ALA:HB3	1.97	0.47
2:F:2858:LYS:HG2	2:F:2872:LEU:HD22	1.97	0.47
1:G:28:GLY:N	1:G:37:ASP:O	2.37	0.47
2:H:1310:CYS:HB2	2:H:1536:SER:HA	1.96	0.47
2:H:2488:LEU:O	2:H:2492:GLY:N	2.48	0.47
2:H:4642:PRO:HG2	2:H:4648:LYS:HD2	1.96	0.47
1:A:68:LEU:HA	1:A:103:LEU:HD23	1.97	0.47
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.96	0.47
2:B:1043:LYS:HA	2:B:1046:ASN:HB2	1.97	0.47
1:C:42:ARG:HG3	1:C:44:LYS:HB3	1.95	0.47
2:D:1748:LEU:HD22	2:D:1749:PRO:HD2	1.95	0.47
2:D:4591:TYR:OH	2:D:4717:ASP:OD2	2.29	0.47
2:D:4668:SER:HA	2:D:4671:LEU:HD12	1.96	0.47
2:F:125:TYR:CZ	2:F:417:ARG:HB3	2.50	0.47
2:F:656:ARG:HH12	2:F:700:THR:HG22	1.79	0.47
2:F:672:LYS:HA	2:F:760:ASP:HA	1.97	0.47
2:F:1302:TYR:HB2	2:F:1543:VAL:HB	1.96	0.47
2:F:4089:HIS:O	2:F:4093:LYS:N	2.44	0.47
2:F:4857:VAL:CG1	2:H:4863:ILE:HG21	2.43	0.47
1:G:42:ARG:HG3	1:G:44:LYS:HB3	1.95	0.47
2:H:64:ILE:HA	2:H:123:HIS:HE1	1.80	0.47
2:H:218:SER:HB3	2:H:286:GLY:HA3	1.96	0.47
2:H:223:ALA:HB2	2:H:349:MET:HE2	1.96	0.47
2:H:228:LEU:HB3	2:H:289:ILE:HD12	1.96	0.47
2:H:420:ARG:H	2:H:420:ARG:HE	1.63	0.47
2:H:1115:VAL:O	2:H:1137:PHE:N	2.48	0.47
2:H:1648:GLU:HA	2:H:1651:LEU:HB3	1.96	0.47
2:H:1748:LEU:HD22	2:H:1749:PRO:HD2	1.95	0.47
2:H:2256:LEU:HD11	2:H:3815:ALA:HB3	1.96	0.47
2:H:3960:SER:HG	2:H:4070:CYS:HG	1.62	0.47
2:B:673:TRP:HB2	2:B:759:LEU:HB3	1.97	0.47
2:B:1215:MET:HE2	2:B:1217:PHE:HZ	1.80	0.47
2:B:4648:LYS:O	2:B:4652:ARG:NE	2.48	0.47
2:D:653:SER:OG	2:D:794:PHE:O	2.31	0.47
2:D:673:TRP:HB2	2:D:759:LEU:HB3	1.96	0.47
1:E:40:ARG:HB3	2:F:688:ALA:HB1	1.97	0.47
2:F:64:ILE:HA	2:F:123:HIS:HE1	1.79	0.47
2:F:420:ARG:H	2:F:420:ARG:HE	1.63	0.47
2:F:483:LYS:O	2:F:544:ASN:ND2	2.38	0.47
2:F:1310:CYS:HB2	2:F:1536:SER:HA	1.96	0.47
2:F:2135:MET:HA	2:F:2136:GLY:HA3	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2837:ASP:OD1	2:F:2906:ARG:NE	2.42	0.47
2:F:4648:LYS:O	2:F:4652:ARG:NE	2.48	0.47
2:H:4100:ALA:O	2:H:4104:THR:OG1	2.30	0.47
2:B:3956:GLN:HE21	2:B:3976:GLN:HE22	1.63	0.47
2:B:4052:ALA:O	2:B:4056:HIS:ND1	2.47	0.47
2:D:218:SER:HB3	2:D:286:GLY:HA3	1.96	0.47
2:D:420:ARG:HE	2:D:420:ARG:H	1.63	0.47
2:D:4857:VAL:CG1	2:F:4863:ILE:HG21	2.45	0.47
2:F:1934:VAL:HG21	2:F:3618:VAL:HA	1.97	0.47
2:F:2102:ALA:O	2:F:2106:THR:N	2.46	0.47
2:F:4717:ASP:HB3	2:F:4720:PHE:HB3	1.97	0.47
2:H:394:HIS:NE2	2:H:396:GLU:OE1	2.48	0.47
2:H:1215:MET:HE2	2:H:1217:PHE:HZ	1.80	0.47
2:H:2148:GLY:O	2:H:2152:ASN:ND2	2.48	0.47
2:H:4594:LEU:O	2:H:4596:VAL:N	2.47	0.47
2:H:4668:SER:HA	2:H:4671:LEU:HD12	1.96	0.47
1:A:40:ARG:HB3	2:B:688:ALA:HB1	1.97	0.47
2:B:64:ILE:HA	2:B:123:HIS:HE1	1.79	0.47
2:B:223:ALA:HB2	2:B:349:MET:HE2	1.96	0.47
2:B:394:HIS:NE2	2:B:396:GLU:OE1	2.48	0.47
2:B:2148:GLY:O	2:B:2152:ASN:ND2	2.48	0.47
2:B:4642:PRO:HG2	2:B:4648:LYS:HD2	1.96	0.47
2:B:4804:ASP:N	2:B:4804:ASP:OD1	2.47	0.47
1:C:68:LEU:HA	1:C:103:LEU:HD23	1.97	0.47
2:D:1115:VAL:O	2:D:1137:PHE:N	2.48	0.47
2:D:2858:LYS:HG2	2:D:2872:LEU:HD22	1.97	0.47
2:D:4804:ASP:OD1	2:D:4804:ASP:N	2.47	0.47
2:F:1306:MET:HB3	2:F:1575:HIS:CE1	2.50	0.47
2:F:1748:LEU:HD22	2:F:1749:PRO:HD2	1.96	0.47
2:F:4649:PHE:HB3	2:F:4653:LYS:HE3	1.96	0.47
2:F:4668:SER:HA	2:F:4671:LEU:HD12	1.96	0.47
1:G:23:VAL:HB	1:G:105:ASN:H	1.79	0.47
2:H:190:ARG:HG2	2:H:207:PHE:HE1	1.80	0.47
2:H:1306:MET:HB3	2:H:1575:HIS:CE1	2.49	0.47
2:B:681:HIS:HD2	2:B:799:LYS:HD3	1.80	0.46
2:B:848:ARG:NH1	2:B:1605:LYS:O	2.48	0.46
2:B:1115:VAL:O	2:B:1137:PHE:N	2.48	0.46
2:B:1748:LEU:HD22	2:B:1749:PRO:HD2	1.96	0.46
2:B:1929:PHE:HZ	2:B:2030:LEU:HB3	1.80	0.46
2:B:3925:ILE:HD11	2:B:3936:LEU:HD13	1.97	0.46
2:B:4100:ALA:O	2:B:4104:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ARG:HB3	1:C:52:LYS:HE2	1.97	0.46
2:D:223:ALA:HB2	2:D:349:MET:HE2	1.96	0.46
2:D:412:GLU:O	2:D:415:THR:OG1	2.33	0.46
2:D:1306:MET:HB3	2:D:1575:HIS:CE1	2.49	0.46
2:D:1648:GLU:HA	2:D:1651:LEU:HB3	1.97	0.46
2:D:1929:PHE:HZ	2:D:2030:LEU:HB3	1.80	0.46
2:D:3925:ILE:HD11	2:D:3936:LEU:HD13	1.97	0.46
2:F:4518:LEU:HD13	2:F:4521:TYR:HE2	1.80	0.46
2:F:4780:TYR:OH	2:H:4515:ASN:HA	2.15	0.46
2:F:4808:ASP:CG	2:H:4523:VAL:CG2	2.66	0.46
2:H:506:HIS:HE2	2:H:534:TYR:HH	1.60	0.46
2:H:1197:VAL:HA	2:H:1201:PHE:HE2	1.79	0.46
2:H:1302:TYR:HB2	2:H:1543:VAL:HB	1.96	0.46
2:H:4627:ILE:HA	2:H:4630:GLN:HB2	1.96	0.46
2:B:190:ARG:HG2	2:B:207:PHE:HE1	1.80	0.46
2:B:2326:ILE:O	2:H:207:PHE:HB3	2.15	0.46
2:D:64:ILE:HA	2:D:123:HIS:HE1	1.80	0.46
2:D:2102:ALA:O	2:D:2106:THR:N	2.46	0.46
2:D:2488:LEU:O	2:D:2492:GLY:N	2.48	0.46
2:D:2793:THR:OG1	2:D:2901:GLY:O	2.30	0.46
2:D:3921:LEU:HD23	2:D:3924:TYR:HD2	1.78	0.46
2:D:4648:LYS:O	2:D:4652:ARG:NE	2.48	0.46
2:F:207:PHE:HB3	2:H:2326:ILE:O	2.15	0.46
2:F:673:TRP:HB2	2:F:759:LEU:HB3	1.97	0.46
2:F:1699:ARG:HH22	2:F:1821:LEU:HD11	1.80	0.46
2:F:1738:LEU:HD22	2:F:1739:PHE:H	1.79	0.46
2:F:3925:ILE:HD11	2:F:3936:LEU:HD13	1.97	0.46
2:F:4627:ILE:HA	2:F:4630:GLN:HB2	1.96	0.46
2:F:4642:PRO:HG2	2:F:4648:LYS:HD2	1.96	0.46
2:F:4733:GLY:HA3	2:F:4740:PHE:HD1	1.80	0.46
2:H:673:TRP:HB2	2:H:759:LEU:HB3	1.97	0.46
2:H:1934:VAL:HG21	2:H:3618:VAL:HA	1.97	0.46
2:H:3925:ILE:HD11	2:H:3936:LEU:HD13	1.97	0.46
2:B:672:LYS:HA	2:B:760:ASP:HA	1.97	0.46
2:B:1699:ARG:HH22	2:B:1821:LEU:HD11	1.80	0.46
2:B:1738:LEU:HD22	2:B:1739:PHE:H	1.80	0.46
2:B:4013:MET:N	2:B:4013:MET:SD	2.89	0.46
2:B:4649:PHE:HB3	2:B:4653:LYS:HE3	1.96	0.46
2:D:101:MET:HE3	2:D:104:THR:HA	1.97	0.46
2:D:190:ARG:HG2	2:D:207:PHE:HE1	1.80	0.46
2:F:137:ARG:N	2:F:146:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:556:ASP:OD1	2:F:556:ASP:N	2.46	0.46
2:F:2832:VAL:O	2:F:2895:LYS:NZ	2.44	0.46
2:F:4052:ALA:O	2:F:4056:HIS:ND1	2.47	0.46
2:H:1484:ASN:H	2:H:1486:TYR:HA	1.80	0.46
2:H:4623:SER:O	2:H:4630:GLN:NE2	2.48	0.46
2:B:3860:ARG:HH21	2:B:3932:ASN:HB2	1.80	0.46
2:D:707:PRO:HD2	2:D:1604:LEU:HD22	1.98	0.46
2:D:848:ARG:NH1	2:D:1605:LYS:O	2.48	0.46
2:D:4138:GLU:HG2	2:D:4148:ARG:HB3	1.98	0.46
2:D:4733:GLY:HA3	2:D:4740:PHE:HD1	1.80	0.46
1:E:68:LEU:HA	1:E:103:LEU:HD23	1.97	0.46
2:F:2488:LEU:O	2:F:2492:GLY:N	2.48	0.46
2:F:4046:LYS:N	2:F:4077:GLU:OE1	2.49	0.46
2:H:137:ARG:N	2:H:146:ASP:OD2	2.49	0.46
2:H:419:ILE:HG12	2:H:489:PHE:HE1	1.81	0.46
2:H:506:HIS:HB3	2:H:564:ARG:HH22	1.81	0.46
2:H:848:ARG:NH1	2:H:1605:LYS:O	2.48	0.46
2:H:4113:ASP:O	2:H:4117:GLN:N	2.46	0.46
2:H:4648:LYS:O	2:H:4652:ARG:NE	2.48	0.46
1:A:23:VAL:HB	1:A:105:ASN:H	1.79	0.46
2:B:707:PRO:HD2	2:B:1604:LEU:HD22	1.98	0.46
2:B:1306:MET:HB3	2:B:1575:HIS:CE1	2.49	0.46
2:B:4713:VAL:O	2:B:4716:THR:OG1	2.27	0.46
2:B:4733:GLY:HA3	2:B:4740:PHE:HD1	1.80	0.46
2:D:394:HIS:NE2	2:D:396:GLU:OE1	2.48	0.46
2:D:4013:MET:N	2:D:4013:MET:SD	2.89	0.46
2:F:190:ARG:HG2	2:F:207:PHE:HE1	1.80	0.46
2:F:1215:MET:HE2	2:F:1217:PHE:HZ	1.80	0.46
2:F:3860:ARG:HH21	2:F:3932:ASN:HB2	1.80	0.46
2:F:4138:GLU:HG2	2:F:4148:ARG:HB3	1.98	0.46
2:H:1689:ILE:HG12	2:H:1703:TYR:HE1	1.80	0.46
2:H:4591:TYR:OH	2:H:4717:ASP:OD2	2.29	0.46
2:B:1716:THR:HA	2:B:1719:LEU:HD12	1.98	0.46
2:B:4138:GLU:HG2	2:B:4148:ARG:HB3	1.98	0.46
1:C:40:ARG:HB3	2:D:688:ALA:HB1	1.97	0.46
2:D:1184:ASP:OD2	2:D:1188:SER:OG	2.30	0.46
2:D:3924:TYR:O	2:D:3932:ASN:ND2	2.48	0.46
2:D:4717:ASP:HB3	2:D:4720:PHE:HB3	1.97	0.46
2:F:101:MET:HE3	2:F:104:THR:HA	1.97	0.46
2:F:228:LEU:HD23	2:F:228:LEU:HA	1.82	0.46
2:F:256:GLN:O	2:F:304:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:394:HIS:NE2	2:F:396:GLU:OE1	2.48	0.46
2:F:1686:LEU:HA	2:F:1689:ILE:HD12	1.98	0.46
2:F:1689:ILE:HG12	2:F:1703:TYR:HE1	1.80	0.46
2:F:3956:GLN:HE21	2:F:3976:GLN:HE22	1.63	0.46
2:H:1716:THR:HA	2:H:1719:LEU:HD12	1.98	0.46
2:H:1738:LEU:HD22	2:H:1739:PHE:H	1.79	0.46
2:H:2858:LYS:HG2	2:H:2872:LEU:HD22	1.97	0.46
2:H:3859:LEU:HD22	2:H:3871:ILE:HG21	1.98	0.46
2:H:4046:LYS:N	2:H:4077:GLU:OE1	2.49	0.46
2:H:4197:THR:HG22	2:H:4201:MET:HE3	1.98	0.46
2:B:207:PHE:HB3	2:D:2326:ILE:O	2.16	0.46
2:B:1611:ILE:N	2:B:1620:GLN:O	2.44	0.46
2:D:1043:LYS:HA	2:D:1046:ASN:HB2	1.97	0.46
2:D:2067:MET:HE1	2:D:2085:MET:HB3	1.97	0.46
2:D:4623:SER:O	2:D:4630:GLN:NE2	2.49	0.46
2:F:419:ILE:HG12	2:F:489:PHE:HE1	1.81	0.46
2:F:848:ARG:NH1	2:F:1605:LYS:O	2.48	0.46
2:F:1648:GLU:HA	2:F:1651:LEU:HB3	1.97	0.46
2:F:2148:GLY:O	2:F:2152:ASN:ND2	2.48	0.46
1:G:68:LEU:HA	1:G:103:LEU:HD23	1.97	0.46
2:H:681:HIS:HD2	2:H:799:LYS:HD3	1.80	0.46
2:H:1686:LEU:HA	2:H:1689:ILE:HD12	1.98	0.46
2:H:3956:GLN:HE21	2:H:3976:GLN:HE22	1.63	0.46
2:H:4138:GLU:HG2	2:H:4148:ARG:HB3	1.98	0.46
2:B:137:ARG:N	2:B:146:ASP:OD2	2.49	0.46
2:B:185:SER:OG	2:B:186:VAL:N	2.47	0.46
2:B:1686:LEU:HA	2:B:1689:ILE:HD12	1.98	0.46
2:B:2791:GLU:H	2:B:2903:ALA:HB3	1.81	0.46
2:B:4113:ASP:O	2:B:4117:GLN:N	2.46	0.46
2:D:137:ARG:N	2:D:146:ASP:OD2	2.49	0.46
2:D:681:HIS:HD2	2:D:799:LYS:HD3	1.80	0.46
2:D:1215:MET:HE2	2:D:1217:PHE:HZ	1.80	0.46
2:D:1738:LEU:HD22	2:D:1739:PHE:H	1.79	0.46
2:D:1934:VAL:HG21	2:D:3618:VAL:HA	1.97	0.46
2:D:2116:ASP:OD2	2:D:2154:LYS:N	2.49	0.46
2:D:4046:LYS:N	2:D:4077:GLU:OE1	2.49	0.46
2:D:4197:THR:HG22	2:D:4201:MET:HE3	1.98	0.46
2:F:1736:ILE:HG12	2:F:1753:LEU:HD12	1.98	0.46
2:F:2067:MET:HE1	2:F:2085:MET:HB3	1.97	0.46
2:F:3924:TYR:O	2:F:3932:ASN:ND2	2.49	0.46
1:G:40:ARG:HB3	2:H:688:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:SER:OG	2:H:186:VAL:N	2.47	0.46
2:H:672:LYS:HA	2:H:760:ASP:HA	1.97	0.46
2:H:4002:ASP:HA	2:H:4115:ARG:HH22	1.81	0.46
2:B:506:HIS:HB3	2:B:564:ARG:HH22	1.81	0.46
2:B:1487:MET:HE2	2:B:1520:PHE:HE2	1.81	0.46
2:B:2488:LEU:O	2:B:2492:GLY:N	2.48	0.46
2:B:4160:GLN:HG3	2:B:4205:ALA:HB2	1.98	0.46
2:B:4197:THR:HG22	2:B:4201:MET:HE3	1.98	0.46
2:B:4857:VAL:HG13	2:D:4863:ILE:HG21	1.96	0.46
2:D:125:TYR:CZ	2:D:417:ARG:HB3	2.50	0.46
2:D:2040:LEU:HD11	2:D:3634:GLU:HG2	1.98	0.46
2:D:2148:GLY:O	2:D:2152:ASN:ND2	2.48	0.46
2:D:3860:ARG:HH21	2:D:3932:ASN:HB2	1.80	0.46
2:F:21:VAL:HG13	2:F:217:ILE:HG13	1.98	0.46
2:F:3859:LEU:HD22	2:F:3871:ILE:HG21	1.98	0.46
2:F:4013:MET:N	2:F:4013:MET:SD	2.89	0.46
2:H:115:TYR:HB2	2:H:171:GLU:HA	1.98	0.46
2:H:3924:TYR:O	2:H:3932:ASN:ND2	2.49	0.46
1:A:28:GLY:N	1:A:37:ASP:O	2.37	0.46
2:B:21:VAL:HG13	2:B:217:ILE:HG13	1.98	0.46
2:B:125:TYR:CZ	2:B:417:ARG:HB3	2.50	0.46
2:B:2067:MET:HE1	2:B:2085:MET:HB3	1.97	0.46
2:B:2835:SER:O	2:B:2839:HIS:N	2.38	0.46
2:D:699:SER:OG	2:D:701:GLU:O	2.31	0.46
2:D:1143:GLN:HA	2:D:1151:HIS:HA	1.98	0.46
2:D:1716:THR:HA	2:D:1719:LEU:HD12	1.98	0.46
2:F:506:HIS:HB3	2:F:564:ARG:HH22	1.81	0.46
2:F:2040:LEU:HD11	2:F:3634:GLU:HG2	1.98	0.46
2:F:4160:GLN:HG3	2:F:4205:ALA:HB2	1.98	0.46
2:F:4197:THR:HG22	2:F:4201:MET:HE3	1.98	0.46
2:H:335:LYS:NZ	2:H:401:ASP:OD2	2.46	0.46
2:H:565:LEU:HG	2:H:604:HIS:CE1	2.51	0.46
2:H:4013:MET:SD	2:H:4013:MET:N	2.89	0.46
2:H:4160:GLN:HG3	2:H:4205:ALA:HB2	1.98	0.46
2:B:1443:VAL:O	2:B:1489:CYS:N	2.43	0.45
2:B:3924:TYR:O	2:B:3932:ASN:ND2	2.49	0.45
2:B:4857:VAL:CG1	2:D:4863:ILE:HG21	2.46	0.45
2:D:20:VAL:HG12	2:D:216:PRO:HA	1.99	0.45
2:D:506:HIS:HB3	2:D:564:ARG:HH22	1.81	0.45
2:D:1699:ARG:HH22	2:D:1821:LEU:HD11	1.80	0.45
2:D:3845:GLN:HB2	2:D:3920:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ARG:HB3	1:E:52:LYS:HE2	1.97	0.45
2:F:1210:ALA:N	2:F:1211:GLN:OE1	2.50	0.45
2:F:1484:ASN:H	2:F:1486:TYR:HA	1.80	0.45
2:F:3845:GLN:HB2	2:F:3920:THR:HG22	1.98	0.45
2:H:2837:ASP:OD1	2:H:2906:ARG:NE	2.42	0.45
2:H:3748:SER:O	2:H:3793:SER:OG	2.30	0.45
2:B:115:TYR:HB2	2:B:171:GLU:HA	1.98	0.45
2:B:2102:ALA:O	2:B:2106:THR:N	2.46	0.45
2:B:4519:LEU:HA	2:H:4810:MET:HB3	1.97	0.45
2:D:115:TYR:HB2	2:D:171:GLU:HA	1.98	0.45
2:D:207:PHE:CG	2:F:2326:ILE:HG23	2.51	0.45
2:D:456:LEU:HD12	2:D:536:LEU:HD13	1.99	0.45
2:D:1487:MET:HE2	2:D:1520:PHE:HE2	1.81	0.45
2:D:1736:ILE:HG12	2:D:1753:LEU:HD12	1.98	0.45
2:D:3779:LEU:HD13	2:D:3855:PHE:HD1	1.81	0.45
2:F:565:LEU:HG	2:F:604:HIS:CE1	2.51	0.45
2:F:1487:MET:HE2	2:F:1520:PHE:HE2	1.81	0.45
2:H:195:SER:OG	2:H:196:TYR:N	2.49	0.45
2:H:731:HIS:ND1	2:H:739:ARG:O	2.50	0.45
2:H:1210:ALA:N	2:H:1211:GLN:OE1	2.50	0.45
2:H:1699:ARG:HH22	2:H:1821:LEU:HD11	1.80	0.45
1:A:14:THR:HB	1:A:68:LEU:HB2	1.99	0.45
1:A:49:ARG:HB3	1:A:52:LYS:HE2	1.97	0.45
2:B:456:LEU:HD12	2:B:536:LEU:HD13	1.99	0.45
2:B:2040:LEU:HD11	2:B:3634:GLU:HG2	1.98	0.45
2:B:2116:ASP:OD2	2:B:2154:LYS:N	2.49	0.45
2:B:2858:LYS:HG2	2:B:2872:LEU:HD22	1.97	0.45
2:D:556:ASP:N	2:D:556:ASP:OD1	2.46	0.45
2:D:1686:LEU:HA	2:D:1689:ILE:HD12	1.98	0.45
2:D:2791:GLU:H	2:D:2903:ALA:HB3	1.81	0.45
2:D:4160:GLN:HG3	2:D:4205:ALA:HB2	1.98	0.45
2:F:1143:GLN:HA	2:F:1151:HIS:HA	1.98	0.45
2:F:1929:PHE:HZ	2:F:2030:LEU:HB3	1.80	0.45
2:F:3897:ASP:OD1	2:F:3958:LYS:NZ	2.40	0.45
2:F:4623:SER:O	2:F:4630:GLN:NE2	2.49	0.45
2:H:556:ASP:OD1	2:H:556:ASP:N	2.46	0.45
2:H:935:MET:O	2:H:939:THR:OG1	2.34	0.45
2:H:1736:ILE:HG12	2:H:1753:LEU:HD12	1.98	0.45
2:H:2116:ASP:OD2	2:H:2154:LYS:N	2.49	0.45
2:H:3860:ARG:HH21	2:H:3932:ASN:HB2	1.81	0.45
2:B:1934:VAL:HG21	2:B:3618:VAL:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3831:LEU:HA	2:B:3832:GLN:HA	1.57	0.45
2:D:21:VAL:HG13	2:D:217:ILE:HG13	1.98	0.45
2:D:626:ARG:NH2	2:D:1668:GLY:O	2.36	0.45
2:D:672:LYS:HA	2:D:760:ASP:HA	1.97	0.45
2:D:1210:ALA:N	2:D:1211:GLN:OE1	2.50	0.45
2:F:1447:THR:OG1	2:F:1538:LYS:O	2.32	0.45
2:H:2067:MET:HE1	2:H:2085:MET:HB3	1.97	0.45
2:H:4518:LEU:HD13	2:H:4521:TYR:HE2	1.79	0.45
2:B:1210:ALA:N	2:B:1211:GLN:OE1	2.50	0.45
2:B:3779:LEU:HD13	2:B:3855:PHE:HD1	1.82	0.45
2:B:4590:GLY:O	2:B:4594:LEU:N	2.44	0.45
2:B:4717:ASP:HB3	2:B:4720:PHE:HB3	1.97	0.45
2:B:4814:TYR:CE2	2:B:4815:MET:CE	2.95	0.45
2:D:565:LEU:HG	2:D:604:HIS:CE1	2.51	0.45
2:D:2135:MET:HA	2:D:2136:GLY:HA3	1.68	0.45
2:D:4002:ASP:HA	2:D:4115:ARG:HH22	1.81	0.45
2:F:835:GLU:HG3	2:F:837:SER:H	1.82	0.45
2:F:2116:ASP:OD2	2:F:2154:LYS:N	2.49	0.45
1:G:14:THR:HB	1:G:68:LEU:HB2	1.99	0.45
2:H:713:TRP:CZ3	2:H:1627:PHE:HB2	2.52	0.45
2:H:1143:GLN:HA	2:H:1151:HIS:HA	1.98	0.45
2:H:1929:PHE:HZ	2:H:2030:LEU:HB3	1.80	0.45
2:H:2832:VAL:O	2:H:2895:LYS:NZ	2.44	0.45
2:H:4052:ALA:O	2:H:4056:HIS:ND1	2.47	0.45
2:B:20:VAL:HG12	2:B:216:PRO:HA	1.99	0.45
2:B:4623:SER:O	2:B:4630:GLN:NE2	2.48	0.45
2:D:713:TRP:CZ3	2:D:1627:PHE:HB2	2.52	0.45
2:D:731:HIS:ND1	2:D:739:ARG:O	2.50	0.45
2:D:1846:ILE:HG12	2:D:1894:LEU:HB3	1.99	0.45
2:F:681:HIS:HD2	2:F:799:LYS:HD3	1.80	0.45
2:F:707:PRO:HD2	2:F:1604:LEU:HD22	1.98	0.45
2:H:835:GLU:HG3	2:H:837:SER:H	1.82	0.45
1:A:67:SER:H	1:A:70:GLN:HB3	1.82	0.45
2:B:180:ASP:HB3	2:B:211:LEU:HD22	1.99	0.45
2:B:4518:LEU:HD13	2:B:4521:TYR:HE2	1.80	0.45
2:D:3859:LEU:HD22	2:D:3871:ILE:HG21	1.98	0.45
2:F:2791:GLU:H	2:F:2903:ALA:HB3	1.81	0.45
2:F:3907:PHE:HD2	2:F:3968:LEU:HD11	1.82	0.45
2:F:4104:THR:O	2:F:4107:SER:OG	2.35	0.45
1:G:49:ARG:HB3	1:G:52:LYS:HE2	1.97	0.45
2:H:614:LEU:HD23	2:H:617:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1846:ILE:HG12	2:H:1894:LEU:HB3	1.99	0.45
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.99	0.45
2:B:419:ILE:HG12	2:B:489:PHE:HE1	1.81	0.45
2:B:680:ASP:HB2	2:B:799:LYS:HG3	1.98	0.45
2:B:4002:ASP:HA	2:B:4115:ARG:HH22	1.81	0.45
2:B:4046:LYS:N	2:B:4077:GLU:OE1	2.49	0.45
2:B:4131:GLN:HA	2:B:4134:LEU:HD23	1.99	0.45
2:B:4138:GLU:HA	2:B:4148:ARG:HA	1.99	0.45
2:D:835:GLU:HG3	2:D:837:SER:H	1.82	0.45
2:D:1433:PHE:HB2	2:D:1552:VAL:HA	1.99	0.45
2:D:1484:ASN:H	2:D:1486:TYR:HA	1.80	0.45
2:D:1620:GLN:HE21	2:D:1622:LEU:HD21	1.81	0.45
2:D:3907:PHE:HD2	2:D:3968:LEU:HD11	1.82	0.45
2:D:4869:ASP:OD1	2:F:4875:ARG:HD3	2.17	0.45
2:F:180:ASP:HB3	2:F:211:LEU:HD22	1.99	0.45
2:F:195:SER:OG	2:F:196:TYR:N	2.49	0.45
2:F:207:PHE:CG	2:H:2326:ILE:HG23	2.52	0.45
2:F:1620:GLN:HE21	2:F:1622:LEU:HD21	1.81	0.45
2:F:1846:ILE:HG12	2:F:1894:LEU:HB3	1.99	0.45
2:F:2196:ASN:OD1	2:F:2199:ARG:NH1	2.50	0.45
2:F:4002:ASP:HA	2:F:4115:ARG:HH22	1.81	0.45
1:G:67:SER:H	1:G:70:GLN:HB3	1.82	0.45
2:H:180:ASP:HB3	2:H:211:LEU:HD22	1.99	0.45
2:H:2040:LEU:HD11	2:H:3634:GLU:HG2	1.98	0.45
2:H:2793:THR:OG1	2:H:2901:GLY:O	2.30	0.45
2:H:2988:SER:O	2:H:2992:CYS:N	2.47	0.45
2:H:4138:GLU:HA	2:H:4148:ARG:HA	1.99	0.45
2:H:4717:ASP:HB3	2:H:4720:PHE:HB3	1.97	0.45
2:B:993:GLU:HG2	2:B:1051:ARG:HG2	1.99	0.45
2:B:1040:ASP:HA	2:B:1043:LYS:HB2	1.99	0.45
2:B:1484:ASN:H	2:B:1486:TYR:HA	1.80	0.45
2:B:2837:ASP:OD1	2:B:2906:ARG:NE	2.42	0.45
2:B:3892:TYR:O	2:B:3896:LYS:NZ	2.50	0.45
2:B:3907:PHE:HD2	2:B:3968:LEU:HD11	1.82	0.45
2:D:18:ASP:HB2	2:D:69:LEU:HD12	1.99	0.45
2:D:180:ASP:HB3	2:D:211:LEU:HD22	1.99	0.45
2:D:238:HIS:HB3	2:D:243:GLU:HB3	1.99	0.45
2:D:419:ILE:HG12	2:D:489:PHE:HE1	1.81	0.45
2:D:614:LEU:HD23	2:D:617:LEU:HD12	1.99	0.45
2:D:1732:GLU:O	2:D:1735:SER:OG	2.31	0.45
2:D:4131:GLN:HA	2:D:4134:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:LEU:HD12	2:F:201:LEU:HB3	1.99	0.45
2:F:935:MET:O	2:F:939:THR:OG1	2.34	0.45
2:F:1716:THR:HA	2:F:1719:LEU:HD12	1.98	0.45
2:F:2463:PRO:O	2:F:2520:TYR:OH	2.32	0.45
2:F:4083:GLU:HA	2:F:4087:ARG:HD2	1.98	0.45
2:H:49:LEU:HD12	2:H:201:LEU:HB3	1.99	0.45
2:H:707:PRO:HD2	2:H:1604:LEU:HD22	1.98	0.45
2:B:565:LEU:HG	2:B:604:HIS:CE1	2.51	0.45
2:B:731:HIS:ND1	2:B:739:ARG:O	2.50	0.45
2:B:1736:ILE:HG12	2:B:1753:LEU:HD12	1.98	0.45
2:B:1846:ILE:HG12	2:B:1894:LEU:HB3	1.99	0.45
2:B:3859:LEU:HD22	2:B:3871:ILE:HG21	1.98	0.45
1:C:67:SER:H	1:C:70:GLN:HB3	1.82	0.45
2:D:1221:VAL:HG13	2:D:1224:LEU:HD12	1.99	0.45
2:D:2835:SER:O	2:D:2839:HIS:N	2.38	0.45
2:F:680:ASP:HB2	2:F:799:LYS:HG3	1.98	0.45
2:F:713:TRP:CZ3	2:F:1627:PHE:HB2	2.52	0.45
2:F:745:ASN:HB3	2:F:747:HIS:HB2	1.99	0.45
2:F:1799:VAL:O	2:F:1803:SER:HB3	2.17	0.45
2:F:4804:ASP:OD1	2:F:4804:ASP:N	2.47	0.45
2:H:1261:VAL:HA	2:H:1596:TRP:HH2	1.82	0.45
2:H:3779:LEU:HD13	2:H:3855:PHE:HD1	1.82	0.45
2:H:3845:GLN:HB2	2:H:3920:THR:HG22	1.98	0.45
2:B:195:SER:OG	2:B:196:TYR:N	2.50	0.44
2:B:835:GLU:HG3	2:B:837:SER:H	1.82	0.44
2:B:1799:VAL:O	2:B:1803:SER:HB3	2.17	0.44
2:B:3845:GLN:HB2	2:B:3920:THR:HG22	1.98	0.44
2:B:4104:THR:O	2:B:4107:SER:OG	2.35	0.44
2:B:4875:ARG:HD3	2:H:4869:ASP:OD1	2.18	0.44
1:C:14:THR:HB	1:C:68:LEU:HB2	1.99	0.44
2:D:195:SER:OG	2:D:196:TYR:N	2.49	0.44
2:D:207:PHE:CG	2:F:2326:ILE:CG2	3.00	0.44
2:D:4089:HIS:O	2:D:4093:LYS:N	2.44	0.44
2:F:456:LEU:HD12	2:F:536:LEU:HD13	1.99	0.44
2:F:1115:VAL:O	2:F:1137:PHE:N	2.48	0.44
2:F:1170:GLU:O	2:F:1172:THR:N	2.49	0.44
2:F:1261:VAL:HA	2:F:1596:TRP:HH2	1.82	0.44
2:F:1433:PHE:HB2	2:F:1552:VAL:HA	1.99	0.44
2:H:456:LEU:HD12	2:H:536:LEU:HD13	1.99	0.44
2:H:680:ASP:HB2	2:H:799:LYS:HG3	1.98	0.44
2:H:993:GLU:HG2	2:H:1051:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2157:TYR:HH	2:H:2203:TYR:HH	1.54	0.44
2:H:4733:GLY:HA3	2:H:4740:PHE:HD1	1.80	0.44
2:B:2212:GLN:HE22	2:B:2250:ASP:H	1.65	0.44
1:C:75:THR:HA	1:C:98:ILE:HA	1.99	0.44
2:D:4767:GLN:O	2:D:4771:THR:OG1	2.28	0.44
2:D:4832:ILE:HD11	2:D:4844:ARG:HG3	2.00	0.44
1:E:14:THR:HB	1:E:68:LEU:HB2	1.99	0.44
2:F:115:TYR:HB2	2:F:171:GLU:HA	1.98	0.44
2:F:731:HIS:ND1	2:F:739:ARG:O	2.50	0.44
2:H:1487:MET:HE2	2:H:1520:PHE:HE2	1.81	0.44
2:H:1926:ILE:HD12	2:H:1926:ILE:HA	1.89	0.44
2:H:2127:ILE:HD12	2:H:2127:ILE:HA	1.89	0.44
2:H:2791:GLU:H	2:H:2903:ALA:HB3	1.81	0.44
2:H:3892:TYR:O	2:H:3896:LYS:NZ	2.50	0.44
2:B:713:TRP:CZ3	2:B:1627:PHE:HB2	2.52	0.44
2:D:49:LEU:HD12	2:D:201:LEU:HB3	1.99	0.44
2:D:680:ASP:HB2	2:D:799:LYS:HG3	1.98	0.44
2:D:1799:VAL:O	2:D:1803:SER:HB3	2.17	0.44
2:D:2029:ARG:O	2:D:2032:SER:OG	2.35	0.44
2:D:3831:LEU:HA	2:D:3832:GLN:HA	1.57	0.44
2:D:4635:VAL:O	2:D:4638:THR:OG1	2.31	0.44
2:F:644:LEU:HD22	2:F:1632:ILE:HG22	1.99	0.44
2:F:1221:VAL:HG13	2:F:1224:LEU:HD12	1.99	0.44
2:F:3831:LEU:HA	2:F:3832:GLN:HA	1.57	0.44
2:H:21:VAL:HG13	2:H:217:ILE:HG13	1.98	0.44
2:H:644:LEU:HD22	2:H:1632:ILE:HG22	1.99	0.44
2:H:1602:GLN:HB3	2:H:1604:LEU:HD12	2.00	0.44
2:H:2196:ASN:OD1	2:H:2199:ARG:NH1	2.50	0.44
2:B:207:PHE:HZ	2:D:2326:ILE:HD12	1.72	0.44
2:B:1143:GLN:HA	2:B:1151:HIS:HA	1.98	0.44
2:B:1253:LYS:HE2	2:B:1257:GLN:HE21	1.82	0.44
2:B:2038:THR:OG1	2:B:2039:TYR:N	2.47	0.44
2:B:2103:LEU:HA	2:B:2106:THR:HG22	2.00	0.44
2:D:434:ASP:O	2:D:438:LYS:NZ	2.43	0.44
2:D:745:ASN:HB3	2:D:747:HIS:HB2	1.99	0.44
2:D:935:MET:O	2:D:939:THR:OG1	2.34	0.44
2:D:1040:ASP:HA	2:D:1043:LYS:HB2	1.99	0.44
2:D:4093:LYS:HE2	2:D:4093:LYS:HB3	1.84	0.44
2:F:20:VAL:HG12	2:F:216:PRO:HA	1.99	0.44
2:F:77:ALA:HA	2:H:3891:TRP:CZ3	2.53	0.44
2:F:1253:LYS:HE2	2:F:1257:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1926:ILE:HD12	2:F:1926:ILE:HA	1.89	0.44
2:F:3779:LEU:HD13	2:F:3855:PHE:HD1	1.82	0.44
2:H:1245:ARG:HE	2:H:1692:LYS:HD2	1.83	0.44
2:B:49:LEU:HD12	2:B:201:LEU:HB3	1.99	0.44
2:B:1620:GLN:HE21	2:B:1622:LEU:HD21	1.81	0.44
2:B:1699:ARG:NH1	2:B:1816:PHE:O	2.51	0.44
2:B:1799:VAL:O	2:B:1803:SER:OG	2.30	0.44
2:B:2135:MET:HA	2:B:2136:GLY:HA3	1.68	0.44
2:B:4863:ILE:HG21	2:H:4857:VAL:CG1	2.47	0.44
2:B:4869:ASP:OD1	2:D:4875:ARG:HD3	2.16	0.44
2:D:234:LEU:HD21	2:D:277:LEU:HD12	2.00	0.44
2:D:434:ASP:OD1	2:D:504:ARG:NE	2.41	0.44
2:D:4138:GLU:HA	2:D:4148:ARG:HA	1.99	0.44
2:F:238:HIS:HB3	2:F:243:GLU:HB3	2.00	0.44
2:F:1245:ARG:HE	2:F:1692:LYS:HD2	1.83	0.44
2:H:20:VAL:HG12	2:H:216:PRO:HA	1.99	0.44
2:H:1253:LYS:HE2	2:H:1257:GLN:HE21	1.82	0.44
2:H:1699:ARG:NH1	2:H:1816:PHE:O	2.51	0.44
2:H:2103:LEU:HA	2:H:2106:THR:HG22	2.00	0.44
2:H:4173:PHE:HZ	2:H:4190:PHE:HA	1.83	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.50	0.44
2:B:4810:MET:HB3	2:D:4519:LEU:HA	1.98	0.44
2:D:993:GLU:HG2	2:D:1051:ARG:HG2	1.99	0.44
2:D:1114:ARG:HH12	2:D:1127:GLU:HB3	1.82	0.44
2:D:1245:ARG:HE	2:D:1692:LYS:HD2	1.83	0.44
2:D:3983:LEU:HD12	2:D:3983:LEU:HA	1.87	0.44
2:D:4083:GLU:HA	2:D:4087:ARG:HD2	1.98	0.44
1:E:67:SER:H	1:E:70:GLN:HB3	1.82	0.44
2:F:234:LEU:HD21	2:F:277:LEU:HD12	2.00	0.44
2:F:614:LEU:HD23	2:F:617:LEU:HD12	1.99	0.44
1:G:75:THR:HA	1:G:98:ILE:HA	1.99	0.44
2:H:238:HIS:HB3	2:H:243:GLU:HB3	1.99	0.44
2:H:1620:GLN:HE21	2:H:1622:LEU:HD21	1.81	0.44
2:H:2212:GLN:HE22	2:H:2250:ASP:H	1.65	0.44
2:B:844:ARG:NH1	2:B:849:ASP:OD2	2.51	0.44
2:B:1114:ARG:HH12	2:B:1127:GLU:HB3	1.82	0.44
2:B:4173:PHE:HZ	2:B:4190:PHE:HA	1.83	0.44
2:D:77:ALA:HA	2:F:3891:TRP:CZ3	2.52	0.44
2:D:4173:PHE:HZ	2:D:4190:PHE:HA	1.83	0.44
1:E:75:THR:HA	1:E:98:ILE:HA	1.99	0.44
2:F:993:GLU:HG2	2:F:1051:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4832:ILE:HD11	2:F:4844:ARG:HG3	2.00	0.44
2:F:4869:ASP:OD1	2:H:4875:ARG:HD3	2.17	0.44
2:H:2067:MET:HB3	2:H:2067:MET:HE3	1.79	0.44
2:H:4131:GLN:HA	2:H:4134:LEU:HD23	1.99	0.44
2:H:4832:ILE:HD11	2:H:4844:ARG:HG3	2.00	0.44
2:B:238:HIS:HB3	2:B:243:GLU:HB3	2.00	0.44
2:B:335:LYS:NZ	2:B:401:ASP:OD2	2.46	0.44
2:B:644:LEU:HD22	2:B:1632:ILE:HG22	1.99	0.44
2:B:745:ASN:HB3	2:B:747:HIS:HB2	1.99	0.44
2:B:1245:ARG:HE	2:B:1692:LYS:HD2	1.83	0.44
2:B:1602:GLN:HB3	2:B:1604:LEU:HD12	2.00	0.44
2:D:644:LEU:HD22	2:D:1632:ILE:HG22	1.99	0.44
2:D:2212:GLN:HE22	2:D:2250:ASP:H	1.65	0.44
2:D:4750:GLY:H	2:D:4755:ARG:NE	2.16	0.44
2:F:1228:THR:HA	2:F:1232:LEU:HD12	1.99	0.44
2:F:4857:VAL:HG11	2:H:4863:ILE:HG22	1.98	0.44
2:H:1086:ARG:N	2:H:1207:LEU:O	2.48	0.44
2:H:3800:SER:OG	2:H:3801:CYS:N	2.51	0.44
2:H:4083:GLU:HA	2:H:4087:ARG:HD2	1.99	0.44
2:B:614:LEU:HD23	2:B:617:LEU:HD12	1.99	0.44
2:B:1221:VAL:HG13	2:B:1224:LEU:HD12	1.99	0.44
2:B:1433:PHE:HB2	2:B:1552:VAL:HA	1.99	0.44
2:B:2123:SER:O	2:B:2126:GLN:NE2	2.51	0.44
2:D:2123:SER:O	2:D:2126:GLN:NE2	2.51	0.44
2:D:2196:ASN:OD1	2:D:2199:ARG:NH1	2.50	0.44
2:D:2832:VAL:O	2:D:2895:LYS:NZ	2.44	0.44
2:D:4113:ASP:O	2:D:4117:GLN:N	2.46	0.44
2:F:1570:LEU:HD23	2:F:1570:LEU:HA	1.84	0.44
2:F:2127:ILE:HD12	2:F:2127:ILE:HA	1.89	0.44
2:F:2464:ASP:N	2:F:2464:ASP:OD1	2.50	0.44
2:F:4657:LYS:HD2	2:F:4658:TYR:CZ	2.53	0.44
2:H:18:ASP:HB2	2:H:69:LEU:HD12	1.99	0.44
2:H:1104:GLU:HG2	2:H:1216:ASN:HB2	2.00	0.44
2:H:1272:ARG:NH1	2:H:1587:HIS:O	2.51	0.44
2:B:1104:GLU:HG2	2:B:1216:ASN:HB2	2.00	0.43
2:B:1228:THR:HA	2:B:1232:LEU:HD12	1.99	0.43
2:B:1261:VAL:HA	2:B:1596:TRP:HH2	1.82	0.43
2:D:459:LEU:HD23	2:D:459:LEU:HA	1.86	0.43
2:D:1445:TRP:HB3	2:D:1539:LEU:HD13	2.00	0.43
2:D:3892:TYR:O	2:D:3896:LYS:NZ	2.50	0.43
2:D:4052:ALA:O	2:D:4056:HIS:ND1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:ASP:HB2	2:F:69:LEU:HD12	1.99	0.43
2:F:766:ILE:HB	2:F:779:PHE:HB2	2.00	0.43
2:F:1434:PRO:HD2	2:F:1552:VAL:HG23	2.00	0.43
2:F:1445:TRP:HB3	2:F:1539:LEU:HD13	2.00	0.43
2:F:1699:ARG:NH1	2:F:1816:PHE:O	2.51	0.43
2:F:3892:TYR:O	2:F:3896:LYS:NZ	2.50	0.43
1:G:21:THR:OG1	1:G:49:ARG:NE	2.50	0.43
2:H:1221:VAL:HG13	2:H:1224:LEU:HD12	1.99	0.43
2:H:1799:VAL:O	2:H:1803:SER:HB3	2.17	0.43
2:B:3767:LEU:HA	2:B:3767:LEU:HD23	1.84	0.43
2:D:1261:VAL:HA	2:D:1596:TRP:HH2	1.82	0.43
2:D:4576:LEU:HD13	2:D:4579:LEU:HD22	2.01	0.43
2:F:4138:GLU:HA	2:F:4148:ARG:HA	1.99	0.43
2:F:4750:GLY:H	2:F:4755:ARG:NE	2.16	0.43
2:H:745:ASN:HB3	2:H:747:HIS:HB2	1.99	0.43
2:H:766:ILE:HB	2:H:779:PHE:HB2	2.00	0.43
2:H:1433:PHE:HB2	2:H:1552:VAL:HA	1.99	0.43
2:B:234:LEU:HD21	2:B:277:LEU:HD12	2.00	0.43
2:B:2473:LEU:HD12	2:B:2477:TYR:HD2	1.83	0.43
2:B:4832:ILE:HD11	2:B:4844:ARG:HG3	2.00	0.43
2:B:4857:VAL:HG11	2:D:4863:ILE:HG22	2.01	0.43
2:D:1253:LYS:HE2	2:D:1257:GLN:HE21	1.82	0.43
2:D:1272:ARG:NH1	2:D:1587:HIS:O	2.51	0.43
2:D:4657:LYS:HD2	2:D:4658:TYR:CZ	2.53	0.43
2:F:1272:ARG:NH1	2:F:1587:HIS:O	2.51	0.43
2:F:4131:GLN:HA	2:F:4134:LEU:HD23	1.99	0.43
2:H:234:LEU:HD21	2:H:277:LEU:HD12	2.00	0.43
2:H:2835:SER:O	2:H:2839:HIS:N	2.38	0.43
2:H:4766:LYS:HE3	2:H:4770:LEU:HD11	2.00	0.43
2:B:1272:ARG:NH1	2:B:1587:HIS:O	2.51	0.43
2:B:2029:ARG:O	2:B:2032:SER:OG	2.35	0.43
2:B:4657:LYS:HD2	2:B:4658:TYR:CZ	2.53	0.43
1:C:44:LYS:HA	1:C:45:PRO:HD3	1.90	0.43
2:D:2473:LEU:HD12	2:D:2477:TYR:HD2	1.83	0.43
2:D:4750:GLY:H	2:D:4755:ARG:HE	1.66	0.43
2:F:439:LYS:HD3	2:F:441:LYS:HB2	2.01	0.43
2:F:699:SER:OG	2:F:701:GLU:O	2.31	0.43
2:F:1086:ARG:N	2:F:1207:LEU:O	2.48	0.43
2:F:1602:GLN:HB3	2:F:1604:LEU:HD12	2.00	0.43
2:F:1696:GLY:HA2	2:F:1699:ARG:HB3	2.00	0.43
2:F:2222:LEU:O	2:F:2226:SER:N	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2793:THR:OG1	2:F:2901:GLY:O	2.30	0.43
2:F:4173:PHE:HZ	2:F:4190:PHE:HA	1.83	0.43
2:F:4814:TYR:CE2	2:F:4815:MET:CE	2.95	0.43
2:H:844:ARG:NH1	2:H:849:ASP:OD2	2.51	0.43
2:H:4657:LYS:HD2	2:H:4658:TYR:CZ	2.53	0.43
2:B:935:MET:O	2:B:939:THR:OG1	2.34	0.43
2:B:4083:GLU:HA	2:B:4087:ARG:HD2	1.99	0.43
2:B:4750:GLY:H	2:B:4755:ARG:NE	2.16	0.43
2:B:4808:ASP:CG	2:D:4523:VAL:CG2	2.62	0.43
2:D:620:CYS:N	2:D:623:VAL:O	2.39	0.43
2:D:836:HIS:CE1	2:D:1610:ARG:HB2	2.54	0.43
2:D:1699:ARG:NH1	2:D:1816:PHE:O	2.51	0.43
2:D:4857:VAL:HG11	2:F:4863:ILE:HG22	2.00	0.43
2:F:306:LEU:HG	2:F:314:LEU:HD11	2.00	0.43
2:F:1040:ASP:HA	2:F:1043:LYS:HB2	1.99	0.43
2:F:1114:ARG:HH12	2:F:1127:GLU:HB3	1.82	0.43
2:F:4635:VAL:O	2:F:4638:THR:OG1	2.31	0.43
2:H:306:LEU:HG	2:H:314:LEU:HD11	2.00	0.43
2:H:1040:ASP:HA	2:H:1043:LYS:HB2	2.00	0.43
2:B:861:ALA:HB3	2:B:863:THR:HG23	2.01	0.43
2:B:1505:LEU:O	2:B:1523:ASN:N	2.52	0.43
1:C:29:MET:HB3	1:C:35:LYS:HG2	2.01	0.43
2:D:796:ALA:HB3	2:D:798:ILE:HG13	2.00	0.43
2:D:4611:LEU:HD21	2:D:4617:TYR:HD2	1.84	0.43
2:F:836:HIS:CE1	2:F:1610:ARG:HB2	2.54	0.43
2:F:2103:LEU:HA	2:F:2106:THR:HG22	2.00	0.43
2:F:2123:SER:O	2:F:2126:GLN:NE2	2.51	0.43
2:F:2212:GLN:HE22	2:F:2250:ASP:H	1.65	0.43
2:F:4750:GLY:H	2:F:4755:ARG:HE	1.67	0.43
2:H:1466:THR:HG22	2:H:1482:ARG:HA	2.01	0.43
2:H:2102:ALA:O	2:H:2106:THR:N	2.46	0.43
2:H:2123:SER:O	2:H:2126:GLN:NE2	2.51	0.43
2:B:2793:THR:OG1	2:B:2901:GLY:O	2.30	0.43
2:B:3797:LEU:HD23	2:B:3797:LEU:HA	1.88	0.43
2:B:4766:LYS:HE3	2:B:4770:LEU:HD11	2.00	0.43
2:D:1104:GLU:HG2	2:D:1216:ASN:HB2	2.00	0.43
2:D:1449:ASP:OD1	2:D:1449:ASP:N	2.52	0.43
2:D:1696:GLY:HA2	2:D:1699:ARG:HB3	2.00	0.43
2:D:2198:CYS:HA	2:D:2201:LEU:HD12	2.01	0.43
2:D:3997:GLY:HA2	2:D:4000:MET:SD	2.59	0.43
2:D:4023:LYS:HA	2:D:4026:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4713:VAL:O	2:D:4716:THR:OG1	2.27	0.43
2:F:1176:THR:HG22	2:F:1181:ILE:HG12	2.01	0.43
2:H:1114:ARG:HH12	2:H:1127:GLU:HB3	1.82	0.43
2:H:1190:LEU:HD12	2:H:1193:LYS:HE2	2.00	0.43
2:H:1228:THR:HA	2:H:1232:LEU:HD12	1.99	0.43
2:H:1445:TRP:HB3	2:H:1539:LEU:HD13	2.00	0.43
2:H:1675:ALA:O	2:H:1679:HIS:ND1	2.48	0.43
2:H:3907:PHE:HD2	2:H:3968:LEU:HD11	1.82	0.43
2:H:4713:VAL:O	2:H:4716:THR:OG1	2.27	0.43
1:A:75:THR:HA	1:A:98:ILE:HA	1.99	0.43
2:B:256:GLN:O	2:B:304:LYS:NZ	2.48	0.43
2:B:452:VAL:O	2:B:456:LEU:HB2	2.19	0.43
2:B:1466:THR:HG22	2:B:1482:ARG:HA	2.01	0.43
2:B:3800:SER:OG	2:B:3801:CYS:N	2.51	0.43
2:B:4521:TYR:H	2:H:4810:MET:CG	2.32	0.43
2:D:861:ALA:HB3	2:D:863:THR:HG23	2.01	0.43
2:D:1434:PRO:HD2	2:D:1552:VAL:HG23	2.00	0.43
2:F:35:LEU:HA	2:F:51:SER:HA	2.01	0.43
2:F:207:PHE:CG	2:H:2326:ILE:CG2	3.01	0.43
2:F:1449:ASP:OD1	2:F:1449:ASP:N	2.52	0.43
2:F:1466:THR:HG22	2:F:1482:ARG:HA	2.01	0.43
2:F:3798:MET:SD	2:F:3874:SER:OG	2.77	0.43
2:F:4632:ASP:OD1	2:F:4709:TRP:NE1	2.48	0.43
2:H:233:VAL:HG22	2:H:276:ARG:HB2	2.01	0.43
2:H:297:LEU:HD23	2:H:297:LEU:HA	1.87	0.43
2:H:836:HIS:CE1	2:H:1610:ARG:HB2	2.54	0.43
2:H:2731:ASP:HB3	2:H:2826:ALA:HB2	2.00	0.43
2:H:4778:VAL:O	2:H:4782:TYR:HB2	2.19	0.43
2:B:644:LEU:HB2	2:B:1654:HIS:HD2	1.84	0.43
2:B:796:ALA:HB3	2:B:798:ILE:HG13	2.00	0.43
2:D:1228:THR:HA	2:D:1232:LEU:HD12	1.99	0.43
2:D:2103:LEU:HA	2:D:2106:THR:HG22	2.00	0.43
2:D:2464:ASP:OD1	2:D:2464:ASP:N	2.50	0.43
1:E:29:MET:HB3	1:E:35:LYS:HG2	2.01	0.43
2:F:434:ASP:OD1	2:F:504:ARG:NE	2.40	0.43
2:F:452:VAL:O	2:F:456:LEU:HB2	2.19	0.43
2:F:626:ARG:NH2	2:F:1668:GLY:O	2.36	0.43
2:F:2731:ASP:HB3	2:F:2826:ALA:HB2	2.00	0.43
2:F:3997:GLY:HA2	2:F:4000:MET:SD	2.59	0.43
2:F:4737:ASN:HA	2:F:4740:PHE:HB2	2.01	0.43
2:H:794:PHE:HE2	2:H:1621:CYS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:796:ALA:HB3	2:H:798:ILE:HG13	2.00	0.43
2:H:2198:CYS:HA	2:H:2201:LEU:HD12	2.01	0.43
2:H:2473:LEU:HD12	2:H:2477:TYR:HD2	1.83	0.43
2:H:3831:LEU:HA	2:H:3832:GLN:HA	1.57	0.43
2:H:4737:ASN:HA	2:H:4740:PHE:HB2	2.01	0.43
2:B:647:ARG:HA	2:B:647:ARG:HD2	1.84	0.43
2:B:1170:GLU:O	2:B:1172:THR:N	2.49	0.43
2:B:1190:LEU:HD12	2:B:1193:LYS:HE2	2.00	0.43
2:B:2326:ILE:HG23	2:H:207:PHE:CG	2.53	0.43
2:D:256:GLN:O	2:D:304:LYS:NZ	2.48	0.43
2:F:305:TYR:HE2	2:F:319:LYS:HG2	1.83	0.43
2:F:335:LYS:NZ	2:F:401:ASP:OD2	2.46	0.43
2:F:844:ARG:NH1	2:F:849:ASP:OD2	2.51	0.43
2:F:1190:LEU:HD12	2:F:1193:LYS:HE2	2.00	0.43
2:F:2834:LEU:HB2	2:F:2839:HIS:CE1	2.54	0.43
2:F:4652:ARG:HA	2:F:4655:MET:HB2	2.01	0.43
1:G:29:MET:HB3	1:G:35:LYS:HG2	2.01	0.43
2:H:439:LYS:HD3	2:H:441:LYS:HB2	2.01	0.43
2:H:551:PHE:HD1	2:H:551:PHE:HA	1.70	0.43
2:B:794:PHE:HE2	2:B:1621:CYS:HB2	1.83	0.42
2:B:836:HIS:CE1	2:B:1610:ARG:HB2	2.54	0.42
2:B:1033:VAL:HG23	2:B:1038:LEU:HB3	2.01	0.42
2:B:1250:TRP:HB3	2:B:1600:PRO:HB2	2.01	0.42
2:B:1809:PRO:HA	2:B:1817:LEU:HD13	2.01	0.42
2:B:4046:LYS:HA	2:B:4049:PHE:HB3	2.01	0.42
2:B:4576:LEU:HD13	2:B:4579:LEU:HD22	2.01	0.42
2:D:644:LEU:HB2	2:D:1654:HIS:HD2	1.84	0.42
2:D:1789:ALA:HA	2:D:1792:ILE:HD12	2.01	0.42
2:D:4834:ASP:OD1	2:D:4834:ASP:N	2.52	0.42
2:F:763:ALA:O	2:F:765:SER:N	2.51	0.42
2:F:1104:GLU:HG2	2:F:1216:ASN:HB2	2.00	0.42
2:F:4193:PHE:O	2:F:4197:THR:OG1	2.25	0.42
2:F:4576:LEU:HD13	2:F:4579:LEU:HD22	2.01	0.42
2:H:452:VAL:O	2:H:456:LEU:HB2	2.19	0.42
2:H:644:LEU:HB2	2:H:1654:HIS:HD2	1.84	0.42
2:H:1250:TRP:HB3	2:H:1600:PRO:HB2	2.01	0.42
2:H:1676:LEU:HD23	2:H:1676:LEU:HA	1.87	0.42
2:H:4046:LYS:HA	2:H:4049:PHE:HB3	2.01	0.42
2:H:4652:ARG:HA	2:H:4655:MET:HB2	2.01	0.42
2:H:4750:GLY:H	2:H:4755:ARG:HE	1.66	0.42
1:A:29:MET:HB3	1:A:35:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3730:ALA:HA	2:B:3733:HIS:CE1	2.54	0.42
2:B:4757:ILE:O	2:B:4760:SER:OG	2.29	0.42
2:B:4778:VAL:O	2:B:4782:TYR:HB2	2.19	0.42
2:B:4863:ILE:HG21	2:H:4857:VAL:HG13	1.96	0.42
2:D:233:VAL:HG22	2:D:276:ARG:HB2	2.01	0.42
2:D:1170:GLU:O	2:D:1172:THR:N	2.49	0.42
2:D:1602:GLN:HB3	2:D:1604:LEU:HD12	2.00	0.42
2:D:1611:ILE:N	2:D:1620:GLN:O	2.44	0.42
2:D:3682:LYS:HZ3	2:D:3684:GLU:HG2	1.83	0.42
2:F:1676:LEU:HD23	2:F:1676:LEU:HA	1.87	0.42
2:F:2473:LEU:HD12	2:F:2477:TYR:HD2	1.83	0.42
2:F:4023:LYS:HA	2:F:4026:ASP:HB2	2.01	0.42
2:H:861:ALA:HB3	2:H:863:THR:HG23	2.01	0.42
2:H:1434:PRO:HD2	2:H:1552:VAL:HG23	2.00	0.42
2:H:1757:LEU:HD13	2:H:1757:LEU:HA	1.83	0.42
2:H:1809:PRO:HA	2:H:1817:LEU:HD13	2.01	0.42
2:H:4750:GLY:H	2:H:4755:ARG:NE	2.16	0.42
2:B:1090:ALA:HA	2:B:1249:MET:HG2	2.02	0.42
2:B:1434:PRO:HD2	2:B:1552:VAL:HG23	2.00	0.42
2:B:1789:ALA:HA	2:B:1792:ILE:HD12	2.01	0.42
2:B:3997:GLY:HA2	2:B:4000:MET:SD	2.59	0.42
2:D:77:ALA:HB2	2:F:3891:TRP:CH2	2.54	0.42
2:D:439:LYS:HD3	2:D:441:LYS:HB2	2.01	0.42
2:D:794:PHE:HE2	2:D:1621:CYS:HB2	1.83	0.42
2:D:1086:ARG:N	2:D:1207:LEU:O	2.48	0.42
2:D:1190:LEU:HD12	2:D:1193:LYS:HE2	2.00	0.42
2:D:1809:PRO:HA	2:D:1817:LEU:HD13	2.01	0.42
2:D:4652:ARG:HA	2:D:4655:MET:HB2	2.01	0.42
2:F:794:PHE:HE2	2:F:1621:CYS:HB2	1.83	0.42
2:F:1033:VAL:HG23	2:F:1038:LEU:HB3	2.01	0.42
2:F:1505:LEU:O	2:F:1523:ASN:N	2.52	0.42
2:F:3730:ALA:HA	2:F:3733:HIS:CE1	2.54	0.42
2:F:4202:GLN:O	2:F:4206:GLN:HB3	2.20	0.42
2:H:256:GLN:O	2:H:304:LYS:NZ	2.47	0.42
2:H:1153:GLY:N	2:H:1183:LEU:O	2.53	0.42
2:H:4061:GLN:O	2:H:4064:THR:OG1	2.27	0.42
2:H:4635:VAL:O	2:H:4638:THR:OG1	2.31	0.42
2:B:35:LEU:HA	2:B:51:SER:HA	2.01	0.42
2:B:1696:GLY:HA2	2:B:1699:ARG:HB3	2.00	0.42
2:B:2422:SER:O	2:B:2426:SER:N	2.48	0.42
2:B:4652:ARG:HA	2:B:4655:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4792:LYS:HE3	2:B:4792:LYS:HB3	1.92	0.42
2:D:766:ILE:HB	2:D:779:PHE:HB2	2.00	0.42
2:D:844:ARG:NH1	2:D:849:ASP:OD2	2.51	0.42
2:D:1466:THR:HG22	2:D:1482:ARG:HA	2.01	0.42
2:D:1926:ILE:HD12	2:D:1926:ILE:HA	1.89	0.42
1:E:44:LYS:HA	1:E:45:PRO:HD3	1.90	0.42
2:F:875:PRO:HG2	2:F:878:LEU:HD12	2.02	0.42
2:F:3800:SER:OG	2:F:3801:CYS:N	2.51	0.42
2:F:4766:LYS:HE3	2:F:4770:LEU:HD11	2.00	0.42
2:F:4778:VAL:O	2:F:4782:TYR:HB2	2.19	0.42
2:H:1090:ALA:HA	2:H:1249:MET:HG2	2.02	0.42
2:H:1764:SER:N	2:H:1779:SER:O	2.53	0.42
2:B:207:PHE:CG	2:D:2326:ILE:HG23	2.55	0.42
2:B:306:LEU:HG	2:B:314:LEU:HD11	2.00	0.42
2:B:766:ILE:HB	2:B:779:PHE:HB2	2.00	0.42
2:B:875:PRO:HG2	2:B:878:LEU:HD12	2.02	0.42
2:B:897:LYS:HE2	2:B:915:HIS:CG	2.55	0.42
2:B:2067:MET:HB3	2:B:2067:MET:HE3	1.79	0.42
2:B:4811:LEU:O	2:B:4814:TYR:HB3	2.19	0.42
2:D:2894:LEU:HA	2:D:2897:LEU:HD12	2.02	0.42
2:D:4202:GLN:O	2:D:4206:GLN:HB3	2.20	0.42
2:F:796:ALA:HB3	2:F:798:ILE:HG13	2.00	0.42
2:F:897:LYS:HE2	2:F:915:HIS:CG	2.55	0.42
2:F:1628:MET:HB2	2:F:1687:TYR:HE2	1.84	0.42
2:F:3797:LEU:HD23	2:F:3797:LEU:HA	1.88	0.42
2:F:4611:LEU:HD21	2:F:4617:TYR:HD2	1.84	0.42
2:H:682:THR:H	2:H:751:THR:HG22	1.85	0.42
2:H:763:ALA:O	2:H:765:SER:N	2.52	0.42
2:H:1628:MET:HB2	2:H:1687:TYR:HE2	1.84	0.42
2:H:1696:GLY:HA2	2:H:1699:ARG:HB3	2.00	0.42
2:H:2419:ARG:O	2:H:2422:SER:OG	2.38	0.42
2:H:3997:GLY:HA2	2:H:4000:MET:SD	2.59	0.42
2:H:4104:THR:O	2:H:4107:SER:OG	2.35	0.42
2:H:4811:LEU:O	2:H:4814:TYR:HB3	2.20	0.42
2:B:233:VAL:HG22	2:B:276:ARG:HB2	2.01	0.42
2:B:394:HIS:CD2	2:B:396:GLU:H	2.38	0.42
2:B:1176:THR:HG22	2:B:1181:ILE:HG12	2.01	0.42
2:B:1628:MET:HB2	2:B:1687:TYR:HE2	1.84	0.42
2:B:1764:SER:N	2:B:1779:SER:O	2.53	0.42
2:B:3798:MET:SD	2:B:3874:SER:OG	2.77	0.42
2:B:3834:ASP:OD1	2:B:3834:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4037:ASP:OD2	2:B:4041:LYS:N	2.53	0.42
2:D:416:ALA:HA	2:D:419:ILE:HD12	2.01	0.42
2:D:661:LEU:O	2:D:788:PHE:N	2.53	0.42
2:D:763:ALA:O	2:D:765:SER:N	2.51	0.42
2:D:1176:THR:HG22	2:D:1181:ILE:HG12	2.01	0.42
2:D:3762:LEU:HD12	2:D:3762:LEU:HA	1.86	0.42
2:F:233:VAL:HG22	2:F:276:ARG:HB2	2.00	0.42
2:F:420:ARG:HA	2:F:423:VAL:HB	2.02	0.42
2:F:644:LEU:HB2	2:F:1654:HIS:HD2	1.84	0.42
2:F:1611:ILE:N	2:F:1620:GLN:O	2.43	0.42
2:F:2894:LEU:HA	2:F:2897:LEU:HD12	2.02	0.42
2:H:394:HIS:CD2	2:H:396:GLU:H	2.38	0.42
2:H:897:LYS:HE2	2:H:915:HIS:CG	2.55	0.42
2:H:1505:LEU:O	2:H:1523:ASN:N	2.52	0.42
2:H:2222:LEU:O	2:H:2226:SER:N	2.35	0.42
2:H:3798:MET:SD	2:H:3874:SER:OG	2.77	0.42
2:H:4202:GLN:O	2:H:4206:GLN:HB3	2.20	0.42
2:H:4611:LEU:HD21	2:H:4617:TYR:HD2	1.84	0.42
2:B:52:THR:HG22	2:B:60:PRO:HG3	2.02	0.42
2:B:682:THR:H	2:B:751:THR:HG22	1.85	0.42
2:B:1732:GLU:O	2:B:1735:SER:OG	2.31	0.42
2:B:2464:ASP:OD1	2:B:2464:ASP:N	2.50	0.42
2:B:4093:LYS:HE2	2:B:4093:LYS:HB3	1.84	0.42
2:B:4750:GLY:H	2:B:4755:ARG:HE	1.66	0.42
1:C:21:THR:OG1	1:C:49:ARG:NE	2.50	0.42
2:D:305:TYR:HE2	2:D:319:LYS:HG2	1.84	0.42
2:D:306:LEU:HG	2:D:314:LEU:HD11	2.00	0.42
2:D:678:MET:O	2:D:801:ARG:N	2.46	0.42
2:D:4518:LEU:HD13	2:D:4521:TYR:HE2	1.80	0.42
2:F:77:ALA:HB2	2:H:3891:TRP:CH2	2.54	0.42
2:F:121:LEU:HD23	2:F:121:LEU:HA	1.86	0.42
2:F:647:ARG:HD2	2:F:647:ARG:HA	1.84	0.42
2:F:861:ALA:HB3	2:F:863:THR:HG23	2.01	0.42
2:F:1153:GLY:N	2:F:1183:LEU:O	2.53	0.42
2:F:2198:CYS:HA	2:F:2201:LEU:HD12	2.01	0.42
2:H:35:LEU:HA	2:H:51:SER:HA	2.01	0.42
2:H:1170:GLU:O	2:H:1172:THR:N	2.49	0.42
1:A:82:TYR:OH	2:B:1768:PHE:O	2.28	0.42
2:B:305:TYR:HE2	2:B:319:LYS:HG2	1.84	0.42
2:B:439:LYS:HD3	2:B:441:LYS:HB2	2.01	0.42
2:B:1153:GLY:N	2:B:1183:LEU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1445:TRP:HB3	2:B:1539:LEU:HD13	2.00	0.42
2:B:2198:CYS:HA	2:B:2201:LEU:HD12	2.01	0.42
2:B:2731:ASP:HB3	2:B:2826:ALA:HB2	2.00	0.42
2:B:2988:SER:O	2:B:2992:CYS:N	2.47	0.42
2:D:52:THR:HG22	2:D:60:PRO:HG3	2.02	0.42
2:D:3834:ASP:N	2:D:3834:ASP:OD1	2.53	0.42
2:F:1250:TRP:HB3	2:F:1600:PRO:HB2	2.01	0.42
2:F:1572:LYS:HB3	2:F:1584:PRO:HA	2.01	0.42
2:F:1626:GLN:O	2:F:1687:TYR:OH	2.36	0.42
2:F:2843:GLU:OE2	2:F:2875:TYR:OH	2.34	0.42
2:F:2988:SER:O	2:F:2992:CYS:N	2.47	0.42
2:H:52:THR:HG22	2:H:60:PRO:HG3	2.02	0.42
2:H:305:TYR:HE2	2:H:319:LYS:HG2	1.83	0.42
2:H:4036:TYR:HE2	2:H:4048:ASP:HB3	1.85	0.42
2:H:4093:LYS:HE2	2:H:4093:LYS:HB3	1.84	0.42
2:H:4576:LEU:HD13	2:H:4579:LEU:HD22	2.01	0.42
1:A:15:PHE:HA	1:A:67:SER:HA	2.01	0.42
2:B:661:LEU:O	2:B:788:PHE:N	2.53	0.42
2:B:3891:TRP:CZ3	2:H:77:ALA:HA	2.54	0.42
2:B:4737:ASN:HA	2:B:4740:PHE:HB2	2.01	0.42
2:D:1628:MET:HB2	2:D:1687:TYR:HE2	1.84	0.42
2:D:3730:ALA:HA	2:D:3733:HIS:CE1	2.54	0.42
2:D:4766:LYS:HE3	2:D:4770:LEU:HD11	2.00	0.42
1:E:15:PHE:HA	1:E:67:SER:HA	2.02	0.42
2:F:2419:ARG:O	2:F:2422:SER:OG	2.38	0.42
2:B:554:SER:O	2:B:558:LEU:N	2.49	0.42
2:B:763:ALA:O	2:B:765:SER:N	2.51	0.42
2:B:2731:ASP:OD1	2:B:2822:TYR:OH	2.30	0.42
2:B:2834:LEU:HB2	2:B:2839:HIS:CE1	2.54	0.42
2:B:3897:ASP:OD1	2:B:3958:LYS:NZ	2.40	0.42
2:B:4808:ASP:OD2	2:D:4523:VAL:HG11	2.20	0.42
2:D:452:VAL:O	2:D:456:LEU:HB2	2.19	0.42
2:D:1572:LYS:HB3	2:D:1584:PRO:HA	2.02	0.42
2:D:1607:ASP:HB3	2:D:1608:VAL:HG23	2.02	0.42
2:D:3854:ASP:OD1	2:D:3854:ASP:N	2.53	0.42
2:D:4036:TYR:HE2	2:D:4048:ASP:HB3	1.85	0.42
2:D:4037:ASP:OD2	2:D:4041:LYS:N	2.53	0.42
2:D:4737:ASN:HA	2:D:4740:PHE:HB2	2.01	0.42
2:D:4767:GLN:CG	2:F:4753:THR:OG1	2.67	0.42
2:D:4810:MET:HB3	2:F:4519:LEU:HA	2.01	0.42
2:F:119:ILE:HD13	2:F:162:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:SER:HB3	2:F:202:HIS:HB2	2.02	0.42
2:F:394:HIS:CD2	2:F:396:GLU:H	2.38	0.42
2:F:1732:GLU:O	2:F:1735:SER:OG	2.31	0.42
2:H:1176:THR:HG22	2:H:1181:ILE:HG12	2.01	0.42
2:H:2834:LEU:HB2	2:H:2839:HIS:CE1	2.54	0.42
2:B:123:HIS:CD2	2:B:126:SER:H	2.38	0.41
2:B:626:ARG:NH2	2:B:1668:GLY:O	2.36	0.41
2:B:3677:LEU:HD23	2:B:3677:LEU:HA	1.91	0.41
2:B:4863:ILE:HG22	2:H:4857:VAL:HG13	1.98	0.41
2:D:394:HIS:CD2	2:D:396:GLU:H	2.38	0.41
2:D:682:THR:H	2:D:751:THR:HG22	1.85	0.41
2:D:897:LYS:HE2	2:D:915:HIS:CG	2.55	0.41
2:D:1090:ALA:HA	2:D:1249:MET:HG2	2.02	0.41
2:D:1250:TRP:HB3	2:D:1600:PRO:HB2	2.01	0.41
2:F:620:CYS:N	2:F:623:VAL:O	2.39	0.41
2:F:4036:TYR:HE2	2:F:4048:ASP:HB3	1.85	0.41
2:F:4046:LYS:HA	2:F:4049:PHE:HB3	2.01	0.41
2:F:4834:ASP:N	2:F:4834:ASP:OD1	2.52	0.41
2:H:1033:VAL:HG23	2:H:1038:LEU:HB3	2.01	0.41
2:H:2834:LEU:HD22	2:H:2838:LEU:HB3	2.02	0.41
2:H:4037:ASP:OD2	2:H:4041:LYS:N	2.53	0.41
2:B:1607:ASP:HB3	2:B:1608:VAL:HG23	2.02	0.41
2:B:2326:ILE:CG2	2:H:207:PHE:CG	3.02	0.41
2:B:2894:LEU:HA	2:B:2897:LEU:HD12	2.02	0.41
2:B:3983:LEU:HD12	2:B:3983:LEU:HA	1.88	0.41
2:D:35:LEU:HA	2:D:51:SER:HA	2.01	0.41
2:D:119:ILE:HD13	2:D:162:ILE:HD11	2.02	0.41
2:D:875:PRO:HG2	2:D:878:LEU:HD12	2.02	0.41
2:D:4808:ASP:OD2	2:F:4523:VAL:HG11	2.19	0.41
2:F:52:THR:HG22	2:F:60:PRO:HG3	2.02	0.41
2:F:290:ARG:HA	2:F:353:GLU:HG2	2.02	0.41
2:F:1809:PRO:HA	2:F:1817:LEU:HD13	2.02	0.41
2:F:3993:ASN:HD22	2:F:4110:MET:HA	1.84	0.41
2:H:130:LEU:HA	2:H:149:LEU:HD23	2.03	0.41
2:H:195:SER:HB3	2:H:202:HIS:HB2	2.02	0.41
2:H:420:ARG:HA	2:H:423:VAL:HB	2.02	0.41
2:H:585:ALA:HA	2:H:588:ILE:HD12	2.02	0.41
2:H:647:ARG:HD2	2:H:647:ARG:HA	1.84	0.41
2:H:2730:HIS:CE1	2:H:2764:LEU:HD11	2.56	0.41
2:H:4023:LYS:HA	2:H:4026:ASP:HB2	2.01	0.41
2:B:551:PHE:HD1	2:B:551:PHE:HA	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4810:MET:CG	2:D:4521:TYR:H	2.34	0.41
2:D:195:SER:HB3	2:D:202:HIS:HB2	2.02	0.41
2:D:2731:ASP:HB3	2:D:2826:ALA:HB2	2.00	0.41
2:D:3993:ASN:HD22	2:D:4110:MET:HA	1.84	0.41
2:D:4046:LYS:HA	2:D:4049:PHE:HB3	2.01	0.41
2:D:4778:VAL:O	2:D:4782:TYR:HB2	2.19	0.41
1:E:21:THR:OG1	1:E:49:ARG:NE	2.50	0.41
2:F:64:ILE:H	2:F:64:ILE:HG13	1.74	0.41
2:F:1090:ALA:HA	2:F:1249:MET:HG2	2.01	0.41
2:F:1607:ASP:HB3	2:F:1608:VAL:HG23	2.02	0.41
2:F:3760:LEU:HD23	2:F:3760:LEU:HA	1.89	0.41
2:F:3854:ASP:N	2:F:3854:ASP:OD1	2.53	0.41
2:F:4037:ASP:OD2	2:F:4041:LYS:N	2.53	0.41
2:F:4810:MET:HB3	2:H:4519:LEU:HA	2.01	0.41
2:H:412:GLU:O	2:H:415:THR:OG1	2.33	0.41
2:H:1253:LYS:HD2	2:H:1255:LEU:HB2	2.02	0.41
2:H:1607:ASP:HB3	2:H:1608:VAL:HG23	2.02	0.41
2:H:2464:ASP:N	2:H:2464:ASP:OD1	2.50	0.41
2:H:3730:ALA:HA	2:H:3733:HIS:CE1	2.54	0.41
2:B:77:ALA:HA	2:D:3891:TRP:CZ3	2.56	0.41
2:B:372:LEU:HD11	2:B:391:ALA:HB1	2.03	0.41
2:B:416:ALA:O	2:B:420:ARG:NH2	2.51	0.41
2:B:782:PHE:HZ	2:B:1467:VAL:HG22	1.86	0.41
2:B:2730:HIS:CE1	2:B:2764:LEU:HD11	2.56	0.41
2:D:1505:LEU:O	2:D:1523:ASN:N	2.52	0.41
2:D:2834:LEU:HB2	2:D:2839:HIS:CE1	2.54	0.41
2:D:4011:VAL:HA	2:D:4014:ILE:HG12	2.03	0.41
2:F:682:THR:H	2:F:751:THR:HG22	1.85	0.41
2:F:1843:LEU:O	2:F:1846:ILE:N	2.54	0.41
2:B:195:SER:HB3	2:B:202:HIS:HB2	2.02	0.41
2:B:416:ALA:HA	2:B:419:ILE:HD12	2.02	0.41
2:B:2834:LEU:HD22	2:B:2838:LEU:HB3	2.02	0.41
2:D:420:ARG:HA	2:D:423:VAL:HB	2.02	0.41
2:D:1843:LEU:O	2:D:1846:ILE:N	2.54	0.41
2:F:1764:SER:N	2:F:1779:SER:O	2.53	0.41
2:F:3983:LEU:HD12	2:F:3983:LEU:HA	1.87	0.41
2:F:4189:LEU:HA	2:F:4192:ASN:HD22	1.86	0.41
2:H:123:HIS:CD2	2:H:126:SER:H	2.38	0.41
2:H:1156:TRP:CZ3	2:H:1158:ALA:HA	2.56	0.41
2:H:1572:LYS:HB3	2:H:1584:PRO:HA	2.02	0.41
2:H:1738:LEU:HD21	2:H:2039:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2843:GLU:OE2	2:H:2875:TYR:OH	2.34	0.41
2:H:3797:LEU:HA	2:H:3797:LEU:HD23	1.88	0.41
2:H:3834:ASP:OD1	2:H:3834:ASP:N	2.53	0.41
2:H:4189:LEU:HA	2:H:4192:ASN:HD22	1.86	0.41
2:B:585:ALA:HA	2:B:588:ILE:HD12	2.02	0.41
2:B:1169:THR:OG1	2:B:1170:GLU:N	2.54	0.41
2:B:1285:VAL:HG12	2:B:1286:THR:HG23	2.03	0.41
2:B:3854:ASP:OD1	2:B:3854:ASP:N	2.53	0.41
2:B:4863:ILE:HG22	2:H:4857:VAL:HG11	2.01	0.41
1:C:15:PHE:HA	1:C:67:SER:HA	2.02	0.41
2:D:554:SER:O	2:D:558:LEU:N	2.49	0.41
2:D:1033:VAL:HG23	2:D:1038:LEU:HB3	2.01	0.41
2:D:2063:ILE:O	2:D:2067:MET:HG2	2.21	0.41
2:D:3897:ASP:OD1	2:D:3958:LYS:NZ	2.40	0.41
2:D:4811:LEU:O	2:D:4814:TYR:HB3	2.19	0.41
2:F:1156:TRP:CZ3	2:F:1158:ALA:HA	2.56	0.41
2:F:1253:LYS:HD2	2:F:1255:LEU:HB2	2.02	0.41
2:F:1267:HIS:NE2	2:F:1293:GLN:OE1	2.53	0.41
2:F:1738:LEU:HD21	2:F:2039:TYR:HE1	1.86	0.41
2:F:2063:ILE:O	2:F:2067:MET:HG2	2.21	0.41
2:F:4811:LEU:O	2:F:4814:TYR:HB3	2.20	0.41
2:F:4889:CYS:HB2	2:F:4892:CYS:HB3	2.03	0.41
2:H:290:ARG:HA	2:H:353:GLU:HG2	2.02	0.41
2:H:875:PRO:HG2	2:H:878:LEU:HD12	2.02	0.41
2:H:1449:ASP:OD1	2:H:1449:ASP:N	2.52	0.41
2:B:290:ARG:HA	2:B:353:GLU:HG2	2.02	0.41
2:B:1156:TRP:CZ3	2:B:1158:ALA:HA	2.56	0.41
2:B:3748:SER:O	2:B:3793:SER:OG	2.30	0.41
2:B:3993:ASN:HD22	2:B:4110:MET:HA	1.84	0.41
2:B:4189:LEU:HA	2:B:4192:ASN:HD22	1.86	0.41
2:D:123:HIS:CD2	2:D:126:SER:H	2.38	0.41
2:D:585:ALA:HA	2:D:588:ILE:HD12	2.02	0.41
2:D:782:PHE:HZ	2:D:1467:VAL:HG22	1.86	0.41
2:D:1153:GLY:N	2:D:1183:LEU:O	2.53	0.41
2:D:1156:TRP:CZ3	2:D:1158:ALA:HA	2.56	0.41
2:D:4810:MET:CG	2:F:4521:TYR:H	2.34	0.41
2:F:2730:HIS:CE1	2:F:2764:LEU:HD11	2.56	0.41
2:F:4865:GLY:HA2	2:H:4868:ILE:HD11	2.03	0.41
2:H:64:ILE:H	2:H:64:ILE:HG13	1.74	0.41
2:H:372:LEU:HD11	2:H:391:ALA:HB1	2.03	0.41
2:H:554:SER:O	2:H:558:LEU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1169:THR:OG1	2:H:1170:GLU:N	2.54	0.41
2:H:4834:ASP:OD1	2:H:4834:ASP:N	2.52	0.41
2:B:370:LEU:HB2	2:B:393:MET:HE3	2.03	0.41
2:B:411:GLU:HA	2:B:414:ARG:HB2	2.03	0.41
2:B:1843:LEU:O	2:B:1846:ILE:N	2.54	0.41
2:B:2063:ILE:O	2:B:2067:MET:HG2	2.21	0.41
2:D:4814:TYR:CE2	2:D:4815:MET:CE	2.95	0.41
2:F:416:ALA:HA	2:F:419:ILE:HD12	2.02	0.41
2:F:1757:LEU:HA	2:F:1757:LEU:HD13	1.83	0.41
2:F:4125:SER:HA	2:F:4128:ASN:HD22	1.86	0.41
2:F:4857:VAL:HG13	2:H:4863:ILE:HG22	1.96	0.41
2:H:416:ALA:HA	2:H:419:ILE:HD12	2.02	0.41
2:H:1843:LEU:HD23	2:H:1843:LEU:HA	1.88	0.41
2:H:3993:ASN:HD22	2:H:4110:MET:HA	1.84	0.41
2:H:4011:VAL:HA	2:H:4014:ILE:HG12	2.03	0.41
2:H:4518:LEU:HD23	2:H:4518:LEU:H	1.86	0.41
2:H:4757:ILE:O	2:H:4760:SER:OG	2.29	0.41
1:A:21:THR:OG1	1:A:49:ARG:NE	2.50	0.41
2:B:26:ALA:O	2:B:33:GLN:N	2.49	0.41
2:B:130:LEU:HA	2:B:149:LEU:HD23	2.03	0.41
2:B:420:ARG:HA	2:B:423:VAL:HB	2.02	0.41
2:B:1676:LEU:HD23	2:B:1676:LEU:HA	1.87	0.41
2:B:1738:LEU:HD21	2:B:2039:TYR:HE1	1.86	0.41
2:B:3762:LEU:HD12	2:B:3762:LEU:HA	1.86	0.41
2:B:4202:GLN:O	2:B:4206:GLN:HB3	2.20	0.41
2:B:4611:LEU:HD21	2:B:4617:TYR:HD2	1.84	0.41
2:D:130:LEU:HA	2:D:149:LEU:HD23	2.03	0.41
2:D:150:GLN:NE2	2:D:152:ASP:O	2.54	0.41
2:D:370:LEU:HB2	2:D:393:MET:HE3	2.03	0.41
2:D:486:GLN:OE1	2:D:547:ASN:ND2	2.54	0.41
2:D:3767:LEU:HD23	2:D:3767:LEU:HA	1.84	0.41
2:D:4780:TYR:OH	2:F:4518:LEU:HB2	2.21	0.41
2:D:4808:ASP:CG	2:F:4523:VAL:CG2	2.63	0.41
2:D:4889:CYS:HB2	2:D:4892:CYS:HB3	2.03	0.41
2:F:123:HIS:CD2	2:F:126:SER:H	2.38	0.41
2:F:415:THR:O	2:F:419:ILE:HG13	2.21	0.41
2:F:1440:ASN:HB2	2:F:1548:THR:HG21	2.03	0.41
2:F:1789:ALA:HA	2:F:1792:ILE:HD12	2.01	0.41
2:F:1999:ASP:O	2:F:2003:ASP:N	2.54	0.41
1:G:15:PHE:HA	1:G:67:SER:HA	2.02	0.41
2:H:121:LEU:HD23	2:H:121:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1157:GLN:N	2:H:1160:ASP:OD2	2.54	0.41
2:H:1177:LEU:N	2:H:1180:GLU:O	2.54	0.41
2:H:1285:VAL:HG12	2:H:1286:THR:HG23	2.03	0.41
2:H:1999:ASP:O	2:H:2003:ASP:N	2.54	0.41
2:H:2011:GLU:O	2:H:2027:ARG:NH2	2.54	0.41
2:H:2063:ILE:O	2:H:2067:MET:HG2	2.21	0.41
2:H:2894:LEU:HA	2:H:2897:LEU:HD12	2.02	0.41
2:H:3831:LEU:HA	2:H:3831:LEU:HD23	1.85	0.41
2:B:486:GLN:OE1	2:B:547:ASN:ND2	2.54	0.41
2:B:1136:ALA:HB3	2:B:1145:TRP:HB2	2.03	0.41
2:B:2326:ILE:HD12	2:H:207:PHE:HZ	1.72	0.41
2:D:1440:ASN:HB2	2:D:1548:THR:HG21	2.03	0.41
2:D:1753:LEU:HD11	2:D:1921:HIS:CD2	2.56	0.41
2:D:1764:SER:N	2:D:1779:SER:O	2.53	0.41
2:D:2067:MET:HE3	2:D:2067:MET:HB3	1.79	0.41
2:D:2549:LEU:O	2:D:2553:VAL:N	2.54	0.41
2:D:4189:LEU:HA	2:D:4192:ASN:HD22	1.86	0.41
2:F:123:HIS:NE2	2:F:125:TYR:HB3	2.36	0.41
2:F:130:LEU:HA	2:F:149:LEU:HD23	2.03	0.41
2:F:486:GLN:OE1	2:F:547:ASN:ND2	2.54	0.41
2:F:2088:LEU:O	2:F:2092:GLN:HG2	2.21	0.41
2:F:2177:VAL:HG22	2:F:2221:TYR:CZ	2.56	0.41
2:F:4113:ASP:O	2:F:4117:GLN:N	2.46	0.41
2:H:486:GLN:OE1	2:H:547:ASN:ND2	2.54	0.41
2:H:1255:LEU:HA	2:H:1256:PRO:HD3	1.88	0.41
2:H:1611:ILE:N	2:H:1620:GLN:O	2.44	0.41
2:H:1789:ALA:HA	2:H:1792:ILE:HD12	2.01	0.41
2:H:2298:ARG:HD3	2:H:2298:ARG:HA	1.90	0.41
2:H:3767:LEU:HA	2:H:3767:LEU:HD23	1.84	0.41
2:B:123:HIS:NE2	2:B:125:TYR:HB3	2.36	0.40
2:B:1572:LYS:HB3	2:B:1584:PRO:HA	2.02	0.40
2:B:1655:TYR:OH	2:B:1659:ARG:NH2	2.51	0.40
2:B:4113:ASP:HB2	2:B:4116:LEU:HB3	2.03	0.40
2:D:1177:LEU:N	2:D:1180:GLU:O	2.54	0.40
2:D:3800:SER:OG	2:D:3801:CYS:N	2.51	0.40
2:F:4011:VAL:HA	2:F:4014:ILE:HG12	2.03	0.40
2:H:119:ILE:HD13	2:H:162:ILE:HD11	2.02	0.40
2:H:1136:ALA:HB3	2:H:1145:TRP:HB2	2.03	0.40
2:H:1843:LEU:O	2:H:1846:ILE:N	2.54	0.40
2:H:1940:ASN:O	2:H:1944:ARG:HG2	2.21	0.40
2:H:2177:VAL:HG22	2:H:2221:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3663:ASP:HA	2:H:3664:PRO:HD3	1.95	0.40
2:B:1157:GLN:N	2:B:1160:ASP:OD2	2.54	0.40
2:B:1177:LEU:N	2:B:1180:GLU:O	2.54	0.40
2:B:1255:LEU:HA	2:B:1256:PRO:HD3	1.88	0.40
2:B:2177:VAL:HG22	2:B:2221:TYR:CZ	2.56	0.40
2:B:4011:VAL:HA	2:B:4014:ILE:HG12	2.03	0.40
2:B:4036:TYR:HE2	2:B:4048:ASP:HB3	1.85	0.40
2:B:4889:CYS:HB2	2:B:4892:CYS:HB3	2.03	0.40
2:D:411:GLU:HA	2:D:414:ARG:HB2	2.03	0.40
2:D:415:THR:O	2:D:419:ILE:HG13	2.21	0.40
2:D:1253:LYS:HD2	2:D:1255:LEU:HB2	2.02	0.40
2:D:1645:THR:H	2:D:1645:THR:HG23	1.68	0.40
2:D:4957:ASP:OD1	2:D:4957:ASP:N	2.54	0.40
2:F:191:TYR:N	2:F:206:ALA:O	2.54	0.40
2:H:411:GLU:HA	2:H:414:ARG:HB2	2.03	0.40
2:H:782:PHE:HZ	2:H:1467:VAL:HG22	1.86	0.40
2:H:2157:TYR:OH	2:H:2203:TYR:OH	2.26	0.40
2:H:3983:LEU:HD12	2:H:3983:LEU:HA	1.88	0.40
2:B:119:ILE:HD13	2:B:162:ILE:HD11	2.02	0.40
2:B:717:GLY:H	2:B:722:LEU:HB3	1.86	0.40
2:B:1137:PHE:CE2	2:B:1139:GLY:HA2	2.57	0.40
2:B:1709:ILE:HD13	2:B:1709:ILE:HA	1.94	0.40
2:B:1753:LEU:HD11	2:B:1921:HIS:CD2	2.56	0.40
2:B:4023:LYS:HA	2:B:4026:ASP:HB2	2.01	0.40
2:D:1157:GLN:N	2:D:1160:ASP:OD2	2.54	0.40
2:D:1999:ASP:O	2:D:2003:ASP:N	2.54	0.40
2:D:2157:TYR:OH	2:D:2203:TYR:OH	2.26	0.40
2:D:2834:LEU:HD22	2:D:2838:LEU:HB3	2.02	0.40
1:E:78:PRO:HA	1:E:81:ALA:HB3	2.04	0.40
2:F:297:LEU:HD23	2:F:297:LEU:HA	1.87	0.40
2:F:585:ALA:HA	2:F:588:ILE:HD12	2.02	0.40
2:F:2011:GLU:O	2:F:2027:ARG:NH2	2.54	0.40
2:H:415:THR:O	2:H:419:ILE:HG13	2.21	0.40
2:H:517:VAL:HG23	2:H:520:ARG:NE	2.35	0.40
2:H:678:MET:O	2:H:801:ARG:N	2.46	0.40
2:H:3762:LEU:HA	2:H:3762:LEU:HD12	1.86	0.40
2:H:4113:ASP:HB2	2:H:4116:LEU:HB3	2.03	0.40
2:B:3893:TYR:CE2	2:B:3899:ILE:HG23	2.57	0.40
2:D:123:HIS:NE2	2:D:125:TYR:HB3	2.36	0.40
2:D:143:LEU:CB	2:F:2426:SER:C	2.95	0.40
2:D:228:LEU:HD23	2:D:228:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:976:TYR:CZ	2:D:978:PRO:HG3	2.57	0.40
2:D:1136:ALA:HB3	2:D:1145:TRP:HB2	2.03	0.40
2:D:1505:LEU:HD23	2:D:1505:LEU:HA	1.97	0.40
2:D:2088:LEU:O	2:D:2092:GLN:HG2	2.21	0.40
2:D:4518:LEU:H	2:D:4518:LEU:HD23	1.86	0.40
2:F:459:LEU:HD23	2:F:459:LEU:HA	1.86	0.40
2:F:973:THR:HG23	2:F:977:LYS:HB3	2.04	0.40
2:F:976:TYR:CZ	2:F:978:PRO:HG3	2.57	0.40
2:F:1177:LEU:N	2:F:1180:GLU:O	2.54	0.40
2:F:1305:SER:HB2	2:F:1593:HIS:CD2	2.57	0.40
2:F:1707:ILE:HG22	2:F:1712:SER:HB3	2.04	0.40
2:F:4518:LEU:HD23	2:F:4518:LEU:H	1.86	0.40
2:H:626:ARG:NH2	2:H:1668:GLY:O	2.36	0.40
2:H:1902:PRO:HA	2:H:1905:LEU:HB3	2.04	0.40
2:H:4125:SER:HA	2:H:4128:ASN:HD22	1.86	0.40
2:B:1253:LYS:HD2	2:B:1255:LEU:HB2	2.02	0.40
2:B:2088:LEU:O	2:B:2092:GLN:HG2	2.21	0.40
2:B:4518:LEU:H	2:B:4518:LEU:HD23	1.86	0.40
2:D:517:VAL:HG23	2:D:520:ARG:NE	2.35	0.40
2:D:647:ARG:HD2	2:D:647:ARG:HA	1.84	0.40
2:D:4113:ASP:HB2	2:D:4116:LEU:HB3	2.03	0.40
2:F:36:CYS:O	2:F:50:GLU:N	2.55	0.40
2:F:412:GLU:O	2:F:415:THR:OG1	2.33	0.40
2:H:36:CYS:O	2:H:50:GLU:N	2.55	0.40
2:H:1753:LEU:HD11	2:H:1921:HIS:CD2	2.56	0.40
2:H:1833:ILE:HG22	2:H:1834:PHE:H	1.87	0.40
2:H:1905:LEU:HB2	2:H:2081:LEU:HD12	2.04	0.40
2:H:3893:TYR:CE2	2:H:3899:ILE:HG23	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	88/89 (99%)	88 (100%)	0	100	100
1	C	88/89 (99%)	88 (100%)	0	100	100
1	E	88/89 (99%)	88 (100%)	0	100	100
1	G	88/89 (99%)	88 (100%)	0	100	100
2	B	2688/4355 (62%)	2666 (99%)	22 (1%)	73	77
2	D	2688/4355 (62%)	2666 (99%)	22 (1%)	73	77
2	F	2688/4355 (62%)	2666 (99%)	22 (1%)	73	77
2	H	2689/4355 (62%)	2666 (99%)	23 (1%)	70	76
All	All	11105/17776 (62%)	11016 (99%)	89 (1%)	70	77

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	234	LEU
2	B	625	VAL
2	B	791	VAL
2	B	854	THR
2	B	881	ILE
2	B	925	PRO
2	B	939	THR
2	B	989	THR
2	B	990	PRO
2	B	1054	VAL
2	B	1089	ARG
2	B	1552	VAL
2	B	2026	ILE
2	B	2118	ILE
2	B	2211	ASN
2	B	4139	ILE
2	B	4518	LEU
2	B	4519	LEU
2	B	4702	ILE
2	B	4809	ASP
2	B	4900	ASP
2	B	4902	VAL
2	D	234	LEU

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Mol	Chain	Res	Type
2	D	625	VAL
2	D	791	VAL
2	D	854	THR
2	D	881	ILE
2	D	925	PRO
2	D	939	THR
2	D	950	VAL
2	D	989	THR
2	D	990	PRO
2	D	1089	ARG
2	D	1552	VAL
2	D	2026	ILE
2	D	2118	ILE
2	D	2211	ASN
2	D	4139	ILE
2	D	4518	LEU
2	D	4519	LEU
2	D	4702	ILE
2	D	4809	ASP
2	D	4900	ASP
2	D	4902	VAL
2	F	234	LEU
2	F	625	VAL
2	F	791	VAL
2	F	854	THR
2	F	881	ILE
2	F	925	PRO
2	F	939	THR
2	F	950	VAL
2	F	989	THR
2	F	990	PRO
2	F	1089	ARG
2	F	1552	VAL
2	F	2026	ILE
2	F	2118	ILE
2	F	2211	ASN
2	F	4139	ILE
2	F	4518	LEU
2	F	4519	LEU
2	F	4702	ILE
2	F	4809	ASP
2	F	4900	ASP

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Mol	Chain	Res	Type
2	F	4902	VAL
2	H	234	LEU
2	H	625	VAL
2	H	791	VAL
2	H	854	THR
2	H	881	ILE
2	H	925	PRO
2	H	939	THR
2	H	950	VAL
2	H	989	THR
2	H	990	PRO
2	H	1054	VAL
2	H	1089	ARG
2	H	1552	VAL
2	H	2026	ILE
2	H	2118	ILE
2	H	2211	ASN
2	H	4139	ILE
2	H	4518	LEU
2	H	4519	LEU
2	H	4702	ILE
2	H	4809	ASP
2	H	4900	ASP
2	H	4902	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (272) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	44	ASN
2	B	57	ASN
2	B	123	HIS
2	B	150	GLN
2	B	193	HIS
2	B	225	GLN
2	B	238	HIS
2	B	293	GLN
2	B	364	GLN
2	B	375	GLN
2	B	394	HIS
2	B	395	HIS
2	B	398	HIS

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Mol	Chain	Res	Type
2	B	472	HIS
2	B	477	ASN
2	B	531	ASN
2	B	547	ASN
2	B	593	HIS
2	B	604	HIS
2	B	628	ASN
2	B	681	HIS
2	B	745	ASN
2	B	746	GLN
2	B	776	GLN
2	B	1002	ASN
2	B	1147	GLN
2	B	1602	GLN
2	B	1620	GLN
2	B	1656	HIS
2	B	1722	ASN
2	B	1772	ASN
2	B	1836	ASN
2	B	1918	GLN
2	B	1921	HIS
2	B	1940	ASN
2	B	1946	ASN
2	B	2060	GLN
2	B	2152	ASN
2	B	2211	ASN
2	B	2317	ASN
2	B	2319	ASN
2	B	2831	ASN
2	B	2851	ASN
2	B	2898	GLN
2	B	3807	ASN
2	B	3813	ASN
2	B	3856	GLN
2	B	3870	ASN
2	B	3904	GLN
2	B	3906	ASN
2	B	3919	ASN
2	B	3954	HIS
2	B	3956	GLN
2	B	3965	GLN
2	B	3993	ASN

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Mol	Chain	Res	Type
2	B	3999	GLN
2	B	4050	HIS
2	B	4098	ASN
2	B	4128	ASN
2	B	4172	GLN
2	B	4192	ASN
2	B	4499	ASN
2	B	4643	ASN
2	B	4918	ASN
2	D	23	GLN
2	D	44	ASN
2	D	57	ASN
2	D	150	GLN
2	D	193	HIS
2	D	225	GLN
2	D	238	HIS
2	D	261	HIS
2	D	293	GLN
2	D	364	GLN
2	D	375	GLN
2	D	394	HIS
2	D	395	HIS
2	D	398	HIS
2	D	472	HIS
2	D	477	ASN
2	D	531	ASN
2	D	547	ASN
2	D	593	HIS
2	D	604	HIS
2	D	628	ASN
2	D	681	HIS
2	D	745	ASN
2	D	746	GLN
2	D	776	GLN
2	D	888	ASN
2	D	1002	ASN
2	D	1147	GLN
2	D	1589	GLN
2	D	1602	GLN
2	D	1620	GLN
2	D	1656	HIS
2	D	1722	ASN

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Mol	Chain	Res	Type
2	D	1772	ASN
2	D	1836	ASN
2	D	1896	GLN
2	D	1918	GLN
2	D	1921	HIS
2	D	1940	ASN
2	D	1946	ASN
2	D	2060	GLN
2	D	2152	ASN
2	D	2210	GLN
2	D	2317	ASN
2	D	2319	ASN
2	D	2831	ASN
2	D	2851	ASN
2	D	2898	GLN
2	D	3807	ASN
2	D	3813	ASN
2	D	3856	GLN
2	D	3870	ASN
2	D	3904	GLN
2	D	3906	ASN
2	D	3919	ASN
2	D	3954	HIS
2	D	3956	GLN
2	D	3965	GLN
2	D	3993	ASN
2	D	3999	GLN
2	D	4050	HIS
2	D	4128	ASN
2	D	4172	GLN
2	D	4192	ASN
2	D	4499	ASN
2	D	4643	ASN
2	D	4767	GLN
2	D	4918	ASN
2	F	23	GLN
2	F	44	ASN
2	F	57	ASN
2	F	150	GLN
2	F	202	HIS
2	F	225	GLN
2	F	238	HIS

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Mol	Chain	Res	Type
2	F	261	HIS
2	F	293	GLN
2	F	364	GLN
2	F	375	GLN
2	F	394	HIS
2	F	395	HIS
2	F	398	HIS
2	F	472	HIS
2	F	477	ASN
2	F	531	ASN
2	F	547	ASN
2	F	593	HIS
2	F	604	HIS
2	F	628	ASN
2	F	681	HIS
2	F	745	ASN
2	F	776	GLN
2	F	888	ASN
2	F	915	HIS
2	F	1002	ASN
2	F	1147	GLN
2	F	1216	ASN
2	F	1589	GLN
2	F	1602	GLN
2	F	1620	GLN
2	F	1631	HIS
2	F	1656	HIS
2	F	1772	ASN
2	F	1836	ASN
2	F	1918	GLN
2	F	1921	HIS
2	F	1940	ASN
2	F	1946	ASN
2	F	2060	GLN
2	F	2152	ASN
2	F	2211	ASN
2	F	2317	ASN
2	F	2319	ASN
2	F	2831	ASN
2	F	2851	ASN
2	F	2898	GLN
2	F	3807	ASN

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Mol	Chain	Res	Type
2	F	3813	ASN
2	F	3856	GLN
2	F	3870	ASN
2	F	3904	GLN
2	F	3906	ASN
2	F	3919	ASN
2	F	3954	HIS
2	F	3956	GLN
2	F	3965	GLN
2	F	3993	ASN
2	F	3999	GLN
2	F	4050	HIS
2	F	4098	ASN
2	F	4128	ASN
2	F	4172	GLN
2	F	4179	ASN
2	F	4192	ASN
2	F	4499	ASN
2	F	4643	ASN
2	F	4767	GLN
2	F	4817	HIS
2	F	4918	ASN
2	H	23	GLN
2	H	44	ASN
2	H	57	ASN
2	H	123	HIS
2	H	150	GLN
2	H	193	HIS
2	H	225	GLN
2	H	238	HIS
2	H	293	GLN
2	H	364	GLN
2	H	375	GLN
2	H	394	HIS
2	H	395	HIS
2	H	398	HIS
2	H	472	HIS
2	H	477	ASN
2	H	531	ASN
2	H	547	ASN
2	H	593	HIS
2	H	604	HIS

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Mol	Chain	Res	Type
2	H	628	ASN
2	H	681	HIS
2	H	745	ASN
2	H	776	GLN
2	H	1002	ASN
2	H	1147	GLN
2	H	1216	ASN
2	H	1589	GLN
2	H	1602	GLN
2	H	1620	GLN
2	H	1656	HIS
2	H	1684	GLN
2	H	1722	ASN
2	H	1772	ASN
2	H	1836	ASN
2	H	1918	GLN
2	H	1921	HIS
2	H	1940	ASN
2	H	1946	ASN
2	H	2060	GLN
2	H	2119	ASN
2	H	2152	ASN
2	H	2210	GLN
2	H	2211	ASN
2	H	2317	ASN
2	H	2319	ASN
2	H	2831	ASN
2	H	2851	ASN
2	H	2898	GLN
2	H	3807	ASN
2	H	3813	ASN
2	H	3856	GLN
2	H	3870	ASN
2	H	3904	GLN
2	H	3906	ASN
2	H	3919	ASN
2	H	3954	HIS
2	H	3956	GLN
2	H	3965	GLN
2	H	3993	ASN
2	H	3999	GLN
2	H	4050	HIS

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Mol	Chain	Res	Type
2	H	4128	ASN
2	H	4172	GLN
2	H	4192	ASN
2	H	4499	ASN
2	H	4643	ASN
2	H	4918	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.

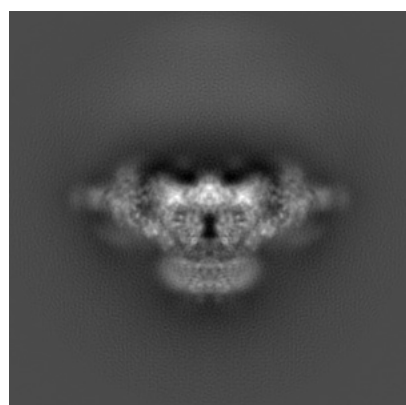
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9824. These allow visual inspection of the internal detail of the map and identification of artifacts.

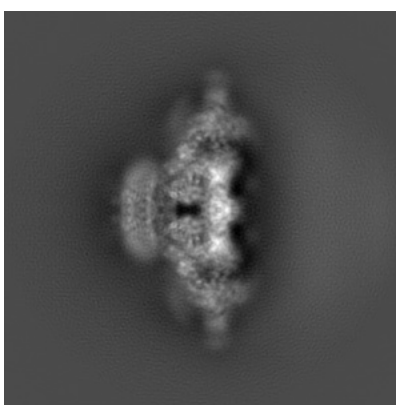
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

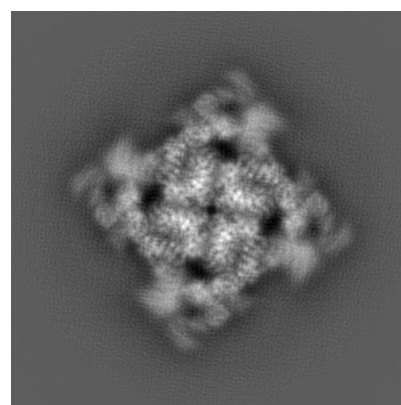
6.1.1 Primary map



X



Y

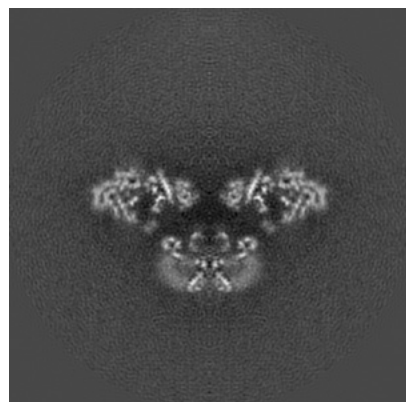


Z

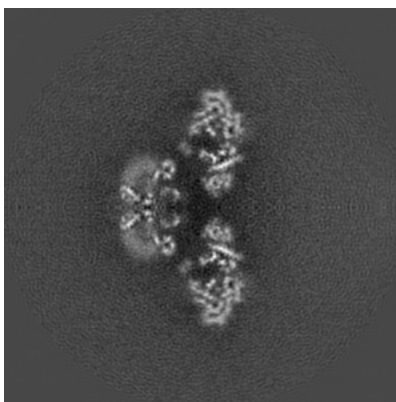
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

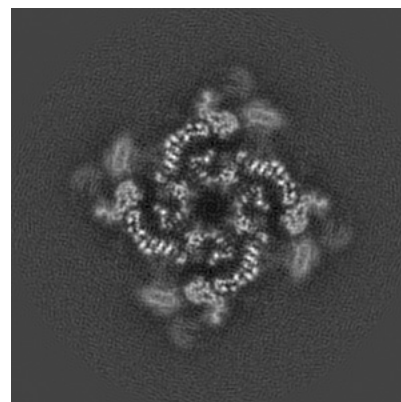
6.2.1 Primary map



X Index: 200



Y Index: 200

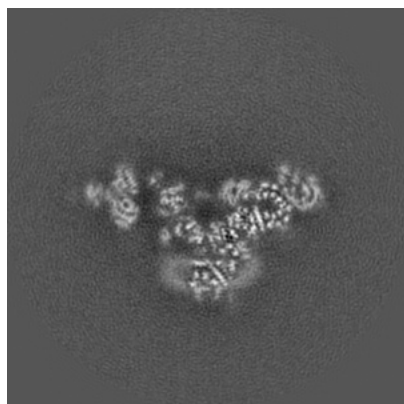


Z Index: 200

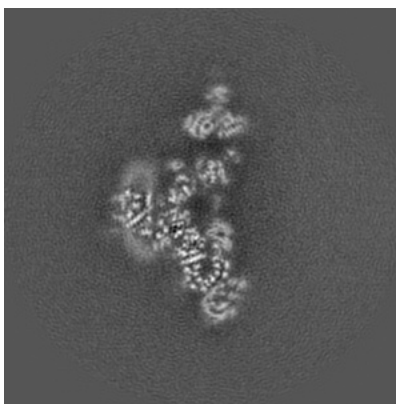
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

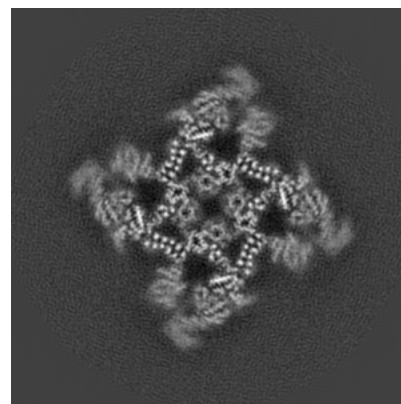
6.3.1 Primary map



X Index: 189



Y Index: 189

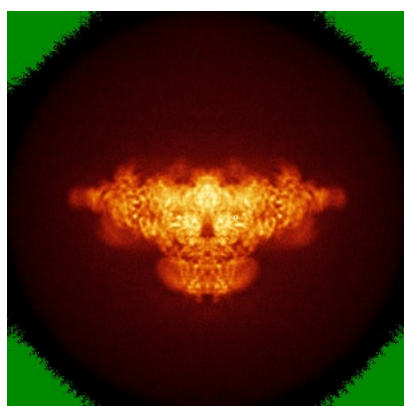


Z Index: 209

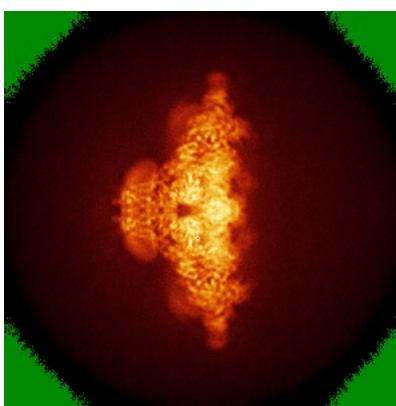
The images above show the largest variance slices of the map in three orthogonal directions.

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

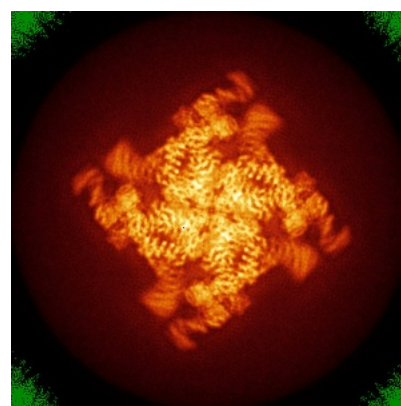
6.4.1 Primary map



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

This section was not generated.

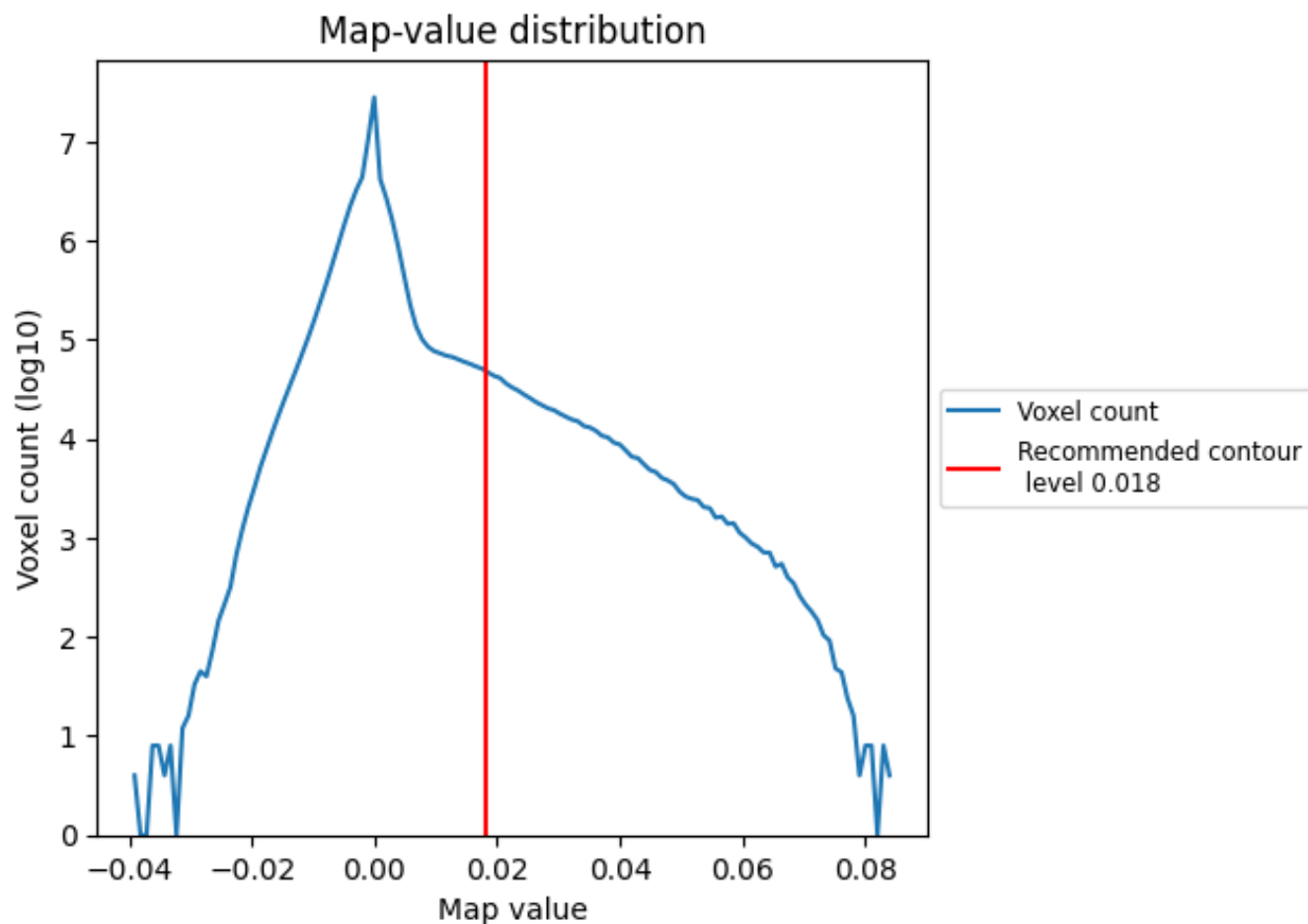
6.6 Mask visualisation

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

7 Map analysis [i](#)

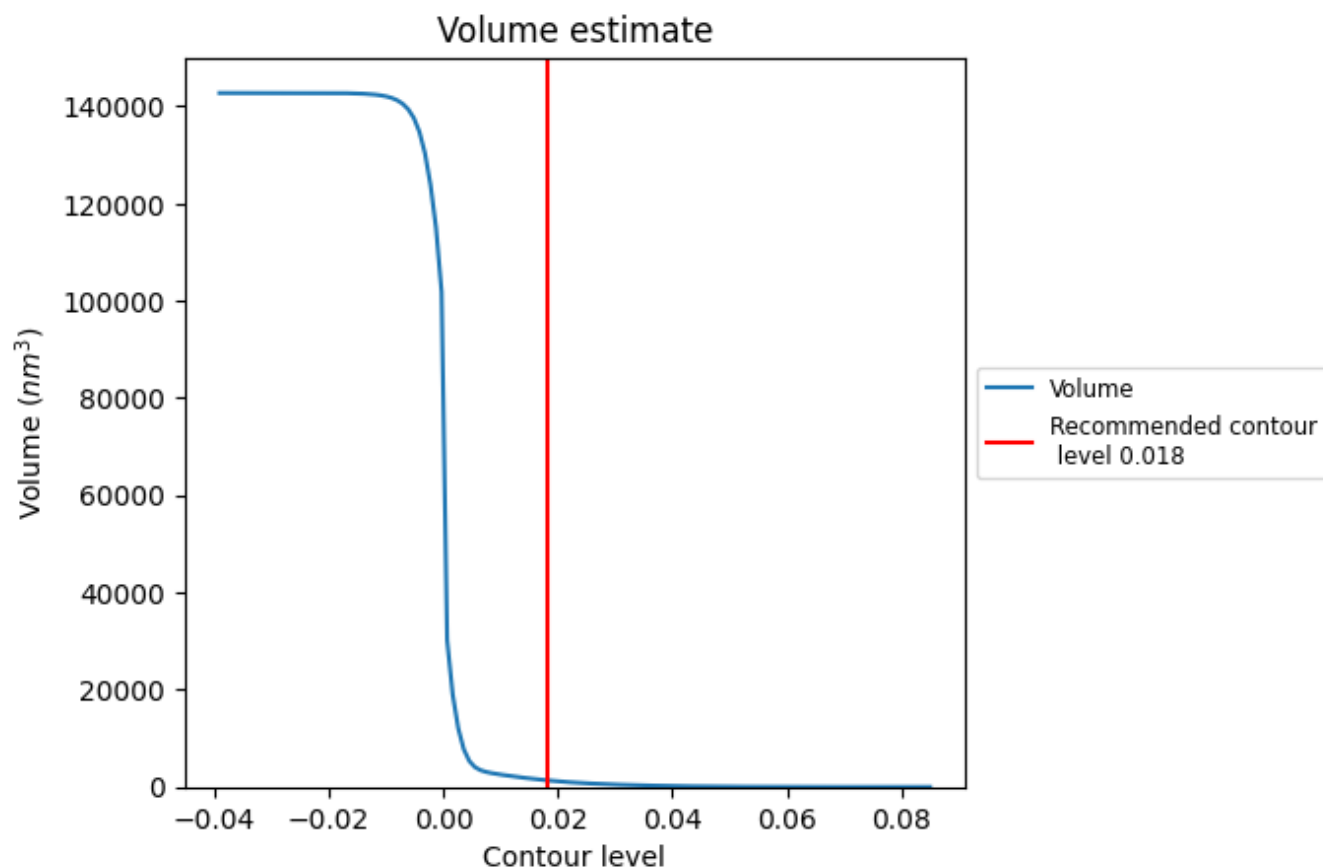
This section contains the results of statistical analysis of the map.

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.

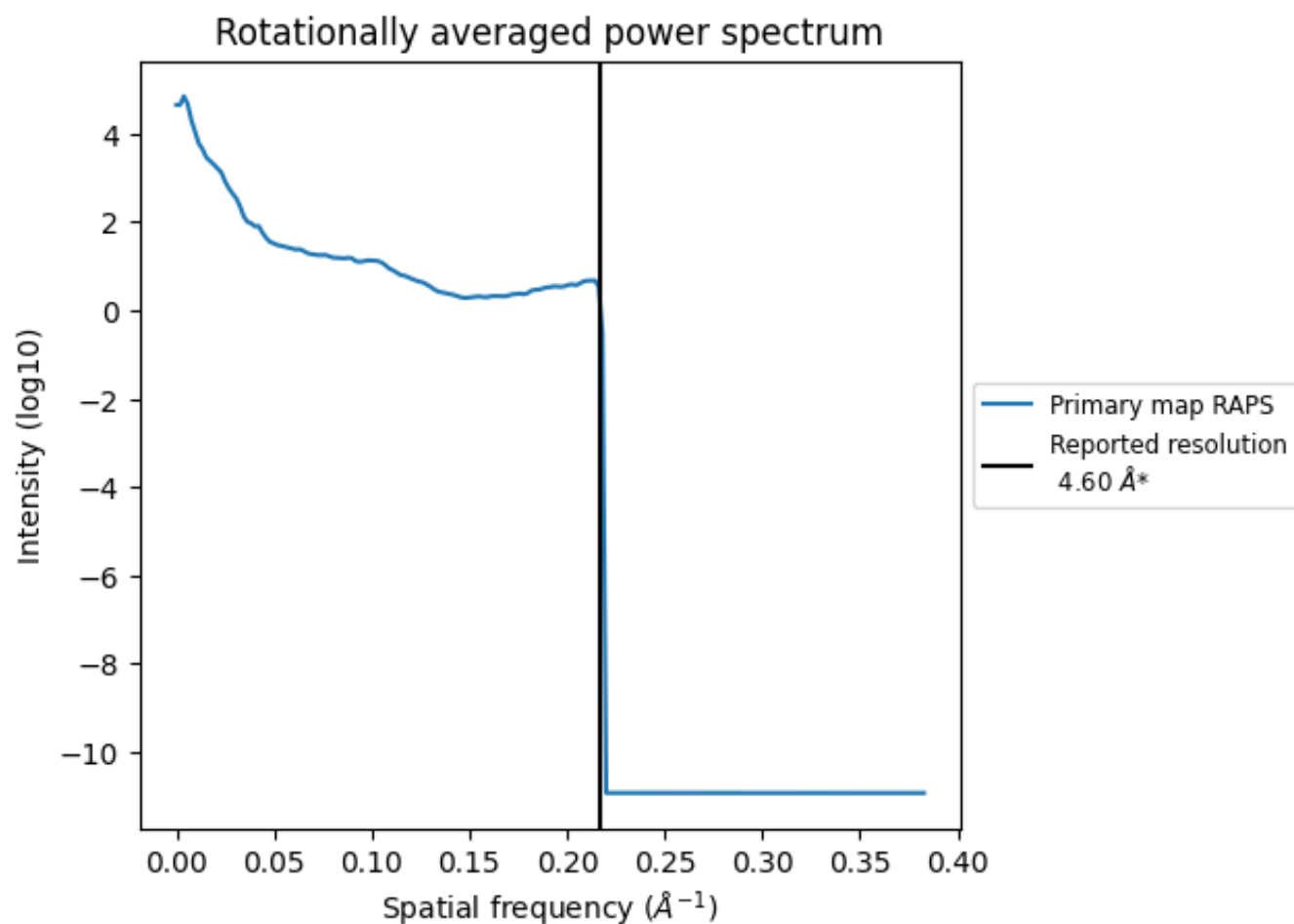
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1373 nm^3 ; this corresponds to an approximate mass of 1240 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 ⓘ

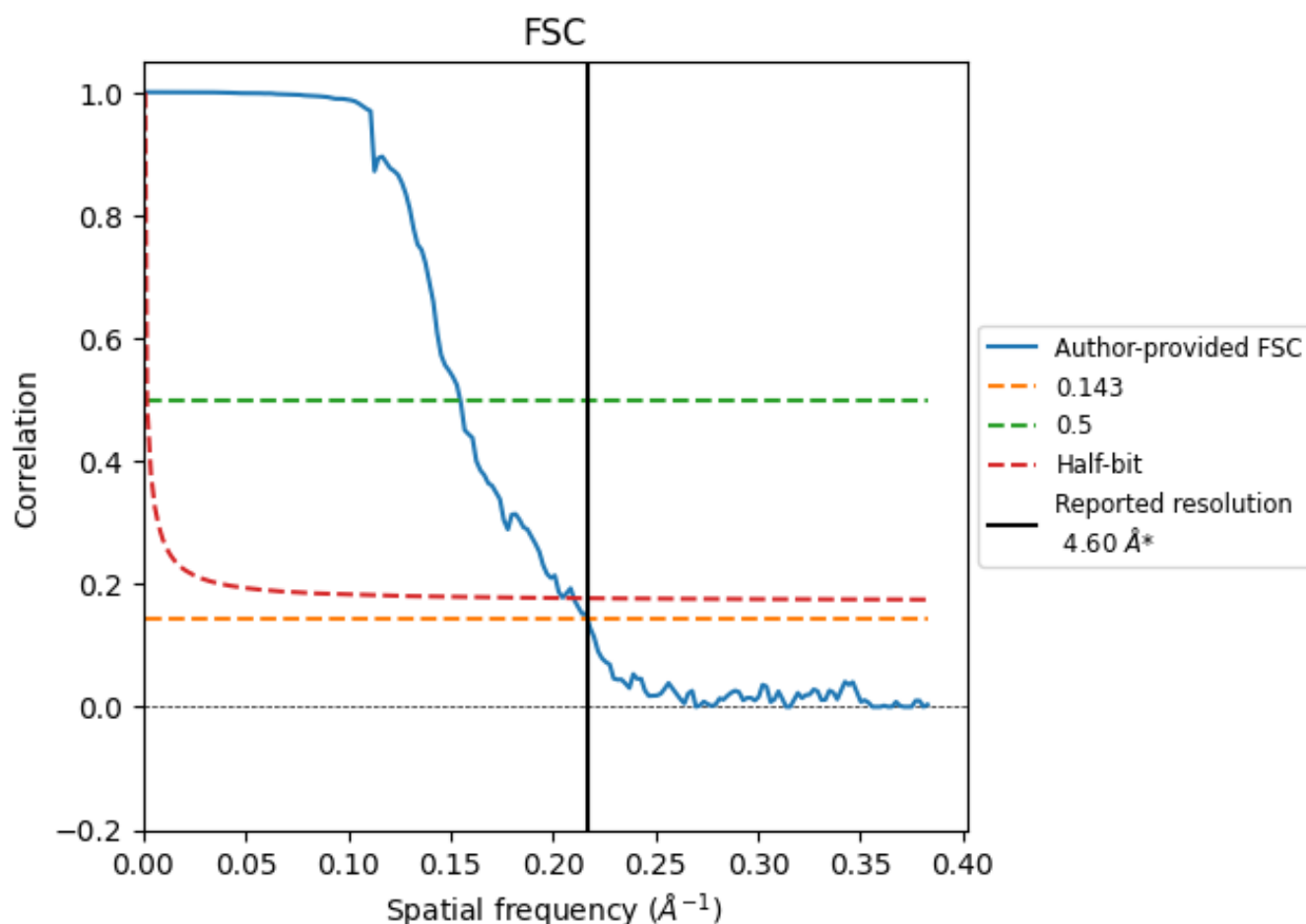


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	6.46	4.76
Unmasked-calculated*	-	-	-

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

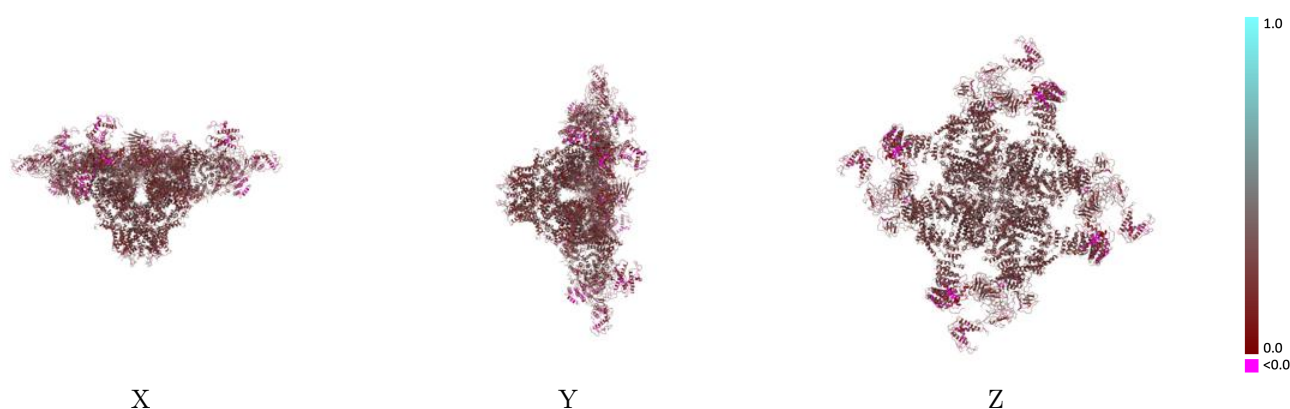
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9824 and PDB model 6JGZ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

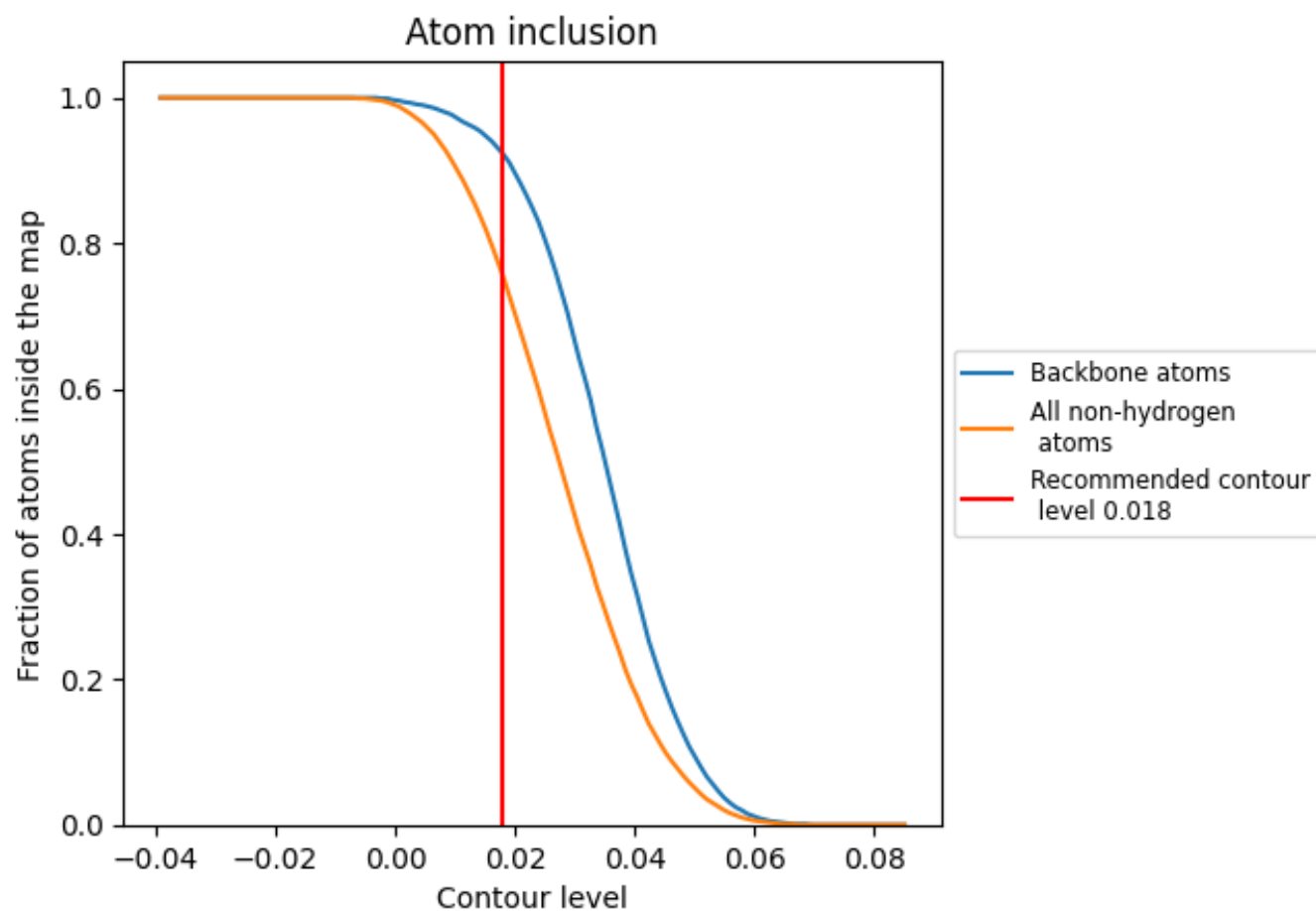


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 76% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.2490
A	0.8170	0.2650
B	0.7530	0.2480
C	0.8190	0.2650
D	0.7530	0.2490
E	0.8170	0.2650
F	0.7530	0.2480
G	0.8140	0.2650
H	0.7530	0.2480

1.0

0.0

<0.0